



## Full wwPDB EM Validation Report ⓘ

Oct 15, 2025 – 03:21 pm BST

PDB ID : 9QZF / pdb\_00009qzf  
EMDB ID : EMD-53471  
Title : Proximal A-C linker of Tetrahymena centriole, six repeating units  
Authors : Cai, B.; Xu, J.W.; Luo, L.; Aarts, E.; Leitner, A.; Ishikawa, T.; Beltro, P.;  
Pilhofer, M.; Wieczorek, M.  
Deposited on : 2025-04-22  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46



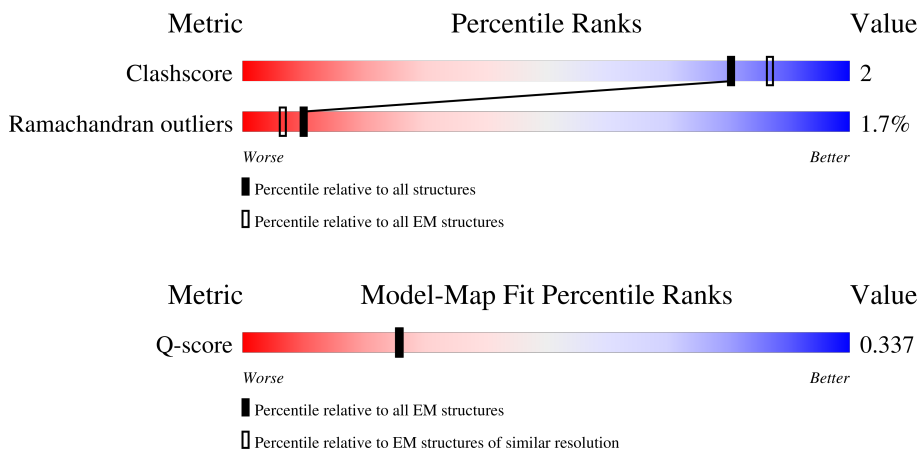
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 210492                      | 15764                       | -  |
| Ramachandran outliers | 207382                      | 16835                       | -  |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |






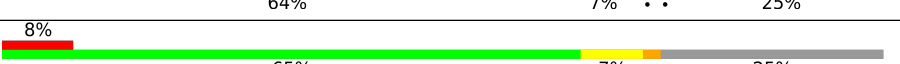
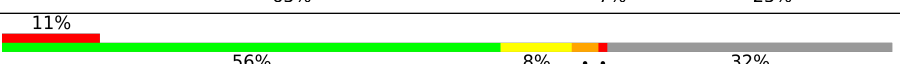
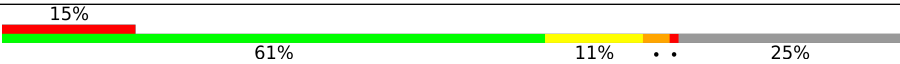


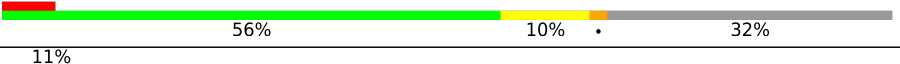
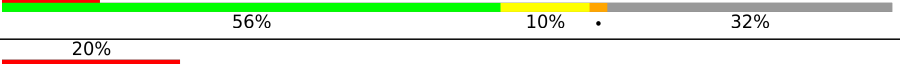

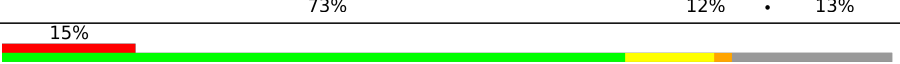
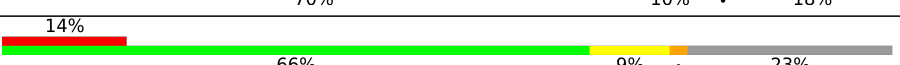


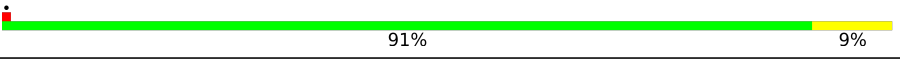
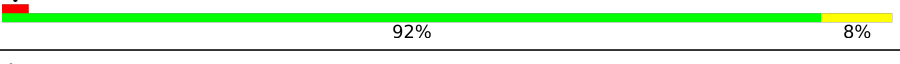
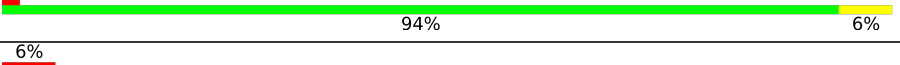
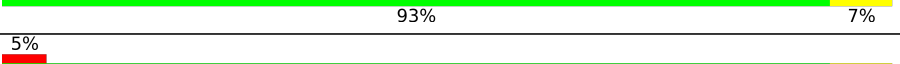
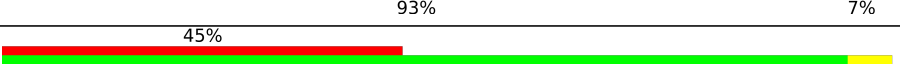
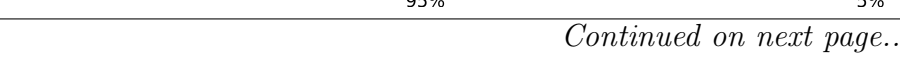


The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 452    | <div> <div>11%</div> <div>83%</div> <div>10%</div> <div>5%</div> </div> |
| 1   | BD    | 452    | <div> <div>6%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>  |
| 1   | C     | 452    | <div> <div>10%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div> |
| 1   | CP    | 452    | <div> <div>5%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>  |
| 1   | Ca    | 452    | <div> <div>11%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | i     | 452    |    |
| 2   | BK    | 380    |    |
| 2   | BR    | 380    |    |
| 2   | CW    | 380    |    |
| 2   | Cd    | 380    |    |
| 2   | Ch    | 380    |    |
| 2   | D     | 380    |    |
| 2   | f     | 380    |    |
| 2   | k     | 380    |    |
| 2   | q     | 380    |    |
| 2   | s     | 380    |   |
| 2   | y     | 380    |  |
| 2   | z     | 380    |  |
| 3   | 1     | 937    |  |
| 3   | 7     | 937    |  |
| 3   | BY    | 937    |  |
| 3   | E     | 937    |  |
| 3   | I     | 937    |  |
| 3   | n     | 937    |  |
| 4   | BO    | 151    |  |
| 4   | BZ    | 151    |  |
| 4   | Bw    | 151    |  |
| 4   | F     | 151    |  |
| 4   | d     | 151    |  |
| 4   | o     | 151    |  |

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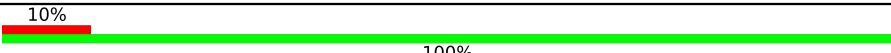

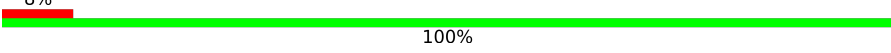
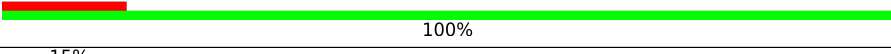
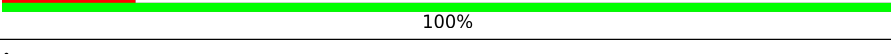
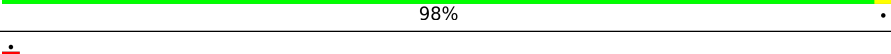
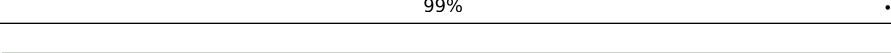
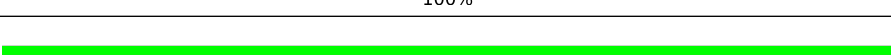
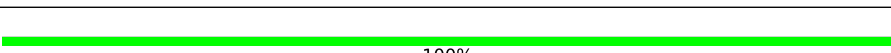
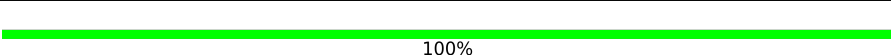
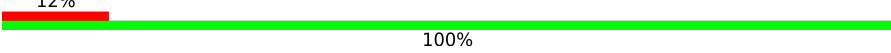
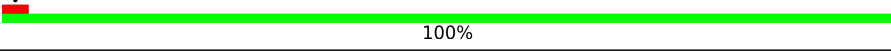
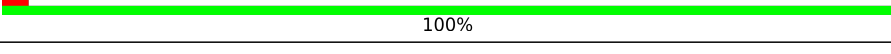
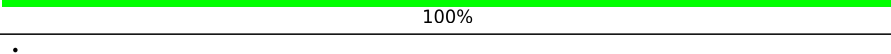
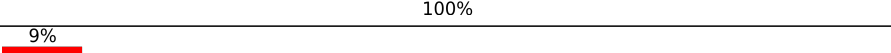
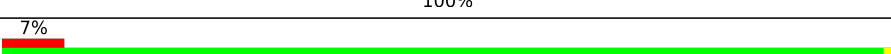
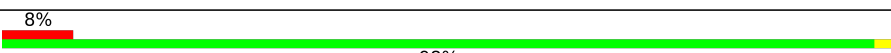
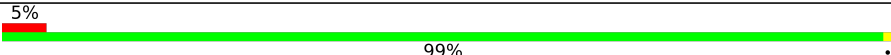
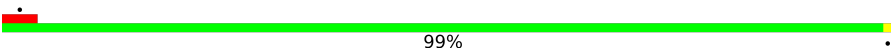
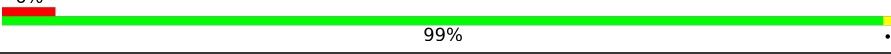
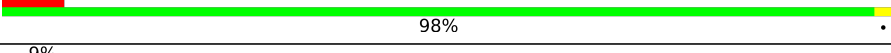
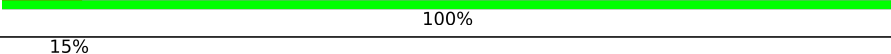
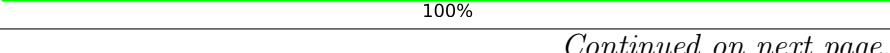


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | 9     | 1202   |                  |
| 5   | AB    | 1202   |                  |
| 5   | AE    | 1202   |                  |
| 5   | AO    | 1202   |                  |
| 5   | AU    | 1202   |                  |
| 5   | Bf    | 1202   |                  |
| 5   | Bt    | 1202   |                  |
| 5   | G     | 1202   |                  |
| 5   | L     | 1202   |                  |
| 5   | M     | 1202   |                  |
| 5   | R     | 1202   |                  |
| 5   | v     | 1202   |                  |
| 6   | B4    | 164    |                  |
| 6   | BV    | 164    |                  |
| 6   | Bg    | 164    |                  |
| 6   | H     | 164    |                  |
| 6   | l     | 164    |                  |
| 6   | w     | 164    |                  |
| 7   | 4     | 634    |                  |
| 7   | AG    | 634    |                  |
| 7   | AM    | 634    |                  |
| 7   | Bm    | 634    |                  |
| 7   | J     | 634    |                  |
| 7   | O     | 634    |                  |
| 8   | 5     | 167    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | Bc    | 167    |    |
| 8   | Bn    | 167    |    |
| 8   | CA    | 167    |    |
| 8   | K     | 167    |    |
| 8   | t     | 167    |    |
| 9   | 2     | 161    |    |
| 9   | AC    | 161    |    |
| 9   | Bj    | 161    |    |
| 9   | Bu    | 161    |    |
| 9   | CH    | 161    |    |
| 9   | N     | 161    |   |
| 10  | AJ    | 32     |  |
| 10  | AW    | 32     |  |
| 10  | Ac    | 32     |  |
| 10  | B1    | 32     |  |
| 10  | P     | 32     |  |
| 10  | U     | 32     |  |
| 11  | 0     | 105    |  |
| 11  | AK    | 105    |  |
| 11  | B2    | 105    |  |
| 11  | Bq    | 105    |  |
| 11  | CO    | 105    |  |
| 11  | Q     | 105    |  |
| 12  | AR    | 33     |  |
| 12  | Ae    | 33     |  |

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| Mol | Chain | Length | Quality of chain             |
|-----|-------|--------|------------------------------|
| 12  | Ak    | 33     | 12%<br>100%                  |
| 12  | B8    | 33     | 6%<br>100%                   |
| 12  | S     | 33     | 6%<br>100%                   |
| 12  | X     | 33     | 12%<br>100%                  |
| 13  | AH    | 127    | 98%<br>.                     |
| 13  | AS    | 127    | 22%<br>99%<br>.              |
| 13  | B9    | 127    | 98%<br>.                     |
| 13  | Bx    | 127    | 98%<br>.                     |
| 13  | CV    | 127    | 98%<br>.                     |
| 13  | T     | 127    | 98%<br>.                     |
| 14  | AZ    | 153    | 9%<br>95%<br>5%<br>.         |
| 14  | Am    | 153    | 33%<br>90%<br>10%            |
| 14  | As    | 153    | 95%<br>5%<br>.               |
| 14  | CE    | 153    | 95%<br>5%<br>.               |
| 14  | V     | 153    | 6%<br>96%<br>..              |
| 14  | a     | 153    | 8%<br>95%<br>5%<br>.         |
| 15  | AP    | 102    | 6%<br>94%<br>5%<br>.         |
| 15  | Aa    | 102    | 21%<br>98%<br>.              |
| 15  | B5    | 102    | 96%<br>..                    |
| 15  | CF    | 102    | 95%<br>..                    |
| 15  | Cc    | 102    | 97%<br>..                    |
| 15  | W     | 102    | 7%<br>97%<br>..              |
| 16  | A7    | 230    | 7%<br>57%<br>10%<br>31%<br>. |
| 16  | Ai    | 230    | 8%<br>54%<br>8%<br>34%<br>.  |
| 16  | An    | 230    | 10%<br>55%<br>8%<br>34%<br>. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | Aq    | 230    |                  |
| 16  | Av    | 230    |                  |
| 16  | Az    | 230    |                  |
| 16  | CB    | 230    |                  |
| 16  | CI    | 230    |                  |
| 16  | CM    | 230    |                  |
| 16  | CT    | 230    |                  |
| 16  | Z     | 230    |                  |
| 16  | c     | 230    |                  |



## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 130144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called WD repeat WRAP73-like protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 1   | A     | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |
| 1   | C     | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |
| 1   | i     | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |
| 1   | BD    | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |
| 1   | CP    | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |
| 1   | Ca    | 429      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2129  | 1271 | 429 | 429 |         |       |

- Molecule 2 is a protein called Centrosomal protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | D     | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |
| 2   | f     | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |
| 2   | k     | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |
| 2   | q     | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |
| 2   | s     | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |
| 2   | y     | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |
| 2   | BK    | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |
| 2   | BR    | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |
| 2   | CW    | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | Cd    | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |
| 2   | Ch    | 284      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1415  | 847 | 284 | 284 |         |       |
| 2   | z     | 258      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1288  | 772 | 258 | 258 |         |       |

- Molecule 3 is a protein called Rab-GAP TBC domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 3   | E     | 724      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3597  | 2149 | 724 | 724 |         |       |
| 3   | I     | 813      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 4040  | 2414 | 813 | 813 |         |       |
| 3   | n     | 665      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3302  | 1972 | 665 | 665 |         |       |
| 3   | 1     | 621      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3082  | 1840 | 621 | 621 |         |       |
| 3   | 7     | 813      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 4040  | 2414 | 813 | 813 |         |       |
| 3   | BY    | 773      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 3841  | 2295 | 773 | 773 |         |       |

- Molecule 4 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4   | F     | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |
| 4   | d     | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |
| 4   | o     | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |
| 4   | BO    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |
| 4   | BZ    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |
| 4   | Bw    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 755   | 453 | 151 | 151 |         |       |

- Molecule 5 is a protein called TBC1 domain family member 31.



| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 5   | G     | 414      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2064  | 1236 | 414 | 414 |         |       |
| 5   | L     | 518      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2584  | 1548 | 518 | 518 |         |       |
| 5   | M     | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |
| 5   | R     | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |
| 5   | v     | 359      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1790  | 1072 | 359 | 359 |         |       |
| 5   | 9     | 303      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1510  | 904  | 303 | 303 |         |       |
| 5   | AB    | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |
| 5   | AE    | 518      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2584  | 1548 | 518 | 518 |         |       |
| 5   | AO    | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |
| 5   | AU    | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |
| 5   | Bf    | 468      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2334  | 1398 | 468 | 468 |         |       |
| 5   | Bt    | 354      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1752  | 1044 | 354 | 354 |         |       |

- Molecule 6 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | H     | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |
| 6   | l     | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |
| 6   | w     | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |
| 6   | BV    | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |
| 6   | Bg    | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |
| 6   | B4    | 164      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 820   | 492 | 164 | 164 |         |       |

- Molecule 7 is a protein called POC1 centriolar protein homolog.



| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 7   | J     | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |
| 7   | O     | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |
| 7   | 4     | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |
| 7   | AG    | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |
| 7   | AM    | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |
| 7   | Bm    | 365      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1806  | 1076 | 365 | 365 |         |       |

- Molecule 8 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 8   | K     | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |
| 8   | t     | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |
| 8   | 5     | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |
| 8   | Bc    | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |
| 8   | Bn    | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |
| 8   | CA    | 167      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 835   | 501 | 167 | 167 |         |       |

- Molecule 9 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 9   | N     | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |
| 9   | 2     | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |
| 9   | AC    | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |
| 9   | Bj    | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |
| 9   | Bu    | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |
| 9   | CH    | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 805   | 483 | 161 | 161 |         |       |



- Molecule 10 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 10  | P     | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |
| 10  | U     | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |
| 10  | AJ    | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |
| 10  | AW    | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |
| 10  | Ac    | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |
| 10  | B1    | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 160   | 96 | 32 | 32 |         |       |

- Molecule 11 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 11  | Q     | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |
| 11  | 0     | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |
| 11  | AK    | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |
| 11  | Bq    | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |
| 11  | B2    | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |
| 11  | CO    | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 525   | 315 | 105 | 105 |         |       |

- Molecule 12 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 12  | S     | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |
| 12  | X     | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |
| 12  | AR    | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |
| 12  | Ae    | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |
| 12  | Ak    | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 12  | B8    | 33       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 165   | 99 | 33 | 33 |         |       |

- Molecule 13 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 13  | T     | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |
| 13  | AH    | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |
| 13  | AS    | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |
| 13  | Bx    | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |
| 13  | B9    | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |
| 13  | CV    | 127      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 635   | 381 | 127 | 127 |         |       |

- Molecule 14 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | V     | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 14  | a     | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 14  | AZ    | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 14  | Am    | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 14  | As    | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |
| 14  | CE    | 153      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 459 | 153 | 153 |         |       |

- Molecule 15 is a protein called Unknown Protein Chain.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | W     | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |
| 15  | AP    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | Aa    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |
| 15  | B5    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |
| 15  | CF    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |
| 15  | Cc    | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 510   | 306 | 102 | 102 |         |       |

- Molecule 16 is a protein called SWIM-type domain-containing protein.

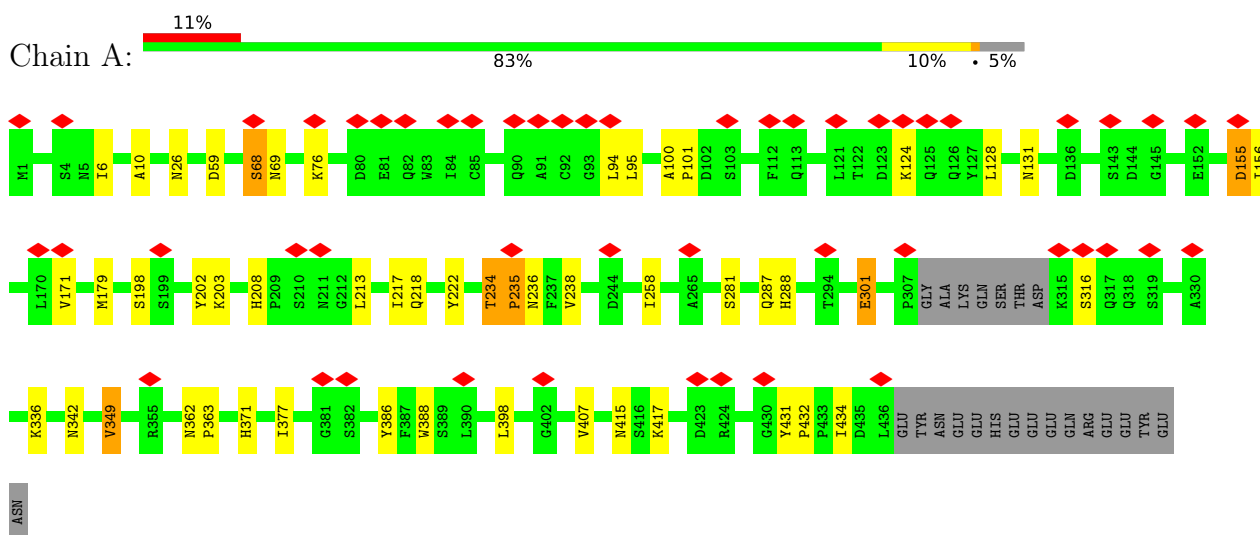
| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16  | Z     | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | c     | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |
| 16  | Ai    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | An    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | Aq    | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |
| 16  | Av    | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |
| 16  | Az    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | A7    | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |
| 16  | CB    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | CI    | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |
| 16  | CM    | 151      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 748   | 446 | 151 | 151 |         |       |
| 16  | CT    | 158      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 783   | 467 | 158 | 158 |         |       |



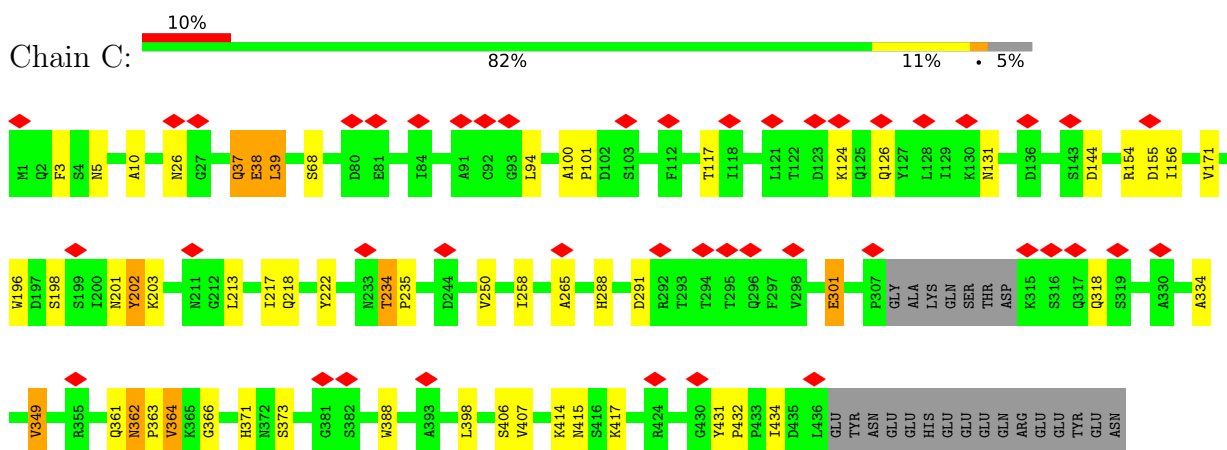
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

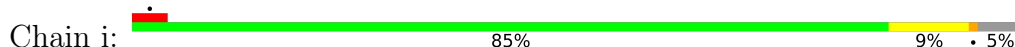
- Molecule 1: WD repeat WRAP73-like protein, putative



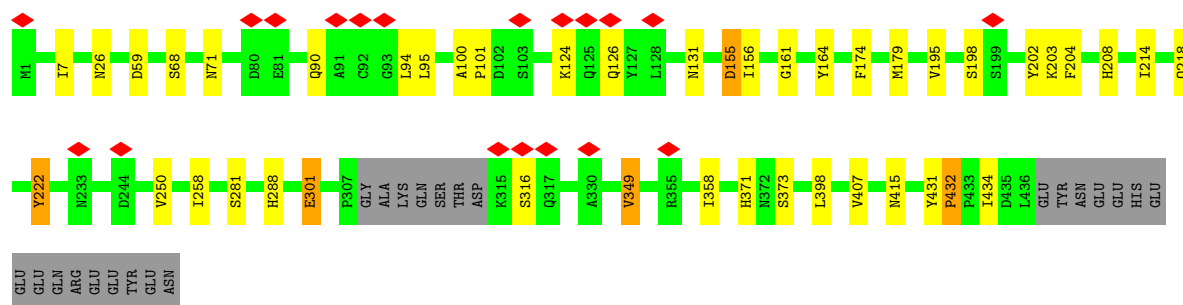
- Molecule 1: WD repeat WRAP73-like protein, putative



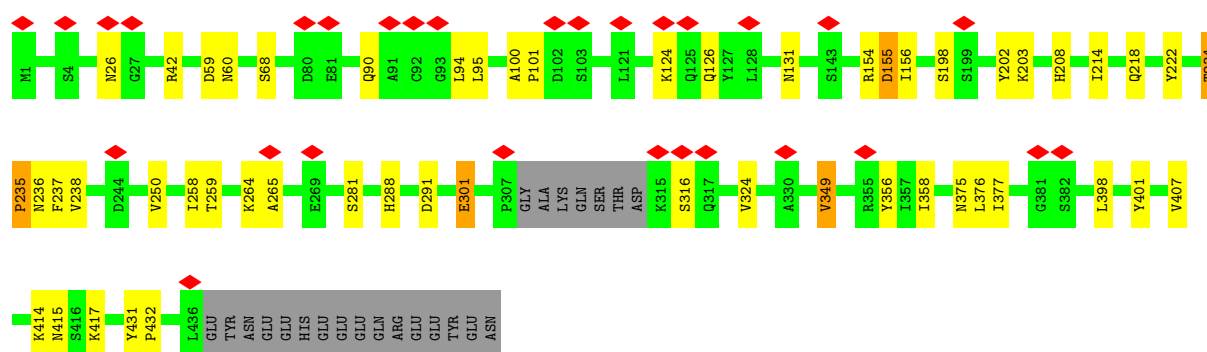
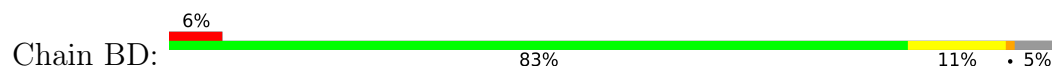
- Molecule 1: WD repeat WRAP73-like protein, putative



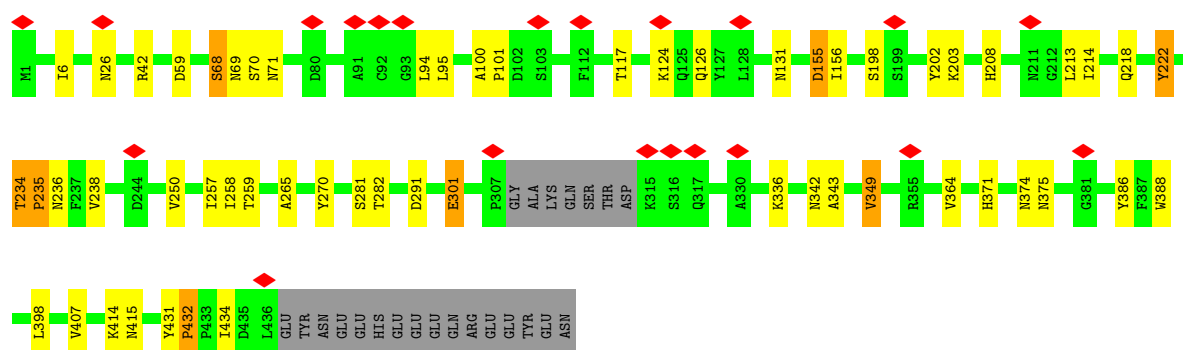
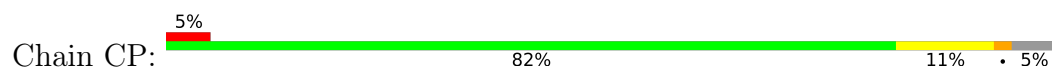




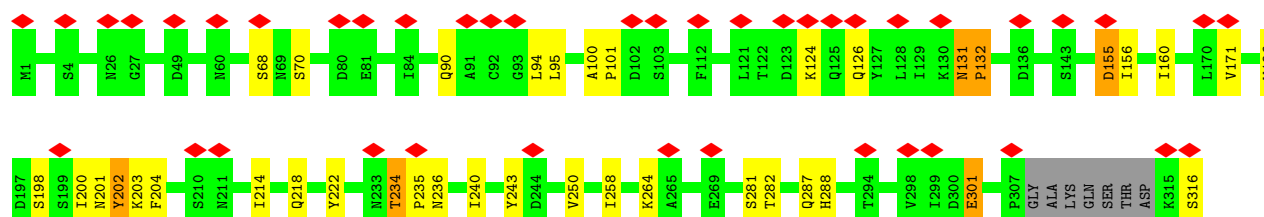
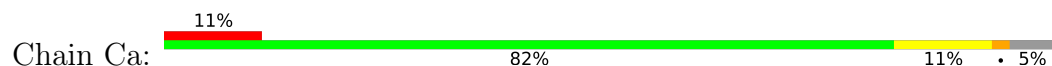
- Molecule 1: WD repeat WRAP73-like protein, putative



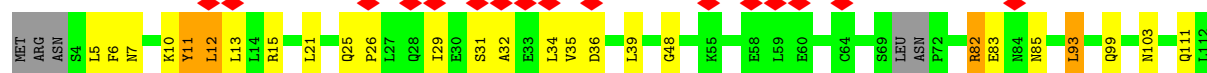
- Molecule 1: WD repeat WRAP73-like protein, putative



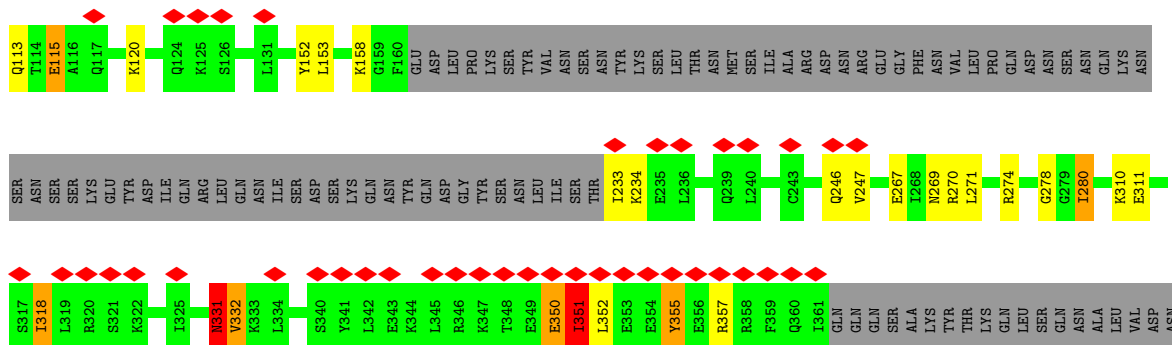
- Molecule 1: WD repeat WRAP73-like protein, putative



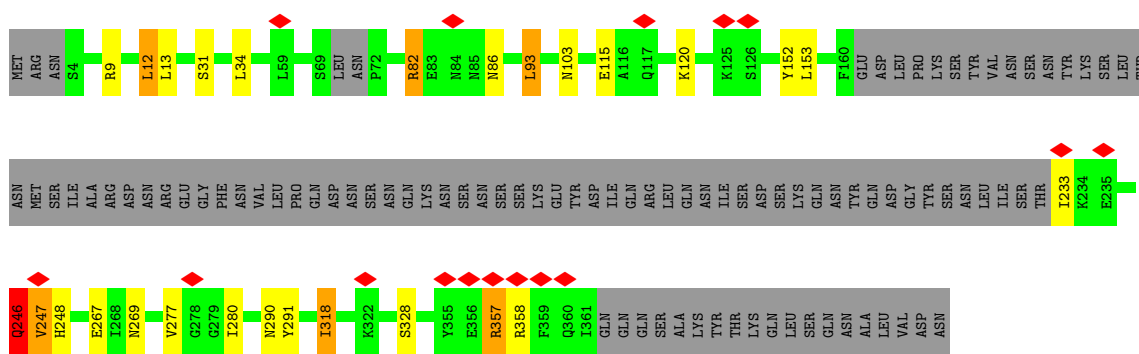




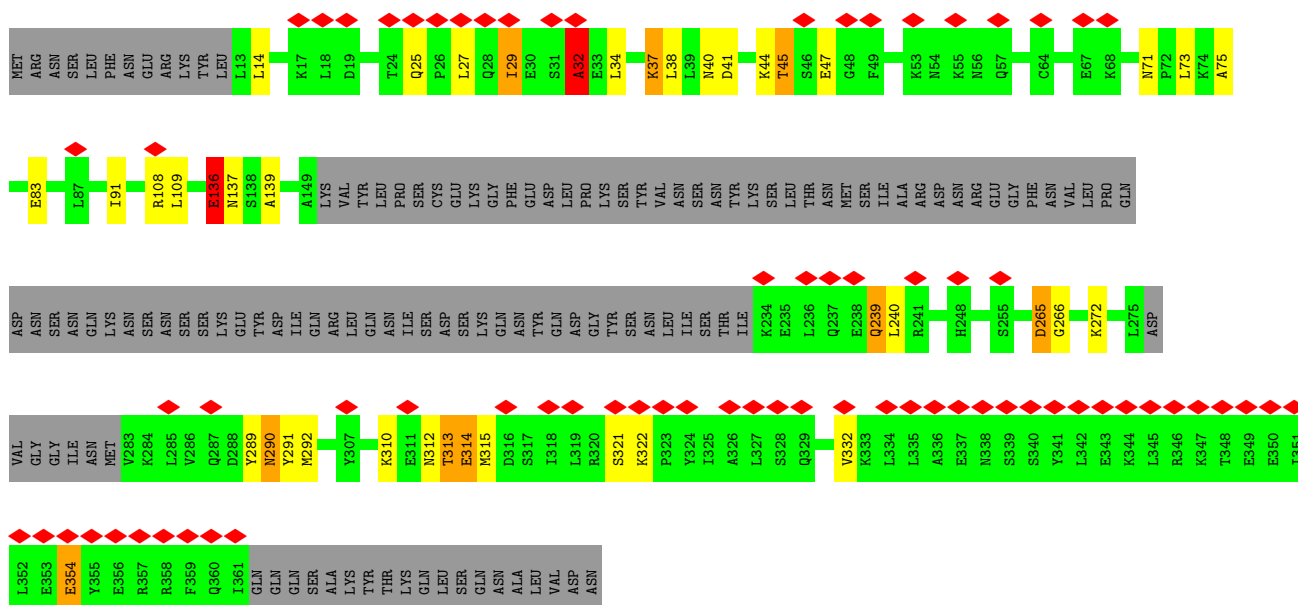




- Molecule 2: Centrosomal protein, putative

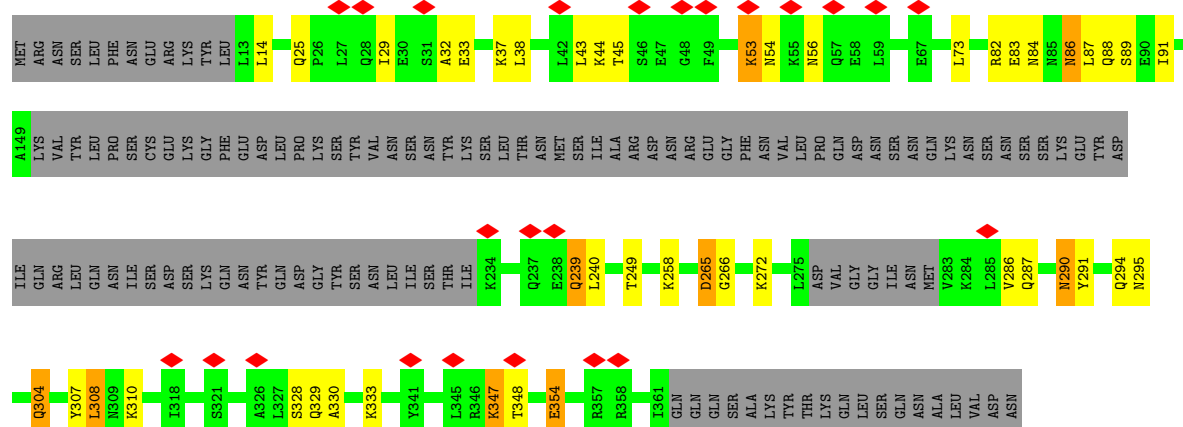


- Molecule 2: Centrosomal protein, putative

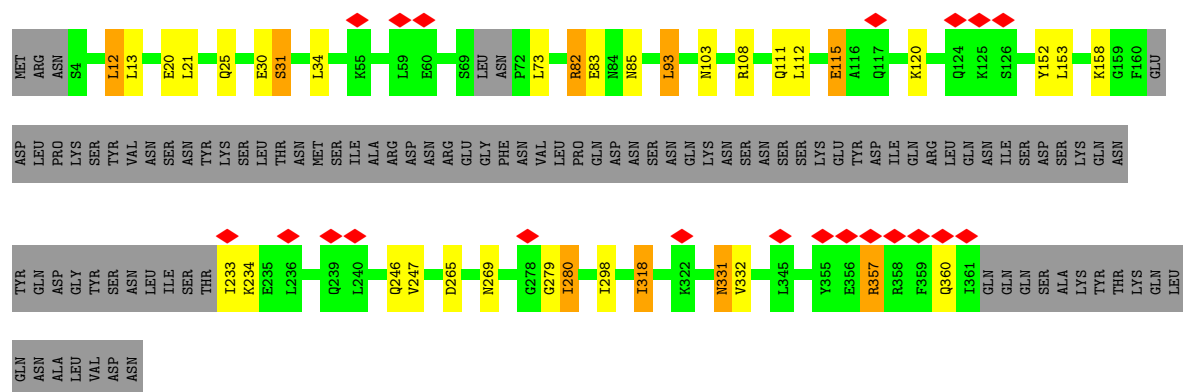


- Molecule 2: Centrosomal protein, putative

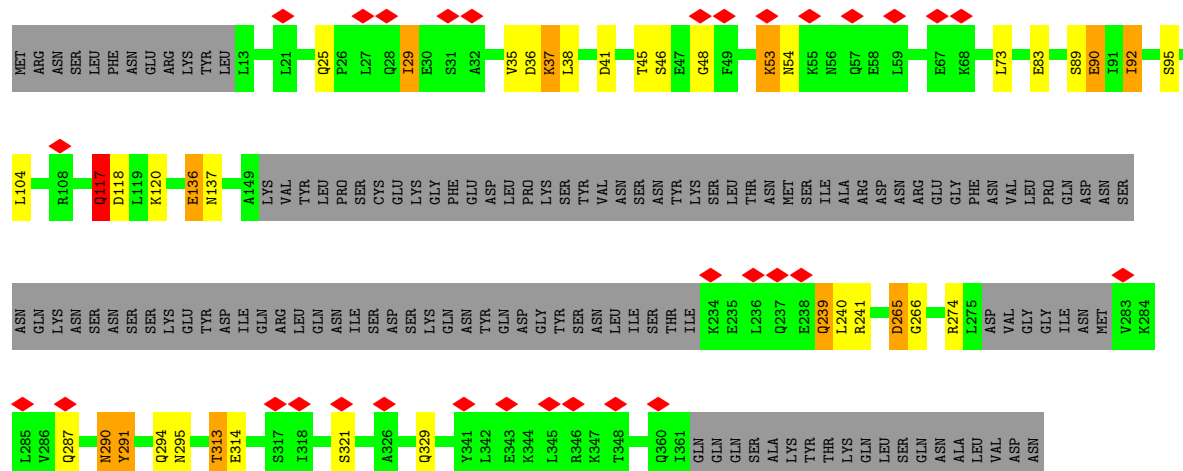




• Molecule 2: Centrosomal protein, putative

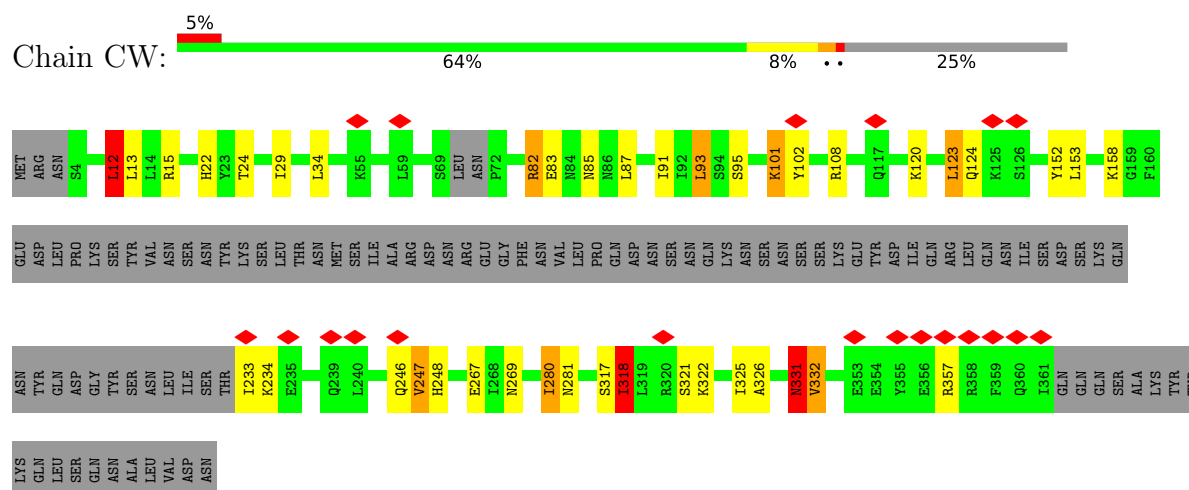


• Molecule 2: Centrosomal protein, putative

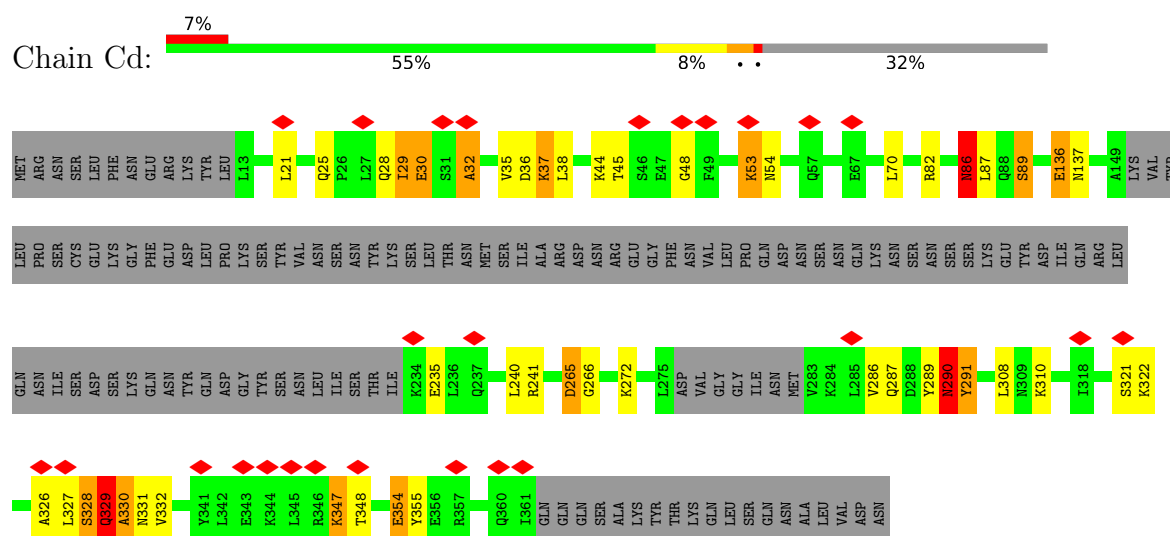




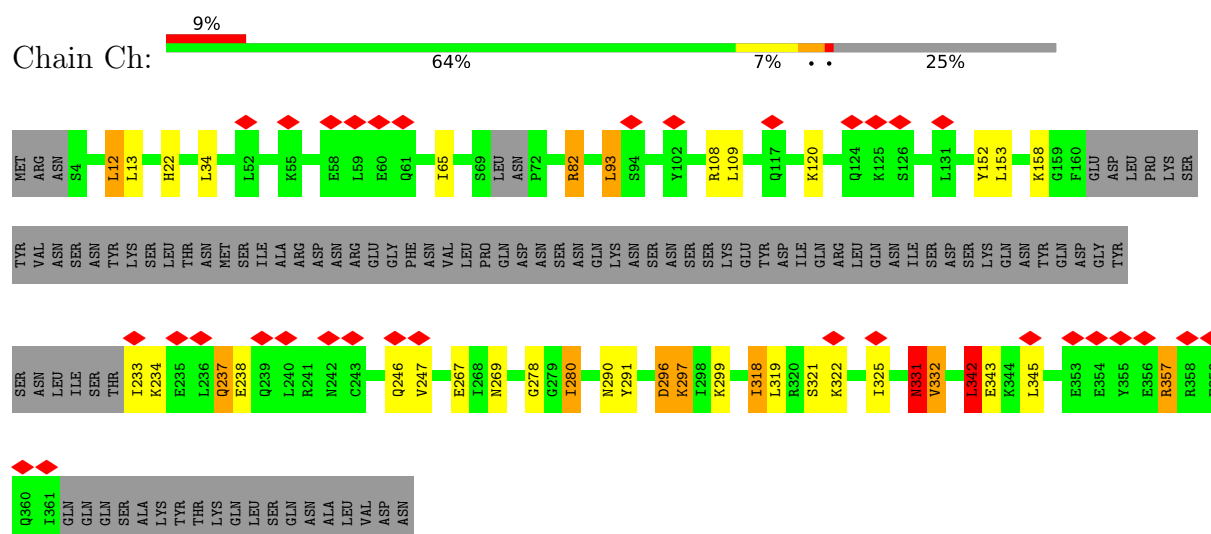
- Molecule 2: Centrosomal protein, putative



- Molecule 2: Centrosomal protein, putative

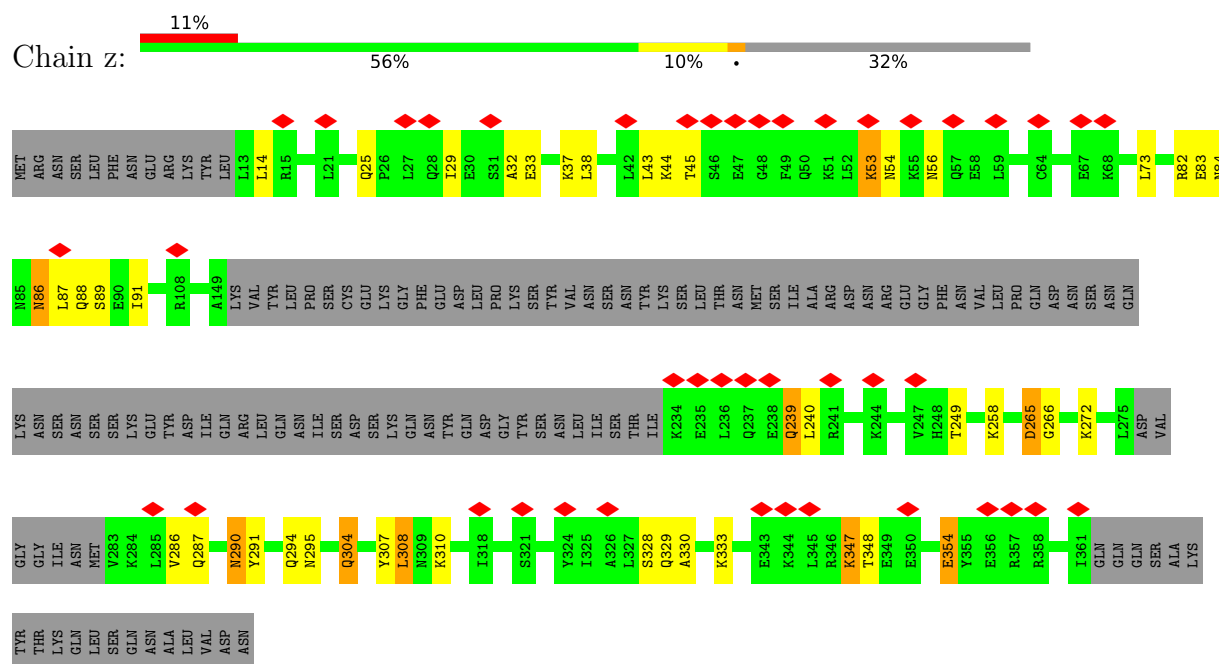


- Molecule 2: Centrosomal protein, putative

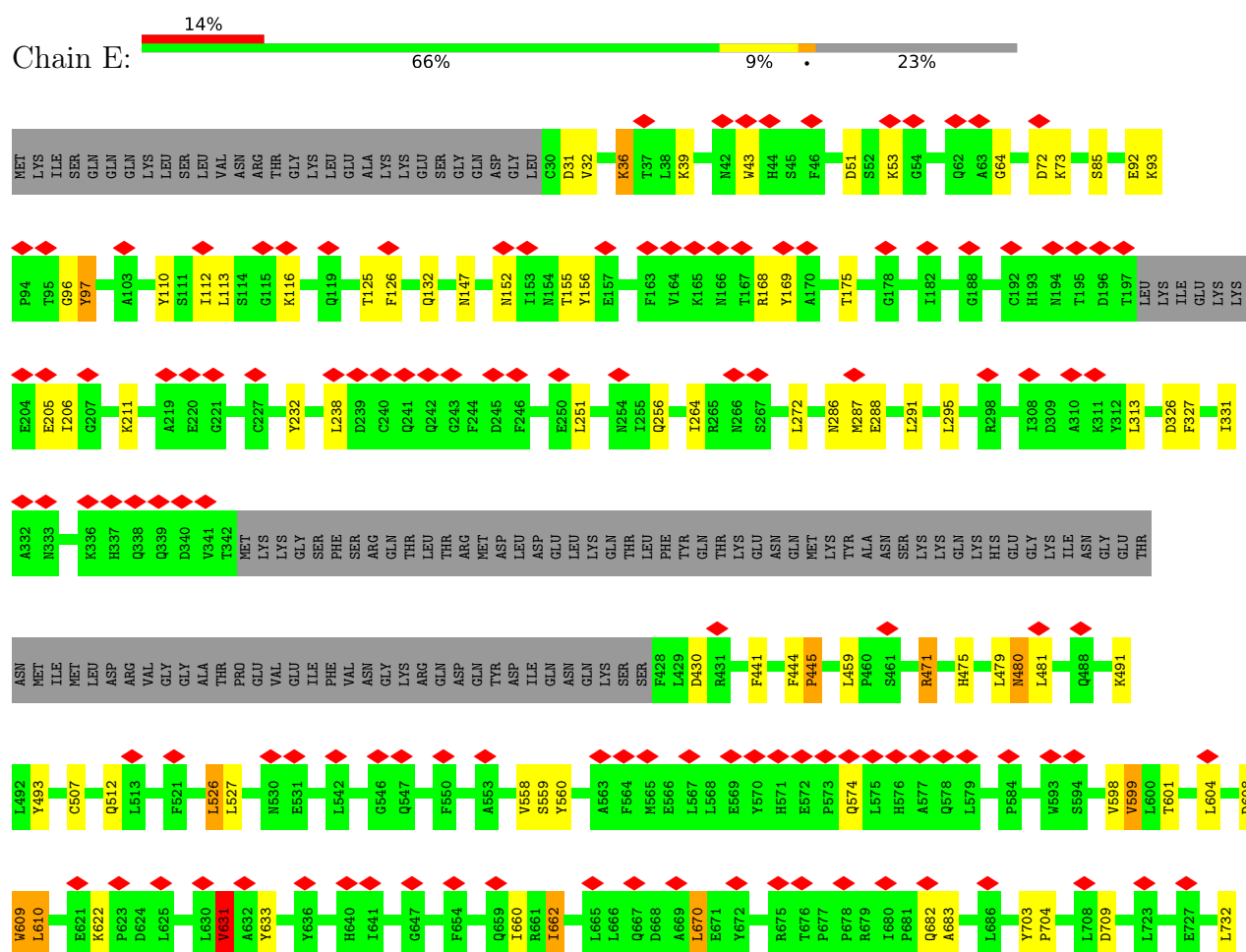




- Molecule 2: Centrosomal protein, putative



- Molecule 3: Rab-GAP TBC domain-containing protein



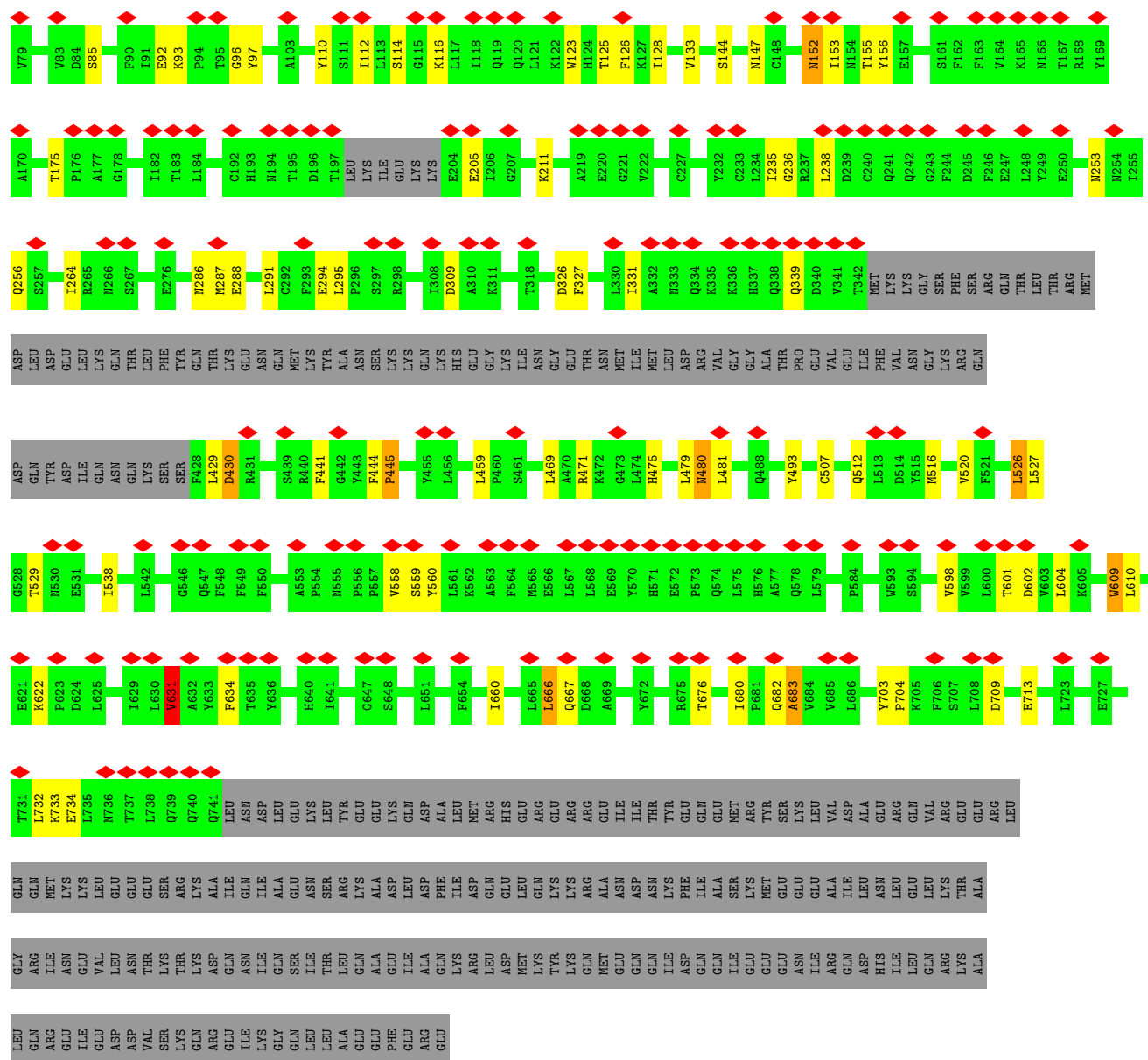




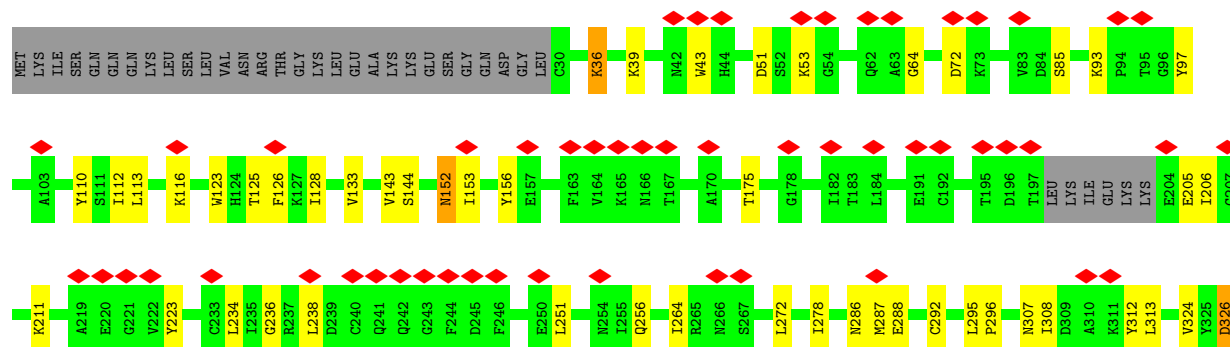
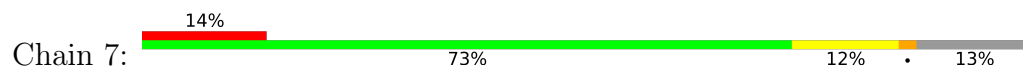




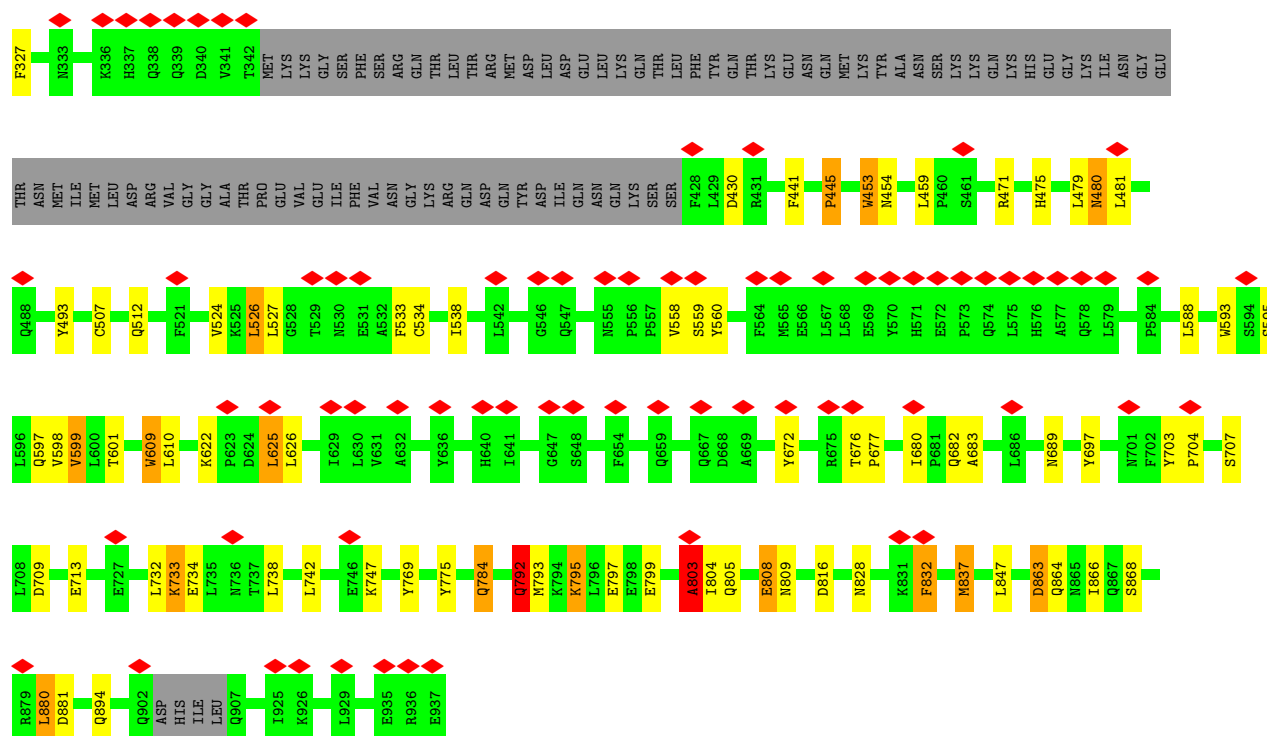




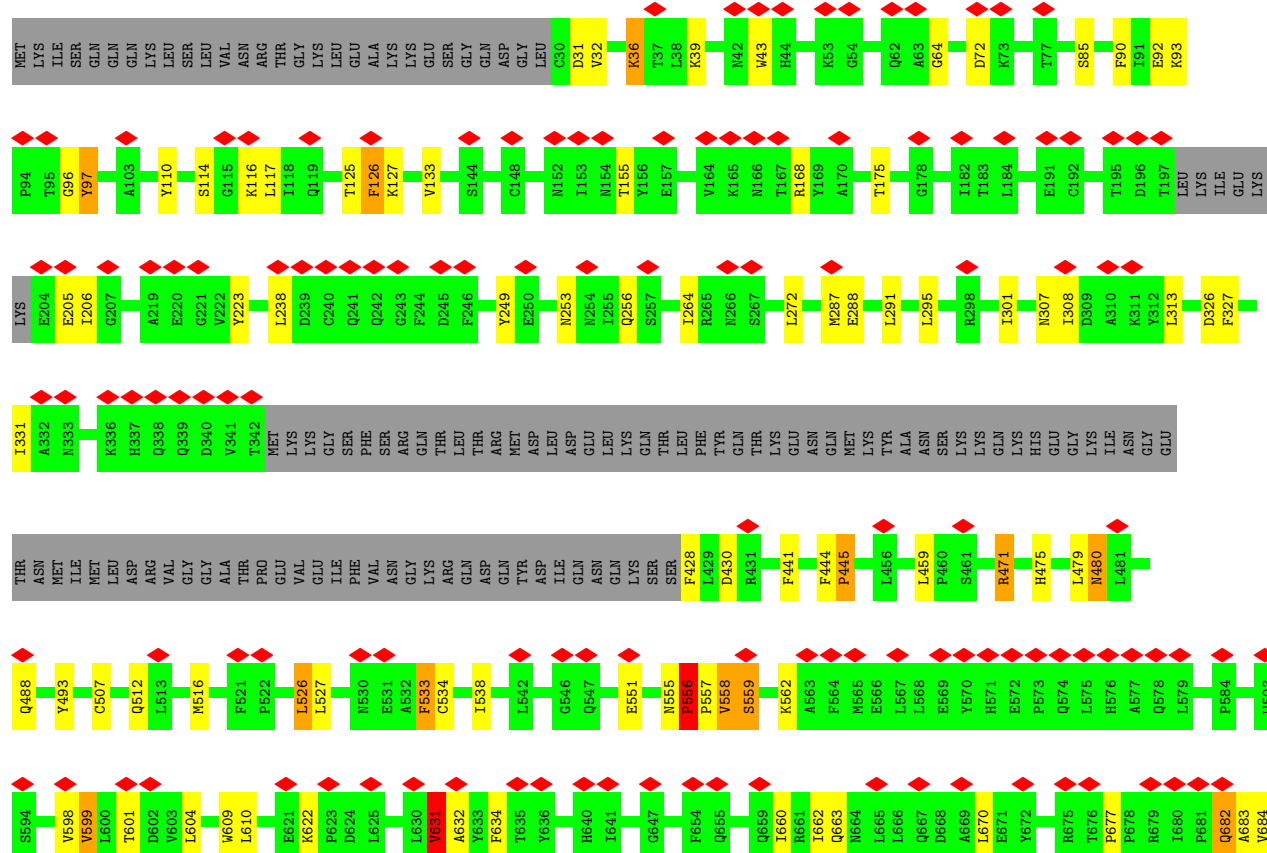
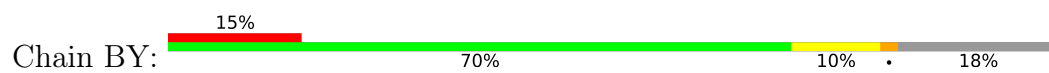
• Molecule 3: Rab-GAP TBC domain-containing protein



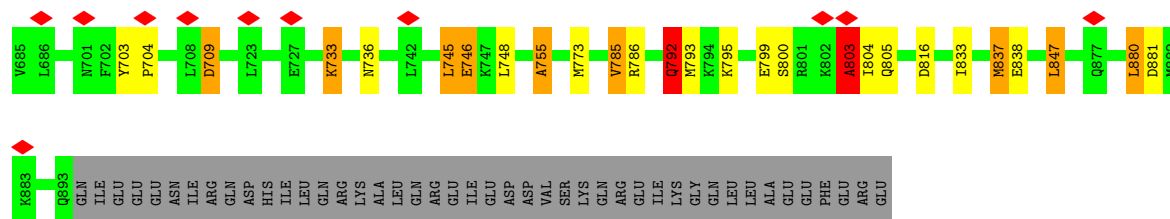




• Molecule 3: Rab-GAP TBC domain-containing protein



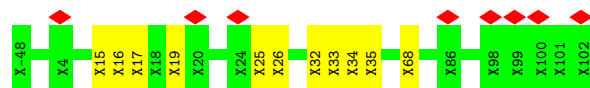
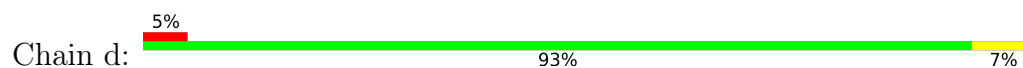




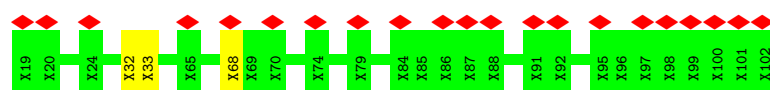
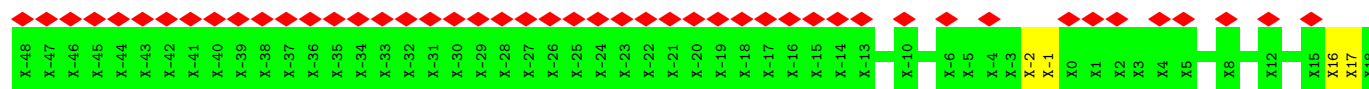
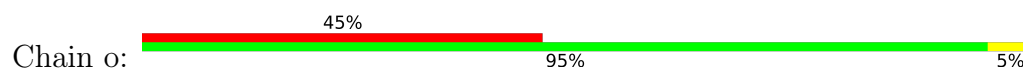
- Molecule 4: Unknown Protein Chain



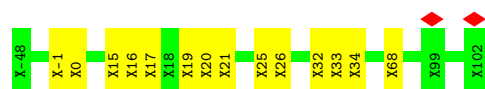
- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain

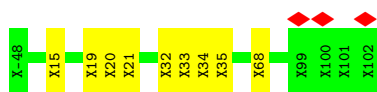


- Molecule 4: Unknown Protein Chain



- Molecule 4: Unknown Protein Chain





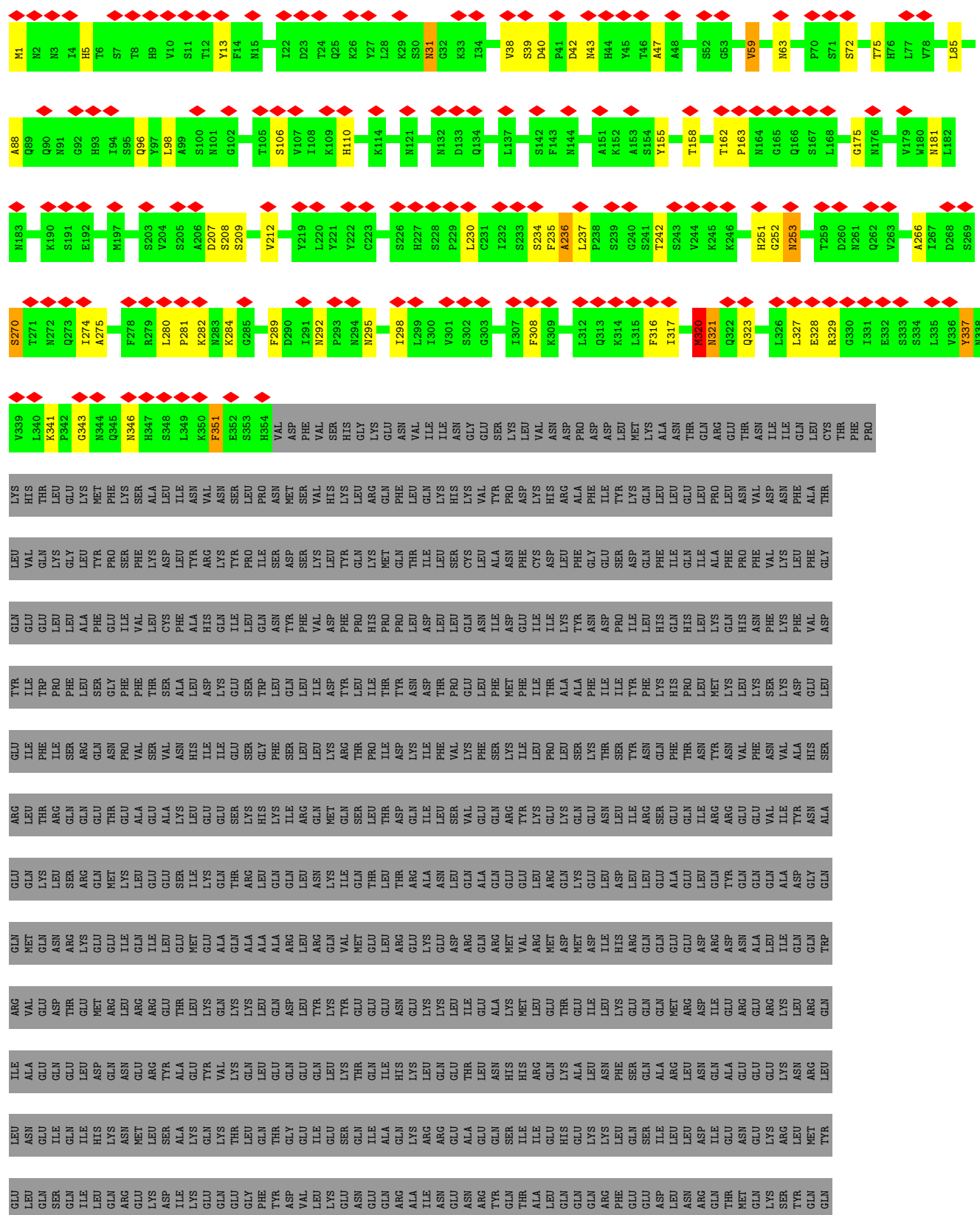
Chain G:  29% 66%







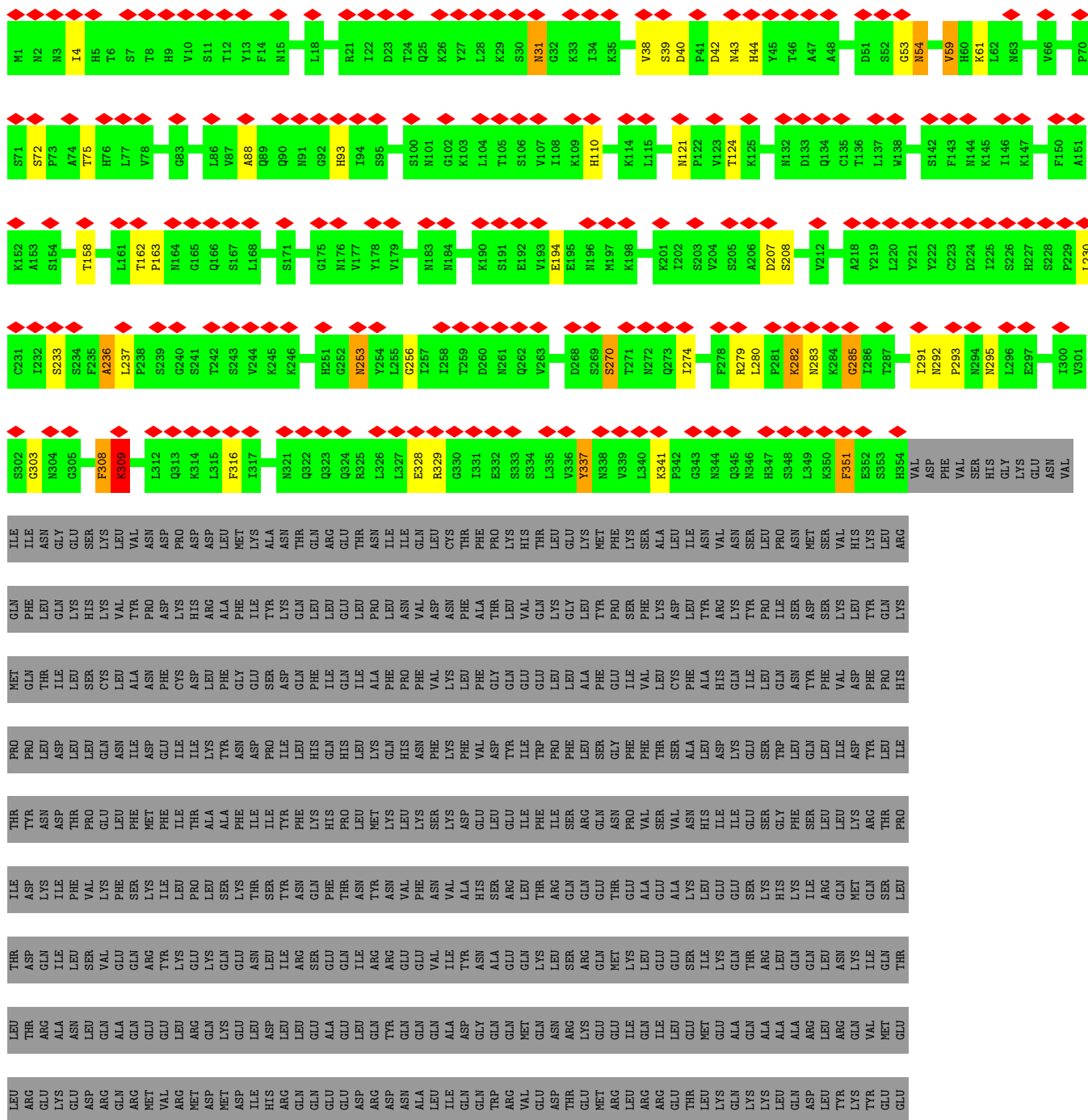






|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | PHE | GLN | ARG | ASN | GLU | HIS | THR | LYS | MET | PRO | SER | GLY | ILE | ASN | GLN | GLU | GLY | GLY | GLN |
| GLN | ARG | LEU | GLN | GLU | GLN | MET | GLN | GLN | ILE | GLN | GLU | GLY | GLY | THR | ASP | GLN | MET | ASN | GLN |

- Molecule 5: TBC1 domain family member 31





[illegible]

- Molecule 5: TBC1 domain family member 31

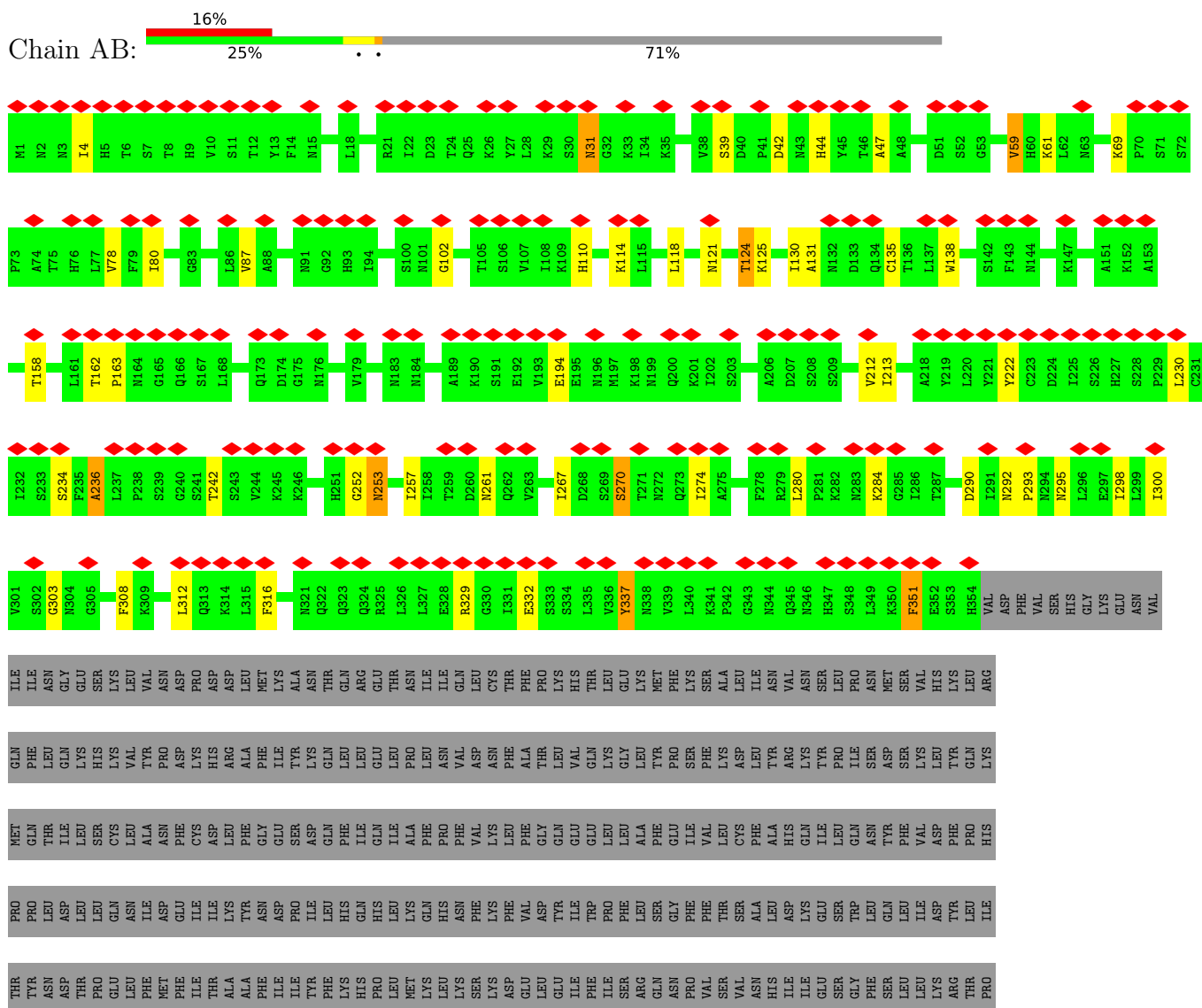
[illegible]







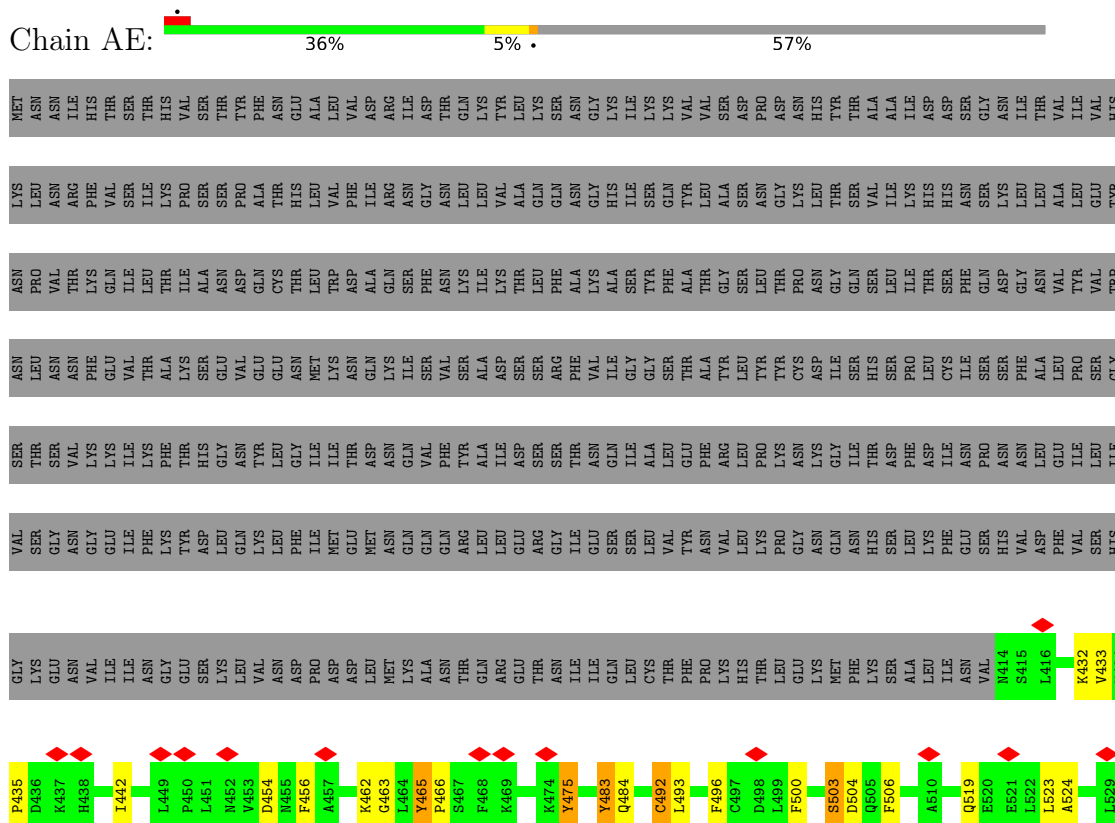
- Molecule 5: TBC1 domain family member 31



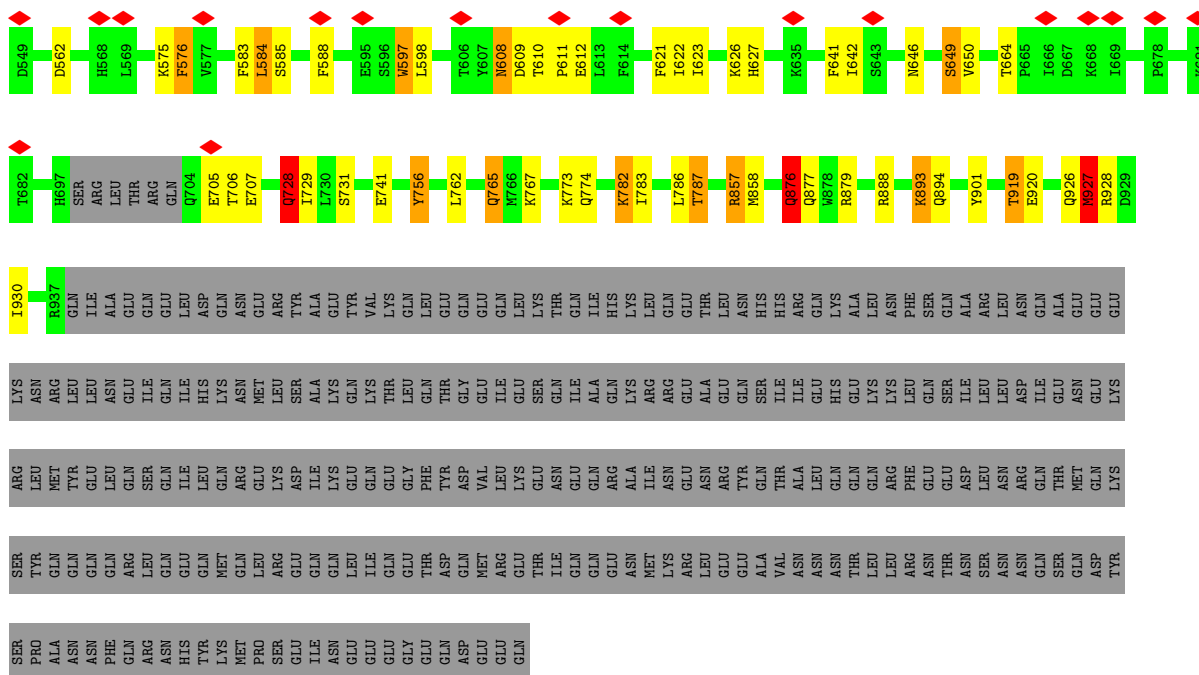


[illegible]

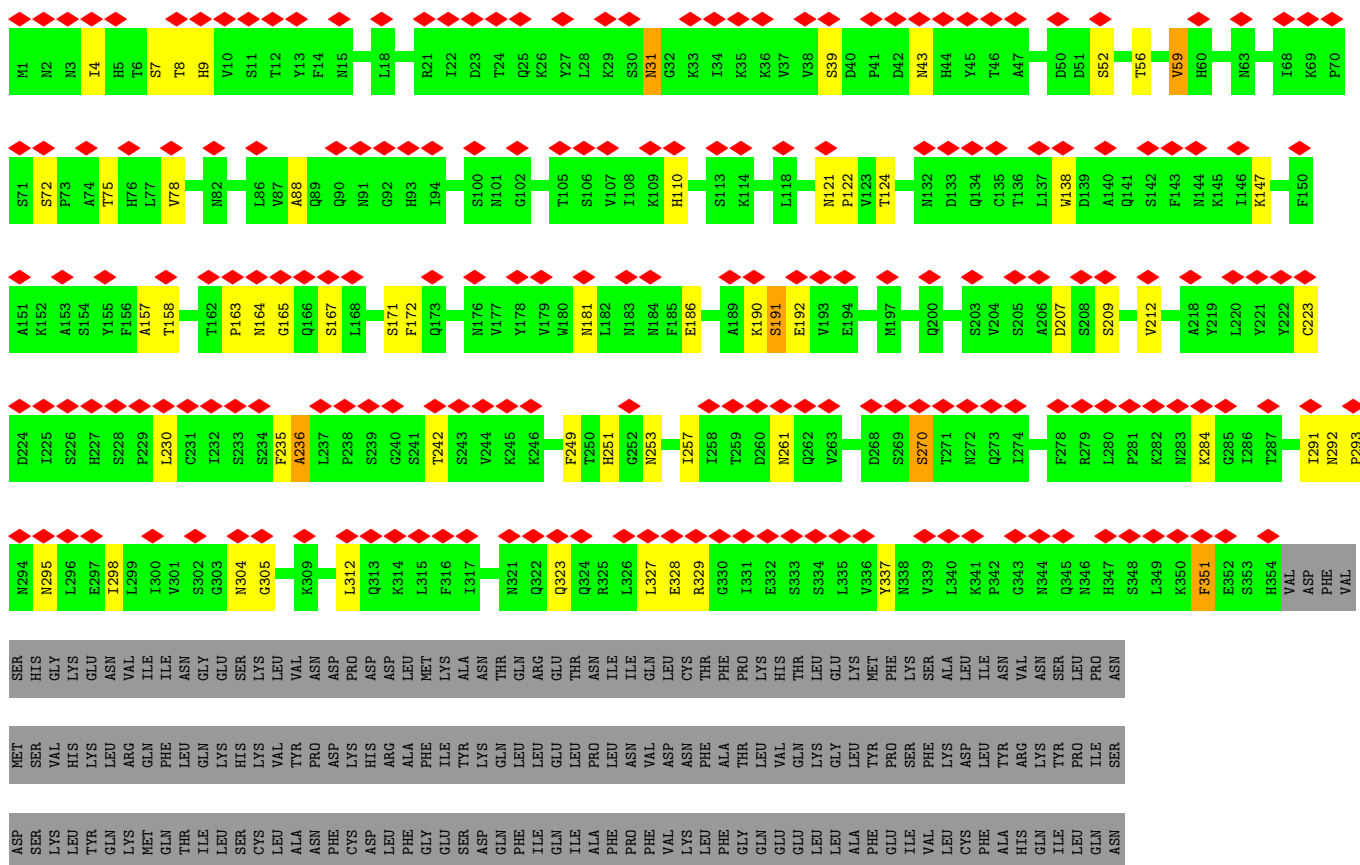
- Molecule 5: TBC1 domain family member 31







• Molecule 5: TBC1 domain family member 31







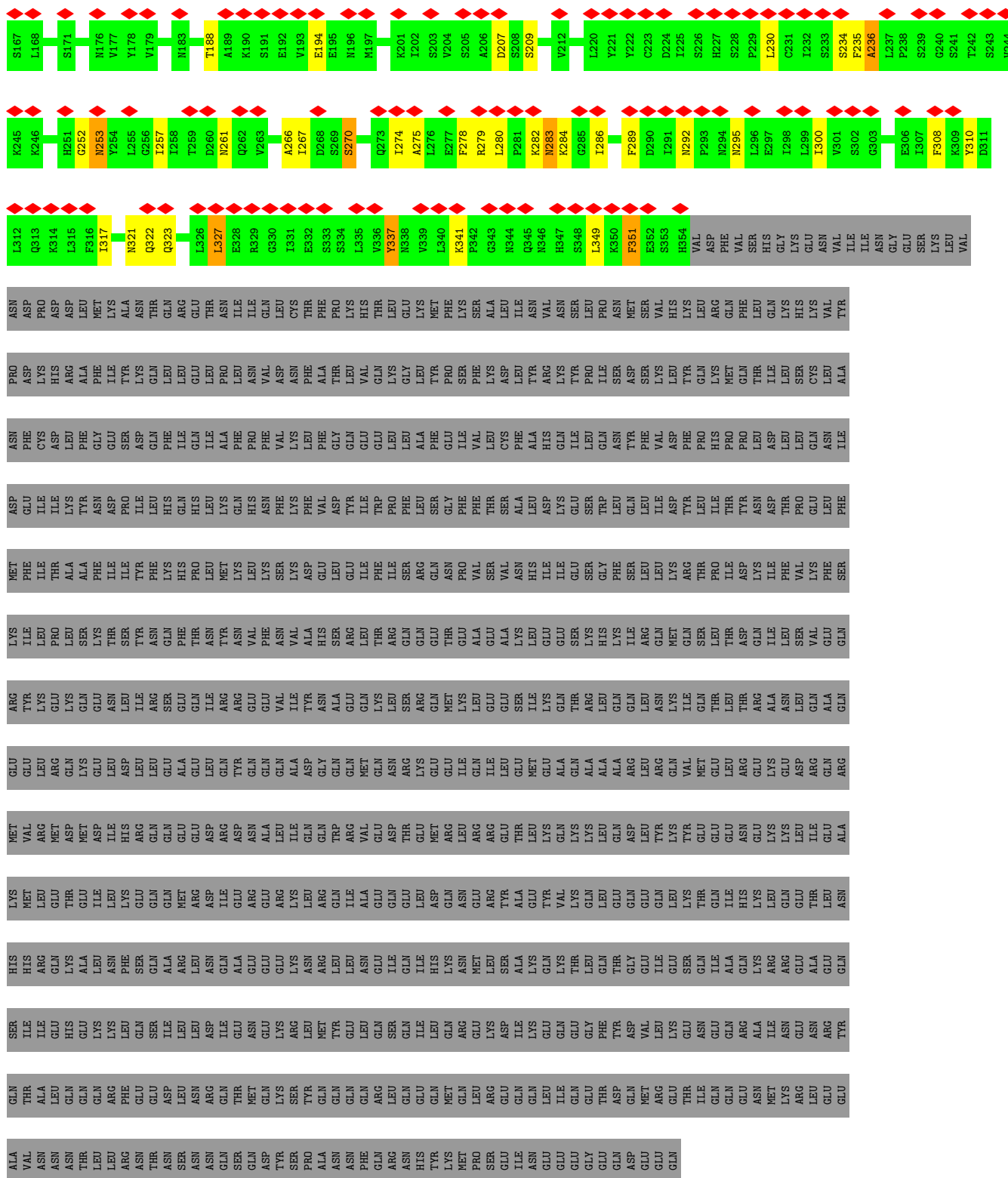




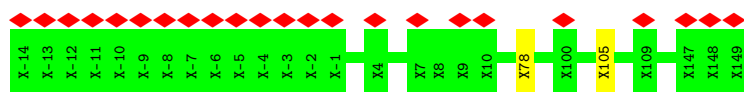




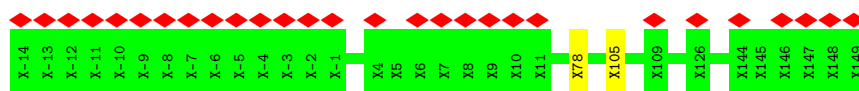




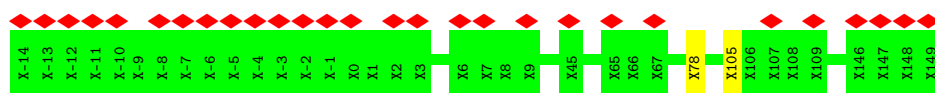




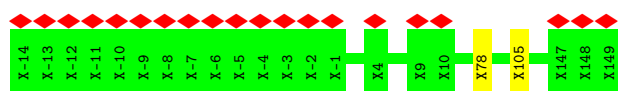
- Molecule 6: Unknown Protein Chain



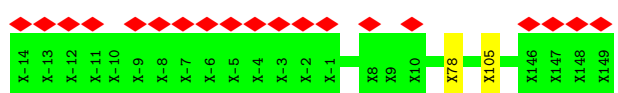
- Molecule 6: Unknown Protein Chain



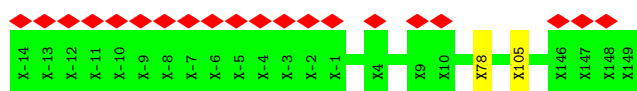
- Molecule 6: Unknown Protein Chain



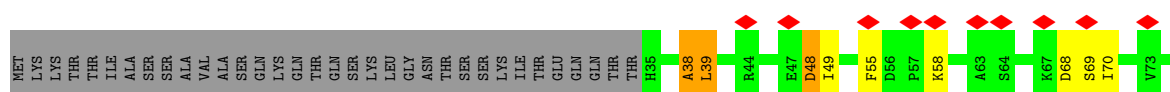
- Molecule 6: Unknown Protein Chain



- Molecule 6: Unknown Protein Chain



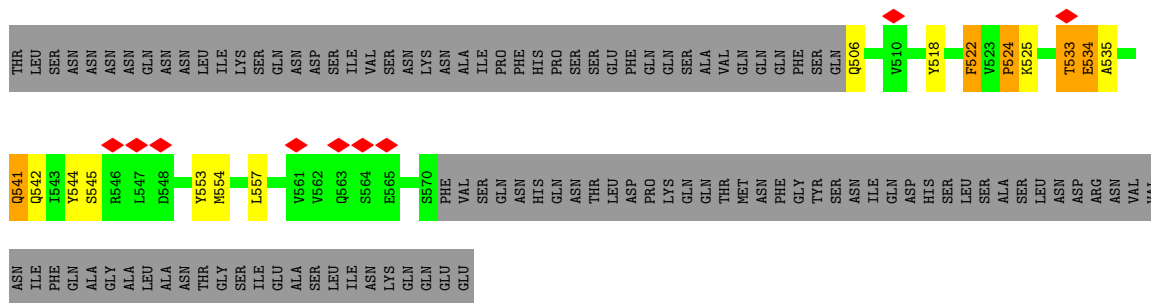
- Molecule 7: POC1 centriolar protein homolog



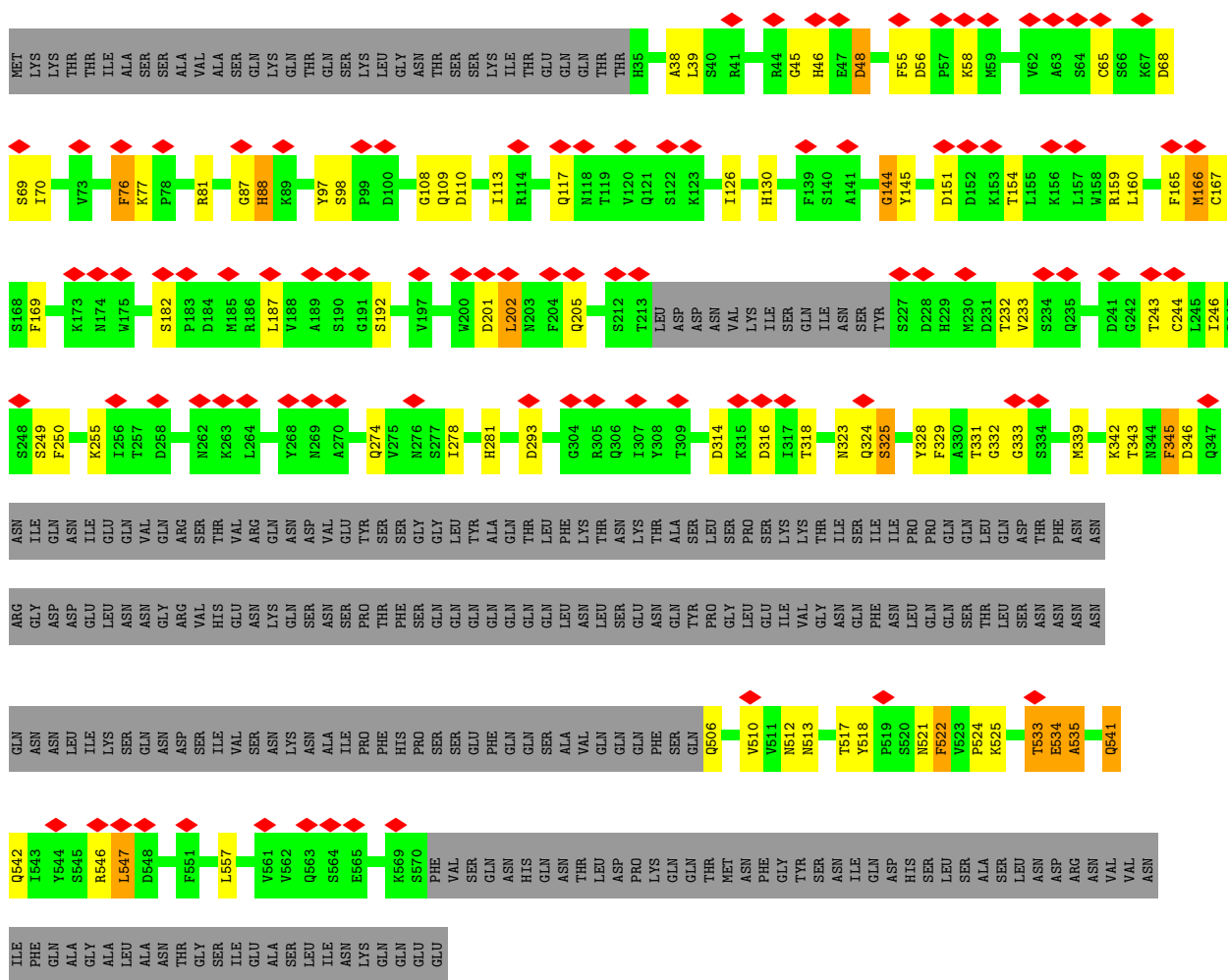
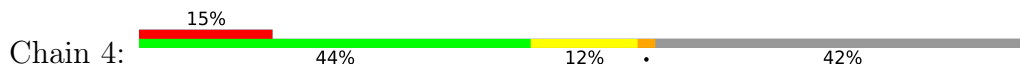




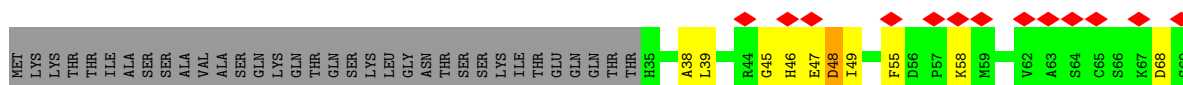
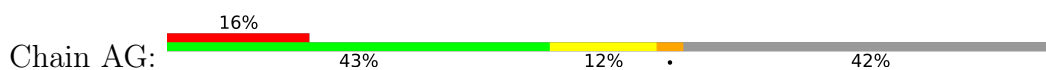




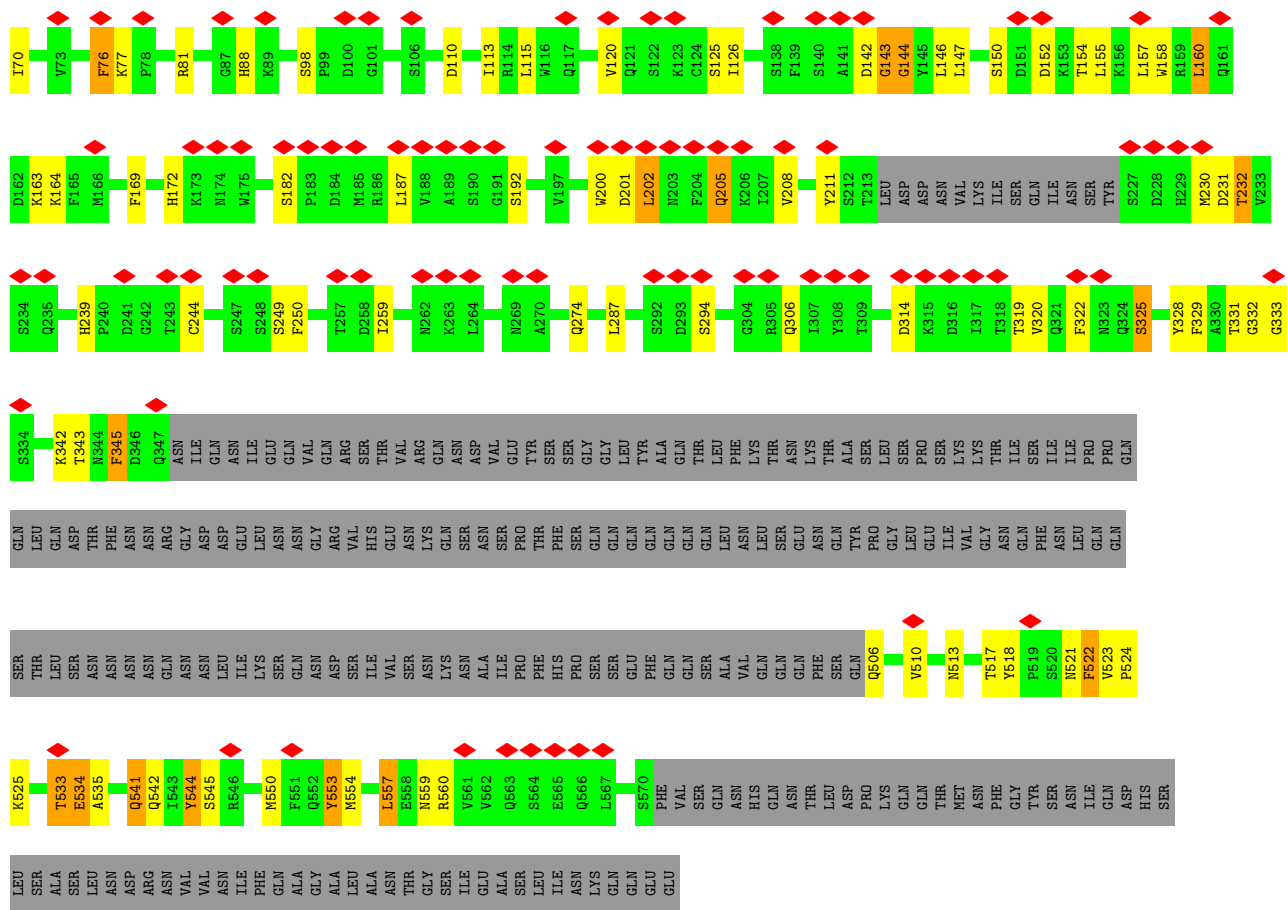
- Molecule 7: POC1 centriolar protein homolog



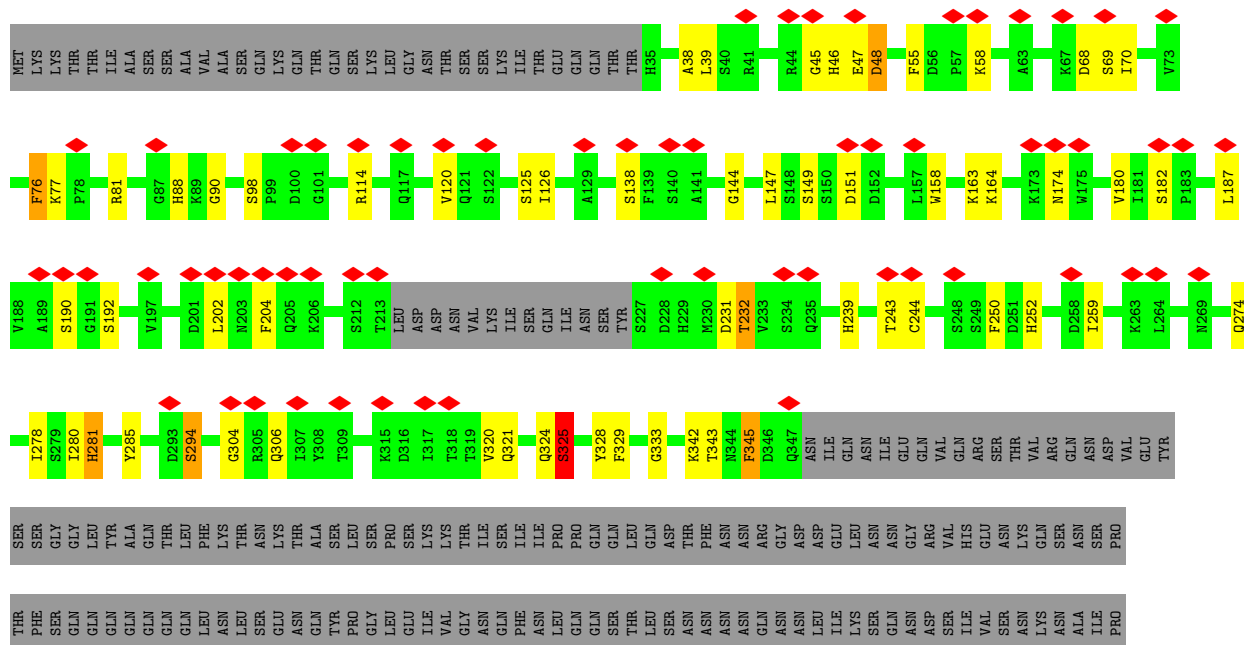
- Molecule 7: POC1 centriolar protein homolog



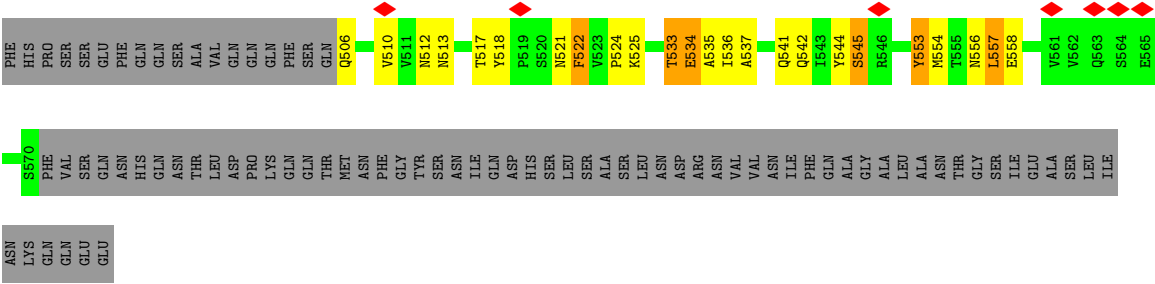




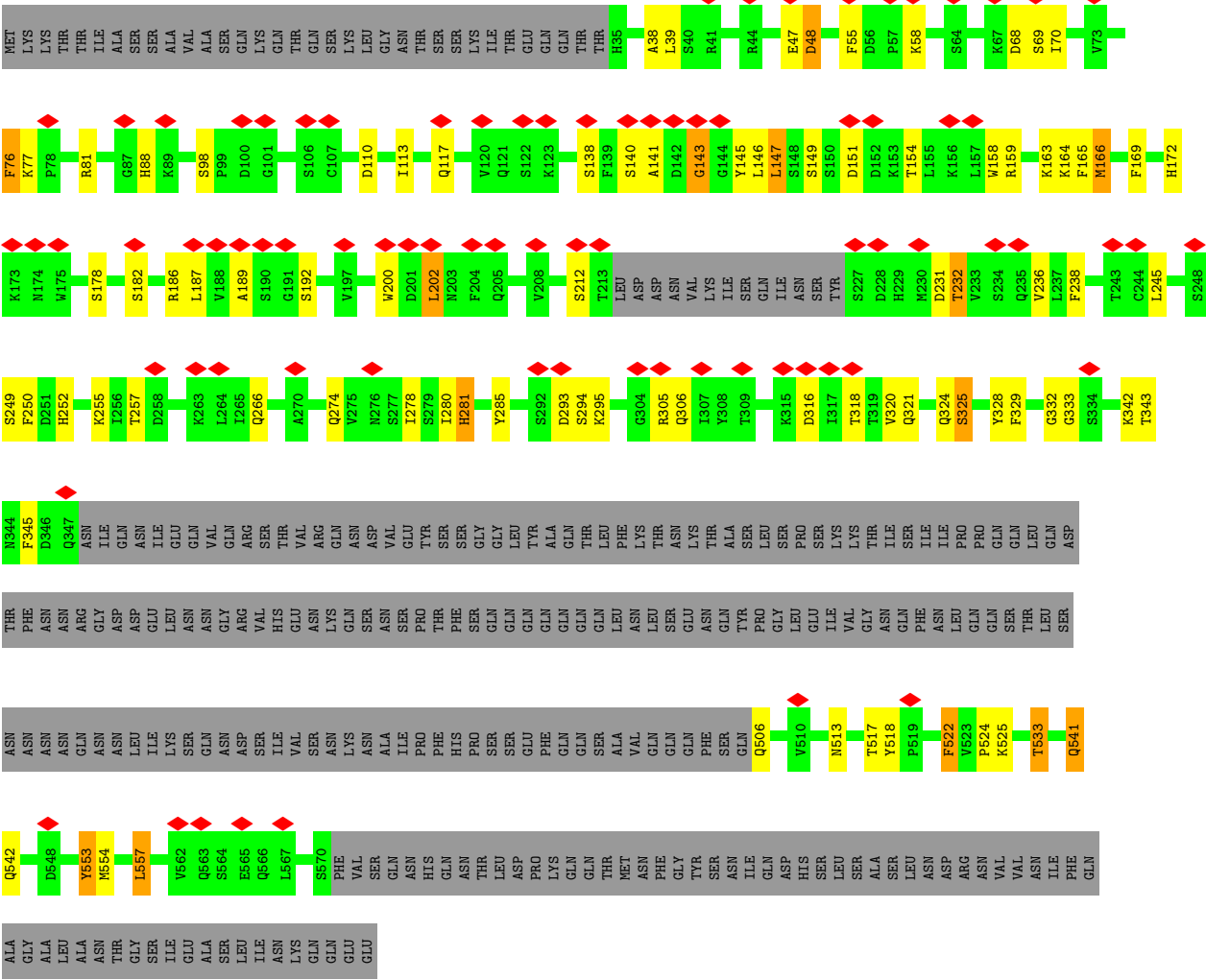
• Molecule 7: POC1 centriolar protein homolog



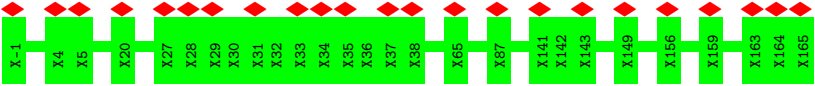




• Molecule 7: POC1 centriolar protein homolog

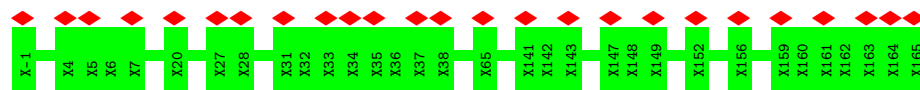


• Molecule 8: Unknown Protein Chain

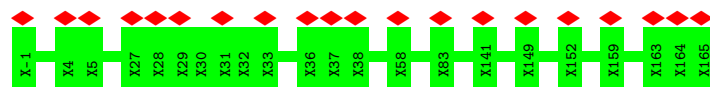




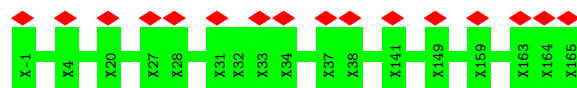
- Molecule 8: Unknown Protein Chain



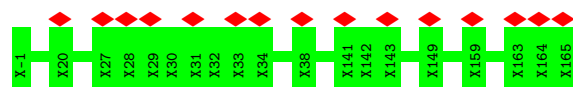
- Molecule 8: Unknown Protein Chain



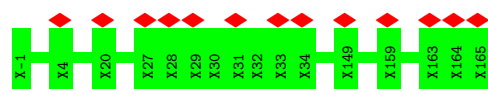
- Molecule 8: Unknown Protein Chain



- Molecule 8: Unknown Protein Chain



- Molecule 8: Unknown Protein Chain



- Molecule 9: Unknown Protein Chain



There are no outlier residues recorded for this chain.

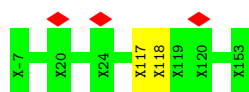
- Molecule 9: Unknown Protein Chain



- Molecule 9: Unknown Protein Chain



Chain AC:  99%



- Molecule 9: Unknown Protein Chain

Chain Bj:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown Protein Chain

Chain Bu:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown Protein Chain

Chain CH:  100%

There are no outlier residues recorded for this chain.

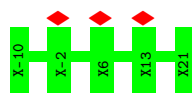
- Molecule 10: Unknown Protein Chain

Chain P:  100%



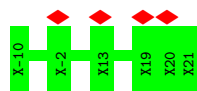
- Molecule 10: Unknown Protein Chain

Chain U:  9%  100%



- Molecule 10: Unknown Protein Chain

Chain AJ:  12%  100%



- Molecule 10: Unknown Protein Chain

Chain AW:  100%





- Molecule 10: Unknown Protein Chain

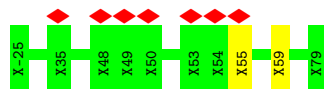


- Molecule 10: Unknown Protein Chain

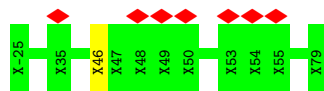


There are no outlier residues recorded for this chain.

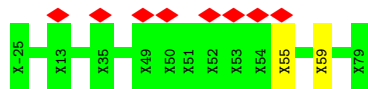
- Molecule 11: Unknown Protein Chain



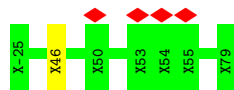
- Molecule 11: Unknown Protein Chain



- Molecule 11: Unknown Protein Chain



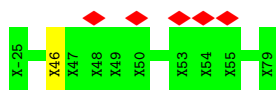
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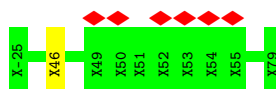
- Molecule 11: Unknown Protein Chain



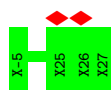




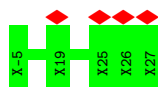
- Molecule 11: Unknown Protein Chain



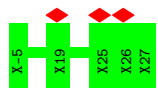
- Molecule 12: Unknown Protein Chain



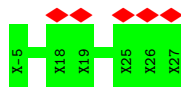
- Molecule 12: Unknown Protein Chain



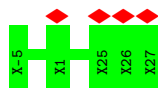
- Molecule 12: Unknown Protein Chain



- Molecule 12: Unknown Protein Chain

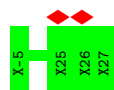


- Molecule 12: Unknown Protein Chain

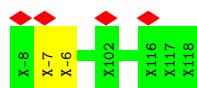


- Molecule 12: Unknown Protein Chain

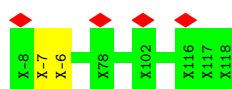




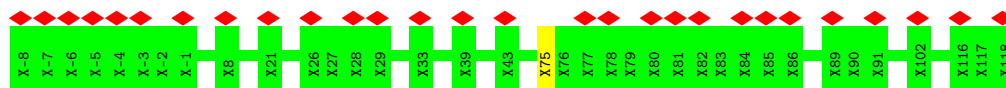
- Molecule 13: Unknown Protein Chain



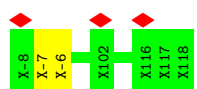
- Molecule 13: Unknown Protein Chain



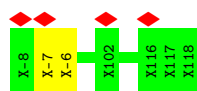
- Molecule 13: Unknown Protein Chain



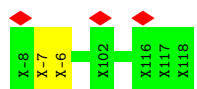
- Molecule 13: Unknown Protein Chain



- Molecule 13: Unknown Protein Chain



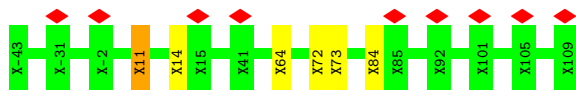
- Molecule 13: Unknown Protein Chain





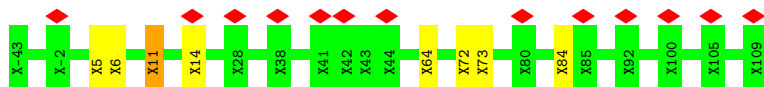
## • Molecule 14: Unknown Protein Chain

Chain V:  6% 96% ..



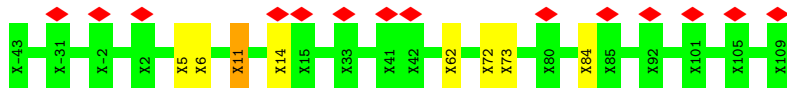
## • Molecule 14: Unknown Protein Chain

Chain a:  8% 95% 5% .




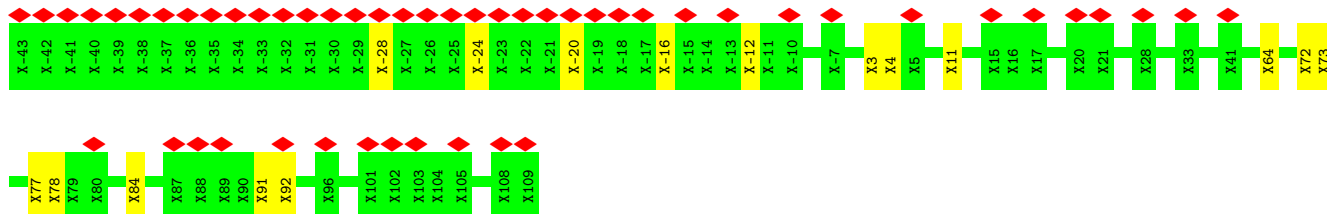
## • Molecule 14: Unknown Protein Chain

Chain AZ:  9% 95% 5% .



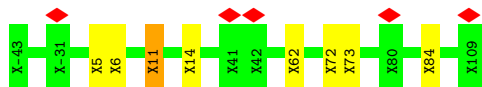
## • Molecule 14: Unknown Protein Chain

Chain Am:  33% 90% 10%



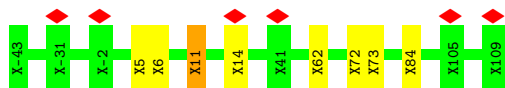
## • Molecule 14: Unknown Protein Chain

Chain As:  95% 5% .



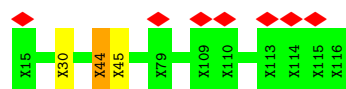
## • Molecule 14: Unknown Protein Chain

Chain CE:  95% 5% .

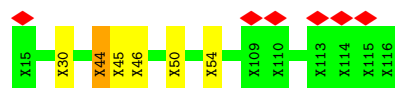


## • Molecule 15: Unknown Protein Chain

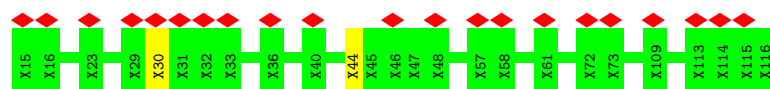




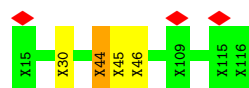
- Molecule 15: Unknown Protein Chain



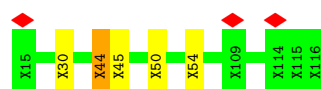
- Molecule 15: Unknown Protein Chain



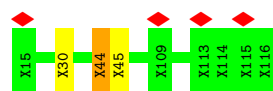
- Molecule 15: Unknown Protein Chain



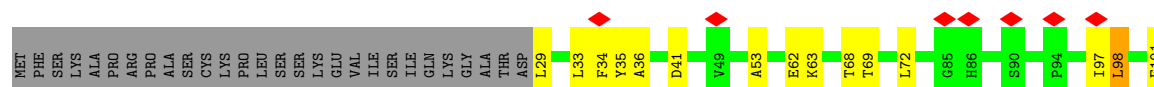
- Molecule 15: Unknown Protein Chain



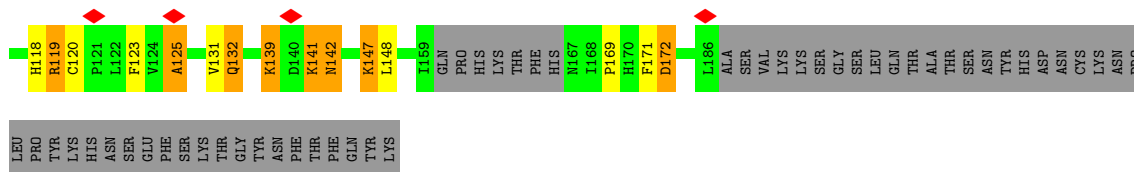
- Molecule 15: Unknown Protein Chain



- Molecule 16: SWIM-type domain-containing protein







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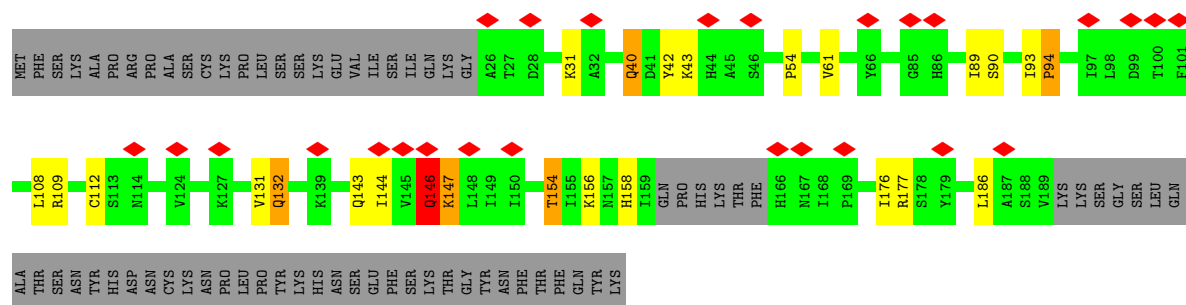
- Molecule 16: SWIM-type domain-containing protein



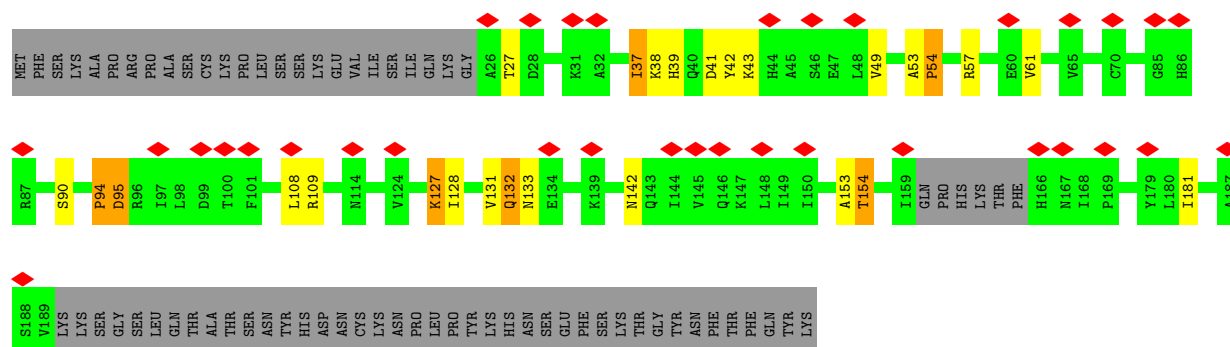
- Molecule 16: SWIM-type domain-containing protein



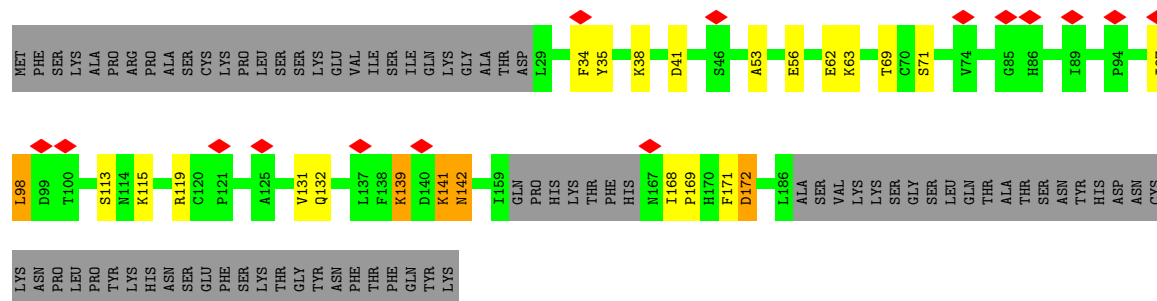




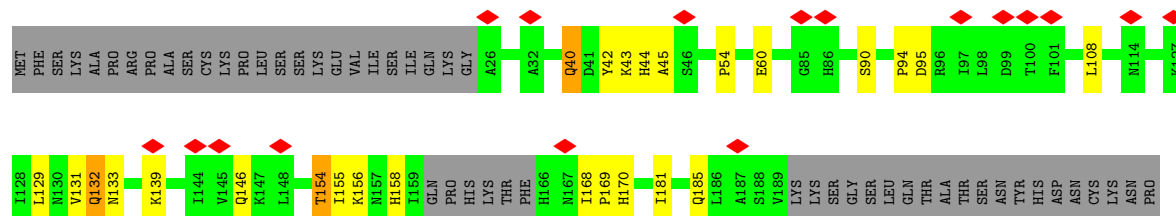
• Molecule 16: SWIM-type domain-containing protein



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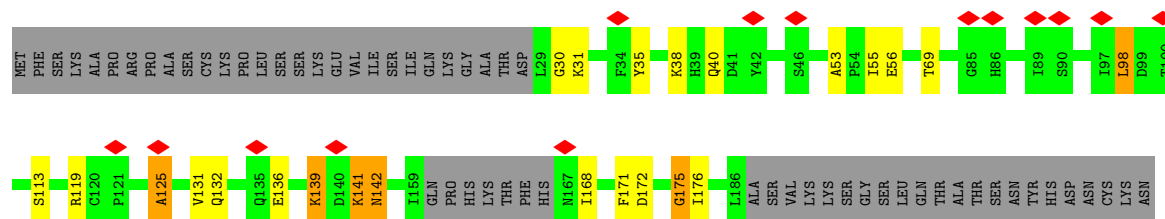
• Molecule 16: SWIM-type domain-containing protein





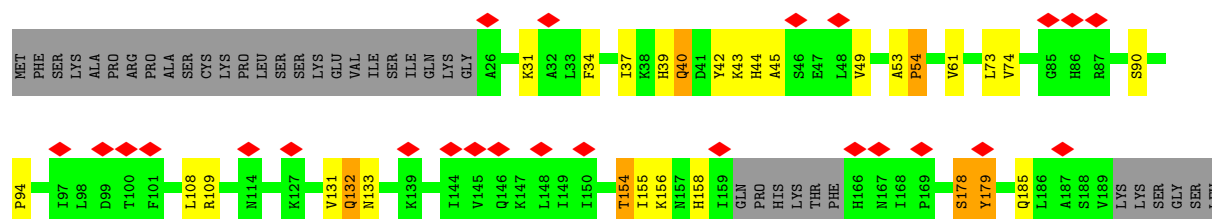
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THR  
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PHE  
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TYR  
LYS

- Molecule 16: SWIM-type domain-containing protein



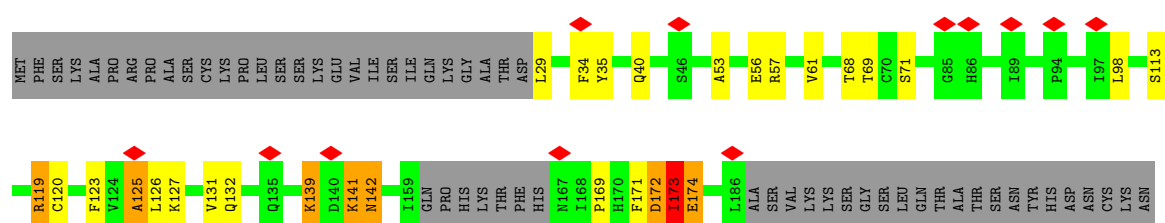
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ASN  
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TYR  
LYS

- Molecule 16: SWIM-type domain-containing protein



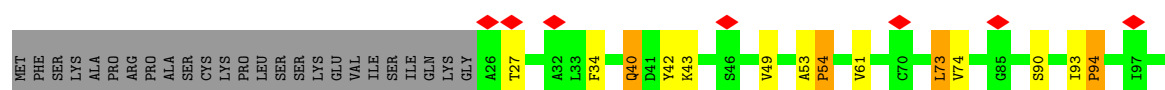
GLN  
THR  
ALA  
THR  
SER  
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TYR  
HIS  
ASP  
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PRO  
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PHE  
GLU  
THR  
PHE  
GLN  
TYR  
LYS

- Molecule 16: SWIM-type domain-containing protein



PRO  
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PHE  
THR  
PHE  
GLN  
TYR  
LYS

- Molecule 16: SWIM-type domain-containing protein









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 155485                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 13.599                                  | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.223                                   | Depositor |
| Map value standard deviation         | 1.035                                   | Depositor |
| Recommended contour level            | 5                                       | Depositor |
| Map size (Å)                         | 631.2, 631.2, 631.2                     | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.315, 1.315, 1.315                     | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | A     | 1.44         | 3/2127 (0.1%) | 1.93        | 50/2965 (1.7%)  |
| 1   | BD    | 1.53         | 4/2127 (0.2%) | 1.91        | 42/2965 (1.4%)  |
| 1   | C     | 1.50         | 1/2127 (0.0%) | 1.87        | 48/2965 (1.6%)  |
| 1   | CP    | 1.55         | 2/2127 (0.1%) | 1.99        | 53/2965 (1.8%)  |
| 1   | Ca    | 1.51         | 2/2127 (0.1%) | 1.96        | 51/2965 (1.7%)  |
| 1   | i     | 1.59         | 4/2127 (0.2%) | 1.88        | 38/2965 (1.3%)  |
| 2   | BK    | 1.32         | 1/1412 (0.1%) | 1.71        | 33/1969 (1.7%)  |
| 2   | BR    | 1.38         | 0/1285        | 2.08        | 43/1793 (2.4%)  |
| 2   | CW    | 1.39         | 4/1412 (0.3%) | 1.89        | 37/1969 (1.9%)  |
| 2   | Cd    | 1.45         | 1/1285 (0.1%) | 1.90        | 47/1793 (2.6%)  |
| 2   | Ch    | 1.31         | 3/1412 (0.2%) | 1.74        | 34/1969 (1.7%)  |
| 2   | D     | 1.28         | 2/1412 (0.1%) | 1.74        | 34/1969 (1.7%)  |
| 2   | f     | 1.34         | 2/1285 (0.2%) | 1.92        | 42/1793 (2.3%)  |
| 2   | k     | 1.35         | 3/1412 (0.2%) | 1.90        | 52/1969 (2.6%)  |
| 2   | q     | 1.30         | 0/1412        | 1.65        | 21/1969 (1.1%)  |
| 2   | s     | 1.31         | 0/1285        | 1.77        | 39/1793 (2.2%)  |
| 2   | y     | 1.42         | 0/1285        | 2.07        | 44/1793 (2.5%)  |
| 2   | z     | 1.42         | 0/1285        | 2.07        | 44/1793 (2.5%)  |
| 3   | 1     | 1.32         | 1/3079 (0.0%) | 1.91        | 97/4292 (2.3%)  |
| 3   | 7     | 1.34         | 6/4036 (0.1%) | 1.84        | 112/5629 (2.0%) |
| 3   | BY    | 1.36         | 5/3838 (0.1%) | 1.93        | 109/5354 (2.0%) |
| 3   | E     | 1.38         | 4/3594 (0.1%) | 1.91        | 101/5013 (2.0%) |
| 3   | I     | 1.25         | 4/4036 (0.1%) | 1.88        | 103/5629 (1.8%) |
| 3   | n     | 1.36         | 6/3299 (0.2%) | 2.00        | 111/4600 (2.4%) |
| 5   | 9     | 1.36         | 1/1508 (0.1%) | 2.02        | 65/2105 (3.1%)  |
| 5   | AB    | 1.40         | 5/1751 (0.3%) | 2.02        | 74/2439 (3.0%)  |
| 5   | AE    | 1.33         | 1/2582 (0.0%) | 1.91        | 82/3608 (2.3%)  |
| 5   | AO    | 1.34         | 1/1751 (0.1%) | 1.94        | 64/2439 (2.6%)  |
| 5   | AU    | 1.38         | 9/1751 (0.5%) | 1.99        | 70/2439 (2.9%)  |
| 5   | Bf    | 1.33         | 0/2332        | 1.87        | 71/3258 (2.2%)  |
| 5   | Bt    | 1.40         | 4/1751 (0.2%) | 2.07        | 69/2439 (2.8%)  |
| 5   | G     | 1.38         | 2/2062 (0.1%) | 1.96        | 75/2880 (2.6%)  |
| 5   | L     | 1.24         | 0/2582        | 1.88        | 91/3608 (2.5%)  |
| 5   | M     | 1.39         | 6/1751 (0.3%) | 2.00        | 64/2439 (2.6%)  |



| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 5   | R     | 1.29         | 1/1751 (0.1%)    | 1.94        | 55/2439 (2.3%)     |
| 5   | v     | 1.35         | 0/1788           | 2.04        | 68/2497 (2.7%)     |
| 7   | 4     | 1.55         | 8/1803 (0.4%)    | 2.06        | 81/2508 (3.2%)     |
| 7   | AG    | 1.55         | 12/1803 (0.7%)   | 2.10        | 90/2508 (3.6%)     |
| 7   | AM    | 1.55         | 2/1803 (0.1%)    | 2.05        | 74/2508 (3.0%)     |
| 7   | Bm    | 1.51         | 5/1803 (0.3%)    | 2.08        | 84/2508 (3.3%)     |
| 7   | J     | 1.52         | 11/1803 (0.6%)   | 2.09        | 80/2508 (3.2%)     |
| 7   | O     | 1.44         | 5/1803 (0.3%)    | 1.91        | 53/2508 (2.1%)     |
| 16  | A7    | 1.49         | 1/781 (0.1%)     | 2.03        | 26/1086 (2.4%)     |
| 16  | Ai    | 1.38         | 0/746            | 2.02        | 35/1037 (3.4%)     |
| 16  | An    | 1.36         | 0/746            | 1.94        | 26/1037 (2.5%)     |
| 16  | Aq    | 1.48         | 1/781 (0.1%)     | 2.07        | 27/1086 (2.5%)     |
| 16  | Av    | 1.52         | 2/781 (0.3%)     | 2.00        | 23/1086 (2.1%)     |
| 16  | Az    | 1.35         | 0/746            | 2.02        | 25/1037 (2.4%)     |
| 16  | CB    | 1.39         | 1/746 (0.1%)     | 2.01        | 28/1037 (2.7%)     |
| 16  | CI    | 1.51         | 1/781 (0.1%)     | 2.05        | 29/1086 (2.7%)     |
| 16  | CM    | 1.38         | 0/746            | 2.09        | 34/1037 (3.3%)     |
| 16  | CT    | 1.54         | 1/781 (0.1%)     | 1.99        | 23/1086 (2.1%)     |
| 16  | Z     | 1.39         | 1/746 (0.1%)     | 2.16        | 34/1037 (3.3%)     |
| 16  | c     | 1.52         | 1/781 (0.1%)     | 1.96        | 22/1086 (2.0%)     |
| All | All   | 1.40         | 140/94166 (0.1%) | 1.95        | 3027/131255 (2.3%) |

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   | A     | 0                   | 7                   |
| 1   | BD    | 0                   | 7                   |
| 1   | C     | 0                   | 5                   |
| 1   | CP    | 0                   | 7                   |
| 1   | Ca    | 0                   | 8                   |
| 1   | i     | 0                   | 6                   |
| 2   | BK    | 0                   | 9                   |
| 2   | BR    | 0                   | 10                  |
| 2   | CW    | 0                   | 11                  |
| 2   | Cd    | 0                   | 15                  |
| 2   | Ch    | 0                   | 11                  |
| 2   | D     | 0                   | 8                   |
| 2   | f     | 0                   | 11                  |
| 2   | k     | 0                   | 11                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | q     | 0                   | 7                   |
| 2   | s     | 0                   | 10                  |
| 2   | y     | 0                   | 11                  |
| 2   | z     | 0                   | 11                  |
| 3   | 1     | 0                   | 10                  |
| 3   | 7     | 0                   | 18                  |
| 3   | BY    | 0                   | 18                  |
| 3   | E     | 0                   | 17                  |
| 3   | I     | 0                   | 18                  |
| 3   | n     | 0                   | 12                  |
| 4   | BO    | 0                   | 1                   |
| 4   | BZ    | 0                   | 1                   |
| 4   | Bw    | 0                   | 1                   |
| 4   | F     | 0                   | 1                   |
| 4   | d     | 0                   | 1                   |
| 4   | o     | 0                   | 1                   |
| 5   | 9     | 0                   | 9                   |
| 5   | AB    | 0                   | 9                   |
| 5   | AE    | 0                   | 18                  |
| 5   | AO    | 0                   | 9                   |
| 5   | AU    | 0                   | 9                   |
| 5   | Bf    | 0                   | 11                  |
| 5   | Bt    | 0                   | 8                   |
| 5   | G     | 0                   | 12                  |
| 5   | L     | 0                   | 17                  |
| 5   | M     | 0                   | 9                   |
| 5   | R     | 0                   | 11                  |
| 5   | v     | 0                   | 10                  |
| 6   | B4    | 0                   | 3                   |
| 6   | BV    | 0                   | 3                   |
| 6   | Bg    | 0                   | 3                   |
| 6   | H     | 0                   | 3                   |
| 6   | l     | 0                   | 3                   |
| 6   | w     | 0                   | 3                   |
| 7   | 4     | 0                   | 13                  |
| 7   | AG    | 0                   | 10                  |
| 7   | AM    | 0                   | 13                  |
| 7   | Bm    | 0                   | 13                  |
| 7   | J     | 0                   | 10                  |
| 7   | O     | 0                   | 12                  |
| 11  | 0     | 0                   | 1                   |
| 11  | B2    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | Bq    | 0                   | 1                   |
| 11  | CO    | 0                   | 1                   |
| 13  | AS    | 0                   | 1                   |
| 14  | AZ    | 0                   | 3                   |
| 14  | Am    | 0                   | 3                   |
| 14  | As    | 0                   | 3                   |
| 14  | CE    | 0                   | 3                   |
| 14  | V     | 0                   | 3                   |
| 14  | a     | 0                   | 3                   |
| 15  | AP    | 0                   | 2                   |
| 15  | Aa    | 0                   | 2                   |
| 15  | B5    | 0                   | 2                   |
| 15  | CF    | 0                   | 2                   |
| 15  | Cc    | 0                   | 2                   |
| 15  | W     | 0                   | 2                   |
| 16  | A7    | 0                   | 5                   |
| 16  | Ai    | 0                   | 5                   |
| 16  | An    | 0                   | 5                   |
| 16  | Aq    | 0                   | 6                   |
| 16  | Av    | 0                   | 6                   |
| 16  | Az    | 0                   | 3                   |
| 16  | CB    | 0                   | 5                   |
| 16  | CI    | 0                   | 5                   |
| 16  | CM    | 0                   | 4                   |
| 16  | CT    | 0                   | 5                   |
| 16  | Z     | 0                   | 5                   |
| 16  | c     | 0                   | 5                   |
| All | All   | 0                   | 579                 |

All (140) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | n     | 752 | LYS  | CA-C  | 9.79  | 1.57        | 1.52     |
| 7   | 4     | 144 | GLY  | CA-C  | -7.76 | 1.43        | 1.52     |
| 5   | Bt    | 283 | ASN  | CA-C  | -7.34 | 1.43        | 1.53     |
| 1   | Ca    | 204 | PHE  | CA-C  | -7.05 | 1.44        | 1.52     |
| 7   | 4     | 130 | HIS  | CA-C  | -6.99 | 1.49        | 1.53     |
| 2   | Cd    | 70  | LEU  | CA-C  | -6.63 | 1.47        | 1.52     |
| 7   | Bm    | 154 | THR  | CA-C  | -6.55 | 1.44        | 1.53     |
| 2   | D     | 34  | LEU  | CA-C  | -6.45 | 1.44        | 1.52     |
| 7   | 4     | 154 | THR  | CA-C  | -6.41 | 1.44        | 1.52     |
| 2   | CW    | 325 | ILE  | N-CA  | -6.34 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | M     | 88  | ALA  | CA-C  | -6.32 | 1.45        | 1.52     |
| 7   | AG    | 314 | ASP  | CA-C  | -6.27 | 1.46        | 1.53     |
| 1   | i     | 198 | SER  | CA-C  | -6.23 | 1.45        | 1.52     |
| 5   | AU    | 300 | ILE  | CA-C  | -6.17 | 1.45        | 1.52     |
| 7   | Bm    | 172 | HIS  | CA-C  | -6.17 | 1.45        | 1.52     |
| 1   | BD    | 198 | SER  | CA-C  | -6.16 | 1.45        | 1.52     |
| 5   | Bt    | 88  | ALA  | CA-C  | -6.14 | 1.45        | 1.52     |
| 5   | AB    | 47  | ALA  | CA-C  | -6.10 | 1.45        | 1.52     |
| 5   | AU    | 181 | ASN  | CA-CB | -6.10 | 1.45        | 1.52     |
| 7   | 4     | 145 | TYR  | N-CA  | -6.07 | 1.38        | 1.46     |
| 7   | AG    | 154 | THR  | CA-C  | -6.05 | 1.44        | 1.52     |
| 5   | AB    | 130 | ILE  | CA-C  | -6.01 | 1.45        | 1.52     |
| 1   | CP    | 198 | SER  | CA-C  | -5.98 | 1.45        | 1.52     |
| 7   | O     | 115 | LEU  | CA-C  | -5.97 | 1.45        | 1.53     |
| 3   | E     | 113 | LEU  | CA-C  | -5.96 | 1.45        | 1.52     |
| 3   | n     | 773 | MET  | CA-CB | -5.91 | 1.43        | 1.53     |
| 5   | G     | 616 | PHE  | CA-C  | -5.87 | 1.45        | 1.52     |
| 5   | AU    | 301 | VAL  | CA-C  | -5.87 | 1.45        | 1.52     |
| 5   | M     | 284 | LYS  | N-CA  | -5.85 | 1.40        | 1.46     |
| 1   | C     | 198 | SER  | CA-C  | -5.84 | 1.45        | 1.52     |
| 5   | AU    | 295 | ASN  | CA-C  | -5.83 | 1.45        | 1.52     |
| 5   | M     | 234 | SER  | CA-CB | -5.83 | 1.43        | 1.53     |
| 16  | Z     | 132 | GLN  | CA-C  | -5.83 | 1.47        | 1.52     |
| 7   | AG    | 211 | TYR  | CA-C  | -5.82 | 1.45        | 1.52     |
| 2   | k     | 26  | PRO  | CA-C  | 5.80  | 1.58        | 1.53     |
| 5   | AU    | 88  | ALA  | CA-C  | -5.75 | 1.45        | 1.52     |
| 3   | 7     | 598 | VAL  | CA-C  | 5.75  | 1.60        | 1.52     |
| 7   | J     | 154 | THR  | CA-C  | -5.74 | 1.45        | 1.53     |
| 7   | AG    | 172 | HIS  | CA-C  | -5.72 | 1.45        | 1.52     |
| 5   | G     | 617 | ILE  | N-CA  | -5.71 | 1.39        | 1.46     |
| 5   | R     | 88  | ALA  | CA-C  | -5.71 | 1.45        | 1.52     |
| 7   | AM    | 192 | SER  | CA-CB | -5.70 | 1.44        | 1.53     |
| 3   | 1     | 598 | VAL  | CA-C  | 5.65  | 1.60        | 1.52     |
| 7   | J     | 279 | SER  | CA-CB | -5.62 | 1.44        | 1.53     |
| 3   | 7     | 272 | LEU  | CA-C  | -5.61 | 1.45        | 1.52     |
| 5   | Bt    | 300 | ILE  | CA-C  | -5.61 | 1.46        | 1.52     |
| 16  | CB    | 35  | TYR  | N-CA  | -5.61 | 1.41        | 1.46     |
| 2   | Ch    | 318 | ILE  | N-CA  | -5.60 | 1.39        | 1.46     |
| 16  | Av    | 181 | ILE  | CA-C  | -5.60 | 1.45        | 1.52     |
| 7   | J     | 237 | LEU  | CA-C  | -5.59 | 1.46        | 1.52     |
| 3   | 7     | 234 | LEU  | CA-C  | -5.58 | 1.46        | 1.52     |
| 7   | AG    | 144 | GLY  | CA-C  | -5.58 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | CW    | 34  | LEU  | CA-C  | -5.57 | 1.45        | 1.52     |
| 2   | Ch    | 325 | ILE  | N-CA  | -5.57 | 1.41        | 1.46     |
| 3   | n     | 272 | LEU  | CA-C  | -5.56 | 1.45        | 1.52     |
| 5   | M     | 88  | ALA  | CA-CB | -5.49 | 1.46        | 1.53     |
| 7   | AG    | 115 | LEU  | CA-C  | -5.49 | 1.45        | 1.53     |
| 2   | f     | 333 | LYS  | CA-C  | -5.44 | 1.45        | 1.52     |
| 1   | Ca    | 198 | SER  | CA-C  | -5.43 | 1.46        | 1.52     |
| 5   | Bt    | 234 | SER  | CA-CB | -5.43 | 1.44        | 1.53     |
| 3   | BY    | 223 | TYR  | CA-C  | -5.42 | 1.46        | 1.52     |
| 7   | O     | 43  | PHE  | CA-C  | -5.41 | 1.46        | 1.52     |
| 3   | E     | 598 | VAL  | CA-C  | 5.41  | 1.59        | 1.52     |
| 1   | A     | 238 | VAL  | CA-C  | -5.38 | 1.46        | 1.52     |
| 7   | J     | 557 | LEU  | CA-C  | -5.37 | 1.45        | 1.52     |
| 7   | O     | 506 | GLN  | C-N   | 5.37  | 1.40        | 1.33     |
| 7   | AG    | 287 | LEU  | CA-C  | -5.37 | 1.46        | 1.52     |
| 3   | 7     | 113 | LEU  | CA-C  | -5.37 | 1.46        | 1.52     |
| 7   | Bm    | 189 | ALA  | CA-CB | -5.36 | 1.44        | 1.53     |
| 3   | BY    | 272 | LEU  | CA-C  | -5.34 | 1.46        | 1.52     |
| 5   | AU    | 301 | VAL  | CA-CB | -5.34 | 1.47        | 1.54     |
| 7   | 4     | 97  | TYR  | CA-C  | -5.33 | 1.46        | 1.52     |
| 2   | CW    | 281 | ASN  | N-CA  | -5.32 | 1.39        | 1.46     |
| 3   | BY    | 598 | VAL  | CA-C  | 5.32  | 1.58        | 1.52     |
| 7   | J     | 518 | TYR  | N-CA  | -5.31 | 1.42        | 1.46     |
| 1   | A     | 198 | SER  | CA-C  | -5.30 | 1.46        | 1.52     |
| 2   | CW    | 83  | GLU  | CA-C  | -5.30 | 1.45        | 1.52     |
| 5   | AB    | 131 | ALA  | CA-CB | -5.30 | 1.45        | 1.53     |
| 1   | BD    | 377 | ILE  | CA-C  | -5.30 | 1.46        | 1.52     |
| 7   | 4     | 165 | PHE  | CA-C  | -5.27 | 1.46        | 1.52     |
| 1   | A     | 377 | ILE  | CA-C  | -5.27 | 1.46        | 1.52     |
| 1   | i     | 195 | VAL  | CA-CB | -5.26 | 1.48        | 1.54     |
| 2   | D     | 83  | GLU  | CA-C  | -5.25 | 1.45        | 1.52     |
| 7   | AG    | 211 | TYR  | N-CA  | -5.23 | 1.39        | 1.46     |
| 7   | J     | 319 | THR  | CA-C  | -5.22 | 1.46        | 1.52     |
| 7   | AG    | 155 | LEU  | N-CA  | -5.22 | 1.40        | 1.46     |
| 7   | AG    | 147 | LEU  | CA-C  | -5.22 | 1.45        | 1.52     |
| 3   | 7     | 610 | LEU  | CA-C  | -5.22 | 1.45        | 1.52     |
| 7   | AG    | 319 | THR  | CA-C  | -5.21 | 1.46        | 1.52     |
| 7   | AM    | 149 | SER  | CA-CB | -5.21 | 1.46        | 1.52     |
| 7   | O     | 279 | SER  | CA-CB | -5.21 | 1.44        | 1.53     |
| 7   | O     | 518 | TYR  | N-CA  | -5.21 | 1.42        | 1.46     |
| 16  | Aq    | 54  | PRO  | CA-C  | -5.21 | 1.46        | 1.52     |
| 3   | I     | 113 | LEU  | CA-C  | -5.20 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | BD    | 154 | ARG  | CA-C  | -5.20 | 1.46        | 1.52     |
| 3   | n     | 764 | ARG  | N-CA  | -5.18 | 1.39        | 1.46     |
| 16  | A7    | 181 | ILE  | CA-C  | -5.18 | 1.46        | 1.52     |
| 3   | E     | 97  | TYR  | CA-C  | -5.17 | 1.48        | 1.53     |
| 2   | k     | 7   | ASN  | N-CA  | -5.17 | 1.40        | 1.46     |
| 7   | 4     | 323 | ASN  | CA-C  | -5.17 | 1.46        | 1.52     |
| 5   | AU    | 181 | ASN  | N-CA  | -5.16 | 1.40        | 1.46     |
| 7   | Bm    | 154 | THR  | N-CA  | -5.16 | 1.39        | 1.45     |
| 2   | Ch    | 318 | ILE  | CA-C  | -5.16 | 1.46        | 1.52     |
| 1   | CP    | 238 | VAL  | CA-C  | -5.16 | 1.46        | 1.52     |
| 7   | J     | 144 | GLY  | CA-C  | -5.15 | 1.44        | 1.51     |
| 1   | i     | 204 | PHE  | CA-C  | -5.15 | 1.46        | 1.52     |
| 16  | Av    | 41  | ASP  | CA-C  | -5.14 | 1.47        | 1.53     |
| 7   | AG    | 320 | VAL  | N-CA  | -5.13 | 1.40        | 1.46     |
| 3   | BY    | 249 | TYR  | CA-C  | -5.13 | 1.46        | 1.52     |
| 2   | BK    | 34  | LEU  | CA-C  | -5.12 | 1.46        | 1.52     |
| 7   | J     | 237 | LEU  | CA-CB | -5.12 | 1.45        | 1.53     |
| 3   | n     | 598 | VAL  | CA-C  | 5.12  | 1.59        | 1.52     |
| 5   | AE    | 500 | PHE  | CA-C  | -5.12 | 1.46        | 1.52     |
| 7   | Bm    | 149 | SER  | CA-CB | -5.11 | 1.46        | 1.52     |
| 5   | AB    | 234 | SER  | CA-CB | -5.10 | 1.44        | 1.53     |
| 3   | 7     | 223 | TYR  | CA-C  | -5.10 | 1.46        | 1.52     |
| 1   | BD    | 238 | VAL  | CA-C  | -5.10 | 1.46        | 1.52     |
| 5   | M     | 47  | ALA  | CA-C  | -5.09 | 1.46        | 1.52     |
| 5   | AU    | 155 | TYR  | CA-C  | -5.09 | 1.46        | 1.52     |
| 16  | c     | 34  | PHE  | CA-C  | -5.09 | 1.45        | 1.52     |
| 3   | I     | 806 | ILE  | N-CA  | -5.09 | 1.40        | 1.46     |
| 7   | J     | 320 | VAL  | N-CA  | -5.09 | 1.40        | 1.46     |
| 3   | I     | 272 | LEU  | CA-C  | -5.09 | 1.46        | 1.52     |
| 5   | AU    | 301 | VAL  | N-CA  | -5.09 | 1.40        | 1.46     |
| 7   | 4     | 192 | SER  | CA-CB | -5.09 | 1.46        | 1.53     |
| 3   | E     | 272 | LEU  | CA-C  | -5.08 | 1.46        | 1.52     |
| 7   | J     | 192 | SER  | CA-CB | -5.08 | 1.45        | 1.53     |
| 3   | n     | 98  | LEU  | CA-C  | -5.07 | 1.46        | 1.52     |
| 7   | J     | 92  | VAL  | CA-CB | -5.06 | 1.48        | 1.54     |
| 2   | f     | 70  | LEU  | CA-C  | -5.06 | 1.48        | 1.52     |
| 5   | AB    | 131 | ALA  | CA-C  | -5.05 | 1.46        | 1.52     |
| 5   | 9     | 610 | THR  | N-CA  | -5.05 | 1.42        | 1.46     |
| 3   | I     | 598 | VAL  | CA-C  | 5.05  | 1.59        | 1.52     |
| 1   | i     | 7   | ILE  | CA-C  | -5.04 | 1.47        | 1.52     |
| 5   | M     | 242 | THR  | CA-C  | -5.04 | 1.49        | 1.52     |
| 5   | AO    | 88  | ALA  | CA-C  | -5.04 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 16  | CI    | 34  | PHE  | CA-CB | -5.03 | 1.45        | 1.53     |
| 2   | k     | 32  | ALA  | CA-CB | -5.03 | 1.46        | 1.52     |
| 3   | BY    | 168 | ARG  | CA-C  | -5.03 | 1.48        | 1.53     |
| 16  | CT    | 34  | PHE  | CA-CB | -5.02 | 1.45        | 1.53     |

All (3027) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 301 | GLU  | CA-C-O | -35.50 | 84.00       | 120.92   |
| 1   | BD    | 301 | GLU  | CA-C-O | -35.40 | 84.11       | 120.92   |
| 1   | i     | 301 | GLU  | CA-C-O | -33.51 | 84.04       | 121.58   |
| 1   | CP    | 301 | GLU  | CA-C-O | -33.50 | 84.06       | 121.58   |
| 1   | Ca    | 301 | GLU  | CA-C-O | -33.44 | 84.12       | 121.58   |
| 1   | C     | 301 | GLU  | CA-C-O | -33.40 | 84.18       | 121.58   |
| 2   | BR    | 294 | GLN  | CA-C-N | 22.26  | 149.38      | 120.44   |
| 2   | BR    | 294 | GLN  | C-N-CA | 22.26  | 149.38      | 120.44   |
| 3   | BY    | 773 | MET  | CA-C-N | 22.12  | 150.52      | 120.44   |
| 3   | BY    | 773 | MET  | C-N-CA | 22.12  | 150.52      | 120.44   |
| 2   | CW    | 280 | ILE  | CA-C-N | 20.91  | 161.48      | 121.54   |
| 2   | CW    | 280 | ILE  | C-N-CA | 20.91  | 161.48      | 121.54   |
| 2   | f     | 294 | GLN  | CA-C-N | 20.81  | 148.74      | 120.44   |
| 2   | f     | 294 | GLN  | C-N-CA | 20.81  | 148.74      | 120.44   |
| 1   | CP    | 68  | SER  | CA-C-N | 20.58  | 151.59      | 120.31   |
| 1   | CP    | 68  | SER  | C-N-CA | 20.58  | 151.59      | 120.31   |
| 3   | I     | 773 | MET  | CA-C-N | 20.44  | 149.31      | 120.29   |
| 3   | I     | 773 | MET  | C-N-CA | 20.44  | 149.31      | 120.29   |
| 3   | n     | 584 | PRO  | CA-C-N | 19.70  | 146.68      | 120.28   |
| 3   | n     | 584 | PRO  | C-N-CA | 19.70  | 146.68      | 120.28   |
| 2   | z     | 294 | GLN  | CA-C-N | 19.43  | 146.86      | 120.44   |
| 2   | z     | 294 | GLN  | C-N-CA | 19.43  | 146.86      | 120.44   |
| 2   | y     | 294 | GLN  | CA-C-N | 19.38  | 146.80      | 120.44   |
| 2   | y     | 294 | GLN  | C-N-CA | 19.38  | 146.80      | 120.44   |
| 3   | E     | 773 | MET  | CA-C-N | 19.11  | 147.43      | 120.29   |
| 3   | E     | 773 | MET  | C-N-CA | 19.11  | 147.43      | 120.29   |
| 2   | y     | 29  | ILE  | CA-C-N | 18.04  | 153.47      | 122.26   |
| 2   | y     | 29  | ILE  | C-N-CA | 18.04  | 153.47      | 122.26   |
| 2   | z     | 29  | ILE  | CA-C-N | 18.04  | 153.47      | 122.26   |
| 2   | z     | 29  | ILE  | C-N-CA | 18.04  | 153.47      | 122.26   |
| 5   | v     | 433 | VAL  | N-CA-C | 17.07  | 127.53      | 111.48   |
| 16  | Az    | 35  | TYR  | CA-C-N | 16.92  | 153.86      | 121.54   |
| 16  | Az    | 35  | TYR  | C-N-CA | 16.92  | 153.86      | 121.54   |
| 7   | J     | 557 | LEU  | N-CA-C | -16.38 | 85.03       | 110.42   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 16  | Ai    | 35  | TYR  | CA-C-N | 16.21  | 152.49      | 121.54   |
| 16  | Ai    | 35  | TYR  | C-N-CA | 16.21  | 152.49      | 121.54   |
| 16  | Z     | 35  | TYR  | CA-C-N | 16.15  | 152.38      | 121.54   |
| 16  | Z     | 35  | TYR  | C-N-CA | 16.15  | 152.38      | 121.54   |
| 16  | CM    | 35  | TYR  | CA-C-N | 15.73  | 151.59      | 121.54   |
| 16  | CM    | 35  | TYR  | C-N-CA | 15.73  | 151.59      | 121.54   |
| 3   | n     | 773 | MET  | CA-C-N | 15.41  | 151.57      | 122.60   |
| 3   | n     | 773 | MET  | C-N-CA | 15.41  | 151.57      | 122.60   |
| 16  | CB    | 35  | TYR  | CA-C-N | 15.32  | 150.81      | 121.54   |
| 16  | CB    | 35  | TYR  | C-N-CA | 15.32  | 150.81      | 121.54   |
| 2   | s     | 29  | ILE  | N-CA-C | 15.21  | 125.59      | 111.45   |
| 2   | BR    | 29  | ILE  | N-CA-C | 15.11  | 124.73      | 110.53   |
| 16  | Aq    | 131 | VAL  | N-CA-C | -14.65 | 98.68       | 113.47   |
| 5   | G     | 433 | VAL  | N-CA-C | 14.54  | 123.67      | 111.90   |
| 3   | BY    | 785 | VAL  | N-CA-C | -14.02 | 99.50       | 113.10   |
| 5   | v     | 557 | ILE  | N-CA-C | -13.99 | 94.39       | 110.21   |
| 5   | AE    | 641 | PHE  | N-CA-C | 13.62  | 126.20      | 111.36   |
| 7   | AG    | 144 | GLY  | N-CA-C | -13.52 | 96.81       | 112.50   |
| 5   | Bf    | 433 | VAL  | N-CA-C | 13.45  | 124.45      | 111.67   |
| 3   | BY    | 598 | VAL  | N-CA-C | 13.41  | 122.76      | 111.90   |
| 3   | 1     | 559 | SER  | N-CA-C | 13.38  | 129.38      | 112.92   |
| 1   | A     | 68  | SER  | CA-C-N | 13.29  | 147.49      | 121.58   |
| 1   | A     | 68  | SER  | C-N-CA | 13.29  | 147.49      | 121.58   |
| 5   | v     | 622 | ILE  | N-CA-C | -13.29 | 95.57       | 110.05   |
| 3   | BY    | 556 | PRO  | N-CA-C | -13.26 | 94.53       | 110.70   |
| 3   | 1     | 598 | VAL  | N-CA-C | 13.10  | 122.83      | 111.56   |
| 5   | G     | 653 | ILE  | N-CA-C | -12.98 | 97.82       | 111.58   |
| 16  | A7    | 131 | VAL  | N-CA-C | -12.82 | 99.45       | 113.43   |
| 3   | I     | 238 | LEU  | N-CA-C | 12.79  | 128.20      | 112.59   |
| 3   | I     | 559 | SER  | CA-C-N | 12.76  | 144.67      | 121.70   |
| 3   | I     | 559 | SER  | C-N-CA | 12.76  | 144.67      | 121.70   |
| 16  | CT    | 131 | VAL  | N-CA-C | -12.76 | 99.53       | 113.43   |
| 3   | 7     | 559 | SER  | N-CA-C | 12.59  | 128.65      | 113.28   |
| 2   | D     | 280 | ILE  | CA-C-N | 12.58  | 144.35      | 121.70   |
| 2   | D     | 280 | ILE  | C-N-CA | 12.58  | 144.35      | 121.70   |
| 3   | E     | 559 | SER  | N-CA-C | 12.57  | 128.74      | 113.16   |
| 3   | I     | 598 | VAL  | N-CA-C | 12.56  | 122.36      | 111.56   |
| 3   | n     | 559 | SER  | N-CA-C | 12.47  | 128.62      | 112.41   |
| 2   | Ch    | 297 | LYS  | N-CA-C | -12.47 | 94.45       | 110.53   |
| 2   | BR    | 329 | GLN  | CA-C-N | 12.45  | 144.11      | 121.70   |
| 2   | BR    | 329 | GLN  | C-N-CA | 12.45  | 144.11      | 121.70   |
| 5   | Bt    | 39  | SER  | N-CA-C | 12.44  | 127.50      | 108.96   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | BY    | 238 | LEU  | N-CA-C | 12.37  | 127.68      | 112.59   |
| 16  | c     | 131 | VAL  | N-CA-C | -12.27 | 100.06      | 113.43   |
| 16  | CI    | 131 | VAL  | N-CA-C | -12.24 | 100.09      | 113.43   |
| 1   | BD    | 234 | THR  | N-CA-C | -12.23 | 96.07       | 110.13   |
| 3   | E     | 238 | LEU  | N-CA-C | 12.20  | 127.47      | 112.59   |
| 5   | L     | 433 | VAL  | N-CA-C | 12.06  | 121.93      | 111.56   |
| 5   | AE    | 433 | VAL  | N-CA-C | 11.98  | 121.86      | 111.56   |
| 3   | n     | 238 | LEU  | N-CA-C | 11.98  | 127.20      | 112.59   |
| 3   | 7     | 238 | LEU  | N-CA-C | 11.97  | 127.19      | 112.59   |
| 1   | BD    | 431 | TYR  | CA-C-N | 11.93  | 132.67      | 120.38   |
| 1   | BD    | 431 | TYR  | C-N-CA | 11.93  | 132.67      | 120.38   |
| 3   | E     | 559 | SER  | CA-C-N | 11.87  | 143.06      | 121.70   |
| 3   | E     | 559 | SER  | C-N-CA | 11.87  | 143.06      | 121.70   |
| 3   | 7     | 559 | SER  | CA-C-N | 11.85  | 143.04      | 121.70   |
| 3   | 7     | 559 | SER  | C-N-CA | 11.85  | 143.04      | 121.70   |
| 5   | 9     | 434 | TYR  | N-CA-C | 11.81  | 118.85      | 108.22   |
| 2   | D     | 269 | ASN  | N-CA-C | 11.79  | 128.16      | 111.30   |
| 3   | I     | 556 | PRO  | N-CA-C | -11.73 | 99.21       | 110.47   |
| 3   | I     | 559 | SER  | N-CA-C | 11.71  | 126.83      | 112.54   |
| 3   | n     | 598 | VAL  | N-CA-C | 11.65  | 121.58      | 111.56   |
| 7   | J     | 250 | PHE  | N-CA-C | -11.62 | 98.61       | 113.72   |
| 3   | n     | 479 | LEU  | CA-C-N | 11.59  | 142.55      | 121.70   |
| 3   | n     | 479 | LEU  | C-N-CA | 11.59  | 142.55      | 121.70   |
| 16  | Av    | 131 | VAL  | N-CA-C | -11.54 | 100.85      | 113.43   |
| 3   | 7     | 512 | GLN  | N-CA-C | 11.54  | 127.70      | 113.50   |
| 1   | CP    | 234 | THR  | N-CA-C | -11.46 | 96.96       | 110.13   |
| 7   | J     | 58  | LYS  | N-CA-C | -11.42 | 99.35       | 113.97   |
| 3   | 1     | 559 | SER  | CA-C-N | 11.41  | 142.25      | 121.70   |
| 3   | 1     | 559 | SER  | C-N-CA | 11.41  | 142.25      | 121.70   |
| 16  | Av    | 90  | SER  | CA-C-N | 11.41  | 142.23      | 121.70   |
| 16  | Av    | 90  | SER  | C-N-CA | 11.41  | 142.23      | 121.70   |
| 16  | CM    | 141 | LYS  | CA-C-N | 11.40  | 142.21      | 121.70   |
| 16  | CM    | 141 | LYS  | C-N-CA | 11.40  | 142.21      | 121.70   |
| 3   | n     | 512 | GLN  | N-CA-C | 11.39  | 127.51      | 113.50   |
| 7   | AG    | 58  | LYS  | N-CA-C | -11.33 | 99.46       | 113.97   |
| 5   | 9     | 433 | VAL  | N-CA-C | 11.33  | 121.08      | 111.90   |
| 3   | I     | 479 | LEU  | CA-C-N | 11.27  | 141.98      | 121.70   |
| 3   | I     | 479 | LEU  | C-N-CA | 11.27  | 141.98      | 121.70   |
| 16  | CI    | 90  | SER  | CA-C-N | 11.25  | 141.95      | 121.70   |
| 16  | CI    | 90  | SER  | C-N-CA | 11.25  | 141.95      | 121.70   |
| 3   | E     | 479 | LEU  | CA-C-N | 11.24  | 141.93      | 121.70   |
| 3   | E     | 479 | LEU  | C-N-CA | 11.24  | 141.93      | 121.70   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 16  | Z     | 141 | LYS  | CA-C-N | 11.20  | 141.85      | 121.70   |
| 16  | Z     | 141 | LYS  | C-N-CA | 11.20  | 141.85      | 121.70   |
| 3   | BY    | 601 | THR  | N-CA-C | -11.17 | 100.19      | 114.04   |
| 3   | BY    | 479 | LEU  | CA-C-N | 11.16  | 141.79      | 121.70   |
| 3   | BY    | 479 | LEU  | C-N-CA | 11.16  | 141.79      | 121.70   |
| 2   | k     | 332 | VAL  | N-CA-C | -11.16 | 98.83       | 111.00   |
| 3   | 7     | 479 | LEU  | CA-C-N | 11.16  | 141.78      | 121.70   |
| 3   | 7     | 479 | LEU  | C-N-CA | 11.16  | 141.78      | 121.70   |
| 3   | 1     | 479 | LEU  | CA-C-N | 11.13  | 141.73      | 121.70   |
| 3   | 1     | 479 | LEU  | C-N-CA | 11.13  | 141.73      | 121.70   |
| 3   | BY    | 512 | GLN  | N-CA-C | 11.12  | 127.06      | 113.38   |
| 16  | A7    | 90  | SER  | CA-C-N | 11.10  | 141.69      | 121.70   |
| 16  | A7    | 90  | SER  | C-N-CA | 11.10  | 141.69      | 121.70   |
| 7   | Bm    | 58  | LYS  | N-CA-C | -11.07 | 99.80       | 113.97   |
| 5   | v     | 432 | LYS  | CA-C-N | -11.06 | 112.13      | 122.97   |
| 5   | v     | 432 | LYS  | C-N-CA | -11.06 | 112.13      | 122.97   |
| 7   | AM    | 58  | LYS  | N-CA-C | -11.06 | 99.82       | 113.97   |
| 5   | M     | 280 | LEU  | CA-C-N | 10.99  | 130.91      | 120.03   |
| 5   | M     | 280 | LEU  | C-N-CA | 10.99  | 130.91      | 120.03   |
| 3   | 1     | 238 | LEU  | N-CA-C | 10.98  | 126.68      | 112.41   |
| 16  | Az    | 141 | LYS  | CA-C-N | 10.96  | 141.43      | 121.70   |
| 16  | Az    | 141 | LYS  | C-N-CA | 10.96  | 141.43      | 121.70   |
| 16  | An    | 141 | LYS  | CA-C-N | 10.96  | 141.42      | 121.70   |
| 16  | An    | 141 | LYS  | C-N-CA | 10.96  | 141.42      | 121.70   |
| 16  | Aq    | 154 | THR  | N-CA-C | -10.90 | 96.46       | 110.53   |
| 3   | E     | 792 | GLN  | N-CA-C | -10.86 | 98.67       | 112.90   |
| 16  | CT    | 90  | SER  | CA-C-N | 10.86  | 141.24      | 121.70   |
| 16  | CT    | 90  | SER  | C-N-CA | 10.86  | 141.24      | 121.70   |
| 16  | CT    | 94  | PRO  | N-CA-C | -10.79 | 94.05       | 111.21   |
| 3   | E     | 785 | VAL  | CA-C-O | -10.75 | 109.21      | 120.71   |
| 5   | Bt    | 283 | ASN  | N-CA-C | -10.75 | 93.70       | 110.36   |
| 2   | k     | 34  | LEU  | N-CA-C | 10.73  | 126.50      | 113.41   |
| 1   | C     | 431 | TYR  | CA-C-N | 10.71  | 131.41      | 120.38   |
| 1   | C     | 431 | TYR  | C-N-CA | 10.71  | 131.41      | 120.38   |
| 16  | c     | 90  | SER  | CA-C-N | 10.70  | 140.96      | 121.70   |
| 16  | c     | 90  | SER  | C-N-CA | 10.70  | 140.96      | 121.70   |
| 3   | E     | 512 | GLN  | N-CA-C | 10.68  | 126.47      | 113.23   |
| 3   | I     | 512 | GLN  | N-CA-C | 10.64  | 126.59      | 113.50   |
| 16  | CB    | 141 | LYS  | CA-C-N | 10.64  | 140.85      | 121.70   |
| 16  | CB    | 141 | LYS  | C-N-CA | 10.64  | 140.85      | 121.70   |
| 7   | 4     | 58  | LYS  | N-CA-C | -10.64 | 100.36      | 113.97   |
| 16  | Aq    | 94  | PRO  | N-CA-C | -10.58 | 94.38       | 111.21   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 7   | 4     | 535 | ALA  | N-CA-C | -10.51 | 96.66       | 110.53   |
| 16  | CT    | 154 | THR  | N-CA-C | -10.45 | 97.05       | 110.53   |
| 2   | BK    | 269 | ASN  | N-CA-C | 10.43  | 126.22      | 111.30   |
| 16  | CI    | 94  | PRO  | N-CA-C | -10.36 | 94.74       | 111.21   |
| 3   | n     | 556 | PRO  | N-CA-C | -10.33 | 98.10       | 110.70   |
| 2   | Ch    | 280 | ILE  | CA-C-N | 10.28  | 140.20      | 121.70   |
| 2   | Ch    | 280 | ILE  | C-N-CA | 10.28  | 140.20      | 121.70   |
| 2   | BK    | 332 | VAL  | N-CA-C | -10.25 | 100.72      | 111.58   |
| 2   | Ch    | 332 | VAL  | N-CA-C | -10.24 | 99.83       | 111.00   |
| 3   | BY    | 556 | PRO  | CA-C-N | 10.22  | 132.62      | 119.84   |
| 3   | BY    | 556 | PRO  | C-N-CA | 10.22  | 132.62      | 119.84   |
| 1   | A     | 431 | TYR  | CA-C-N | 10.22  | 130.90      | 120.38   |
| 1   | A     | 431 | TYR  | C-N-CA | 10.22  | 130.90      | 120.38   |
| 1   | i     | 431 | TYR  | CA-C-N | 10.18  | 130.87      | 120.38   |
| 1   | i     | 431 | TYR  | C-N-CA | 10.18  | 130.87      | 120.38   |
| 7   | 4     | 328 | TYR  | N-CA-C | 10.18  | 122.79      | 108.74   |
| 3   | 1     | 512 | GLN  | N-CA-C | 10.16  | 126.21      | 112.90   |
| 3   | n     | 574 | GLN  | N-CA-C | -10.14 | 103.06      | 114.62   |
| 16  | Aq    | 90  | SER  | CA-C-N | 10.12  | 139.91      | 121.70   |
| 16  | Aq    | 90  | SER  | C-N-CA | 10.12  | 139.91      | 121.70   |
| 3   | BY    | 786 | ARG  | N-CA-C | -10.05 | 99.56       | 112.23   |
| 5   | Bf    | 545 | HIS  | CA-C-N | 10.05  | 130.73      | 120.38   |
| 5   | Bf    | 545 | HIS  | C-N-CA | 10.05  | 130.73      | 120.38   |
| 1   | Ca    | 431 | TYR  | CA-C-N | 10.02  | 130.71      | 120.38   |
| 1   | Ca    | 431 | TYR  | C-N-CA | 10.02  | 130.71      | 120.38   |
| 2   | k     | 280 | ILE  | CA-C-N | 10.00  | 139.69      | 121.70   |
| 2   | k     | 280 | ILE  | C-N-CA | 10.00  | 139.69      | 121.70   |
| 5   | AE    | 545 | HIS  | CA-C-N | 9.98   | 130.66      | 120.38   |
| 5   | AE    | 545 | HIS  | C-N-CA | 9.98   | 130.66      | 120.38   |
| 16  | Av    | 94  | PRO  | N-CA-C | -9.97  | 95.59       | 111.14   |
| 5   | AU    | 39  | SER  | N-CA-C | 9.91   | 123.95      | 108.79   |
| 7   | Bm    | 328 | TYR  | N-CA-C | 9.89   | 122.39      | 108.74   |
| 5   | 9     | 545 | HIS  | CA-C-N | 9.88   | 130.56      | 120.38   |
| 5   | 9     | 545 | HIS  | C-N-CA | 9.88   | 130.56      | 120.38   |
| 3   | E     | 112 | ILE  | N-CA-C | -9.85  | 104.35      | 113.71   |
| 16  | c     | 156 | LYS  | N-CA-C | -9.85  | 95.90       | 110.48   |
| 3   | 1     | 601 | THR  | N-CA-C | -9.83  | 101.39      | 113.97   |
| 3   | 1     | 112 | ILE  | N-CA-C | -9.81  | 104.39      | 113.71   |
| 2   | D     | 332 | VAL  | N-CA-C | -9.78  | 100.34      | 111.00   |
| 1   | CP    | 257 | ILE  | CA-C-N | 9.79   | 139.31      | 121.70   |
| 1   | CP    | 257 | ILE  | C-N-CA | 9.79   | 139.31      | 121.70   |
| 5   | Bf    | 519 | GLN  | CA-C-N | 9.77   | 139.29      | 121.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | Bf    | 519 | GLN  | C-N-CA  | 9.77  | 139.29      | 121.70   |
| 16  | A7    | 154 | THR  | N-CA-C  | -9.77 | 97.93       | 110.53   |
| 16  | CI    | 154 | THR  | CA-C-O  | -9.75 | 111.78      | 122.01   |
| 3   | n     | 559 | SER  | CA-C-N  | 9.74  | 139.23      | 121.70   |
| 3   | n     | 559 | SER  | C-N-CA  | 9.74  | 139.23      | 121.70   |
| 5   | Bt    | 280 | LEU  | CA-C-N  | 9.73  | 129.55      | 120.21   |
| 5   | Bt    | 280 | LEU  | C-N-CA  | 9.73  | 129.55      | 120.21   |
| 16  | Av    | 154 | THR  | CA-C-O  | -9.72 | 110.99      | 121.98   |
| 3   | I     | 112 | ILE  | N-CA-C  | -9.71 | 104.48      | 113.71   |
| 2   | CW    | 332 | VAL  | N-CA-C  | -9.71 | 100.42      | 111.00   |
| 16  | c     | 154 | THR  | CA-C-O  | -9.64 | 111.88      | 122.01   |
| 16  | CI    | 179 | TYR  | N-CA-C  | -9.64 | 97.05       | 110.35   |
| 1   | CP    | 431 | TYR  | CA-C-N  | 9.63  | 130.30      | 120.38   |
| 1   | CP    | 431 | TYR  | C-N-CA  | 9.63  | 130.30      | 120.38   |
| 16  | CM    | 113 | SER  | N-CA-C  | -9.62 | 97.56       | 110.55   |
| 16  | CT    | 154 | THR  | CA-C-O  | -9.61 | 110.89      | 121.94   |
| 5   | AU    | 321 | ASN  | N-CA-C  | -9.61 | 97.09       | 110.35   |
| 7   | 4     | 77  | LYS  | CA-C-N  | 9.58  | 129.33      | 119.56   |
| 7   | 4     | 77  | LYS  | C-N-CA  | 9.58  | 129.33      | 119.56   |
| 2   | BR    | 90  | GLU  | N-CA-C  | -9.57 | 97.14       | 110.35   |
| 3   | 7     | 112 | ILE  | N-CA-C  | -9.56 | 104.62      | 113.71   |
| 1   | Ca    | 288 | HIS  | N-CA-C  | 9.56  | 116.62      | 108.78   |
| 16  | c     | 94  | PRO  | N-CA-C  | -9.55 | 96.24       | 111.14   |
| 2   | Ch    | 269 | ASN  | N-CA-C  | 9.55  | 122.63      | 109.54   |
| 16  | Aq    | 154 | THR  | CA-C-O  | -9.54 | 110.97      | 121.94   |
| 5   | G     | 427 | PHE  | N-CA-C  | -9.54 | 100.96      | 111.36   |
| 7   | J     | 151 | ASP  | N-CA-C  | 9.53  | 124.17      | 112.54   |
| 3   | BY    | 556 | PRO  | CB-CA-C | 9.53  | 122.55      | 110.92   |
| 5   | R     | 39  | SER  | N-CA-C  | 9.53  | 123.55      | 109.07   |
| 3   | 1     | 475 | HIS  | CA-C-N  | 9.52  | 129.27      | 119.56   |
| 3   | 1     | 475 | HIS  | C-N-CA  | 9.52  | 129.27      | 119.56   |
| 16  | Av    | 54  | PRO  | N-CA-C  | -9.52 | 96.38       | 111.03   |
| 7   | AM    | 328 | TYR  | N-CA-C  | 9.47  | 122.21      | 108.86   |
| 7   | 4     | 144 | GLY  | N-CA-C  | -9.45 | 101.54      | 112.50   |
| 16  | A7    | 156 | LYS  | N-CA-C  | -9.41 | 96.60       | 110.52   |
| 3   | n     | 112 | ILE  | N-CA-C  | -9.25 | 104.92      | 113.71   |
| 5   | AU    | 329 | ARG  | N-CA-C  | -9.25 | 102.50      | 113.88   |
| 7   | Bm    | 281 | HIS  | CA-C-N  | 9.25  | 130.20      | 119.47   |
| 7   | Bm    | 281 | HIS  | C-N-CA  | 9.25  | 130.20      | 119.47   |
| 3   | n     | 601 | THR  | N-CA-C  | -9.24 | 102.39      | 114.31   |
| 2   | D     | 87  | LEU  | N-CA-C  | -9.24 | 101.57      | 113.12   |
| 16  | c     | 54  | PRO  | N-CA-C  | -9.22 | 96.83       | 111.03   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | v     | 519 | GLN  | CA-C-N | 9.21  | 138.28      | 121.70   |
| 5   | v     | 519 | GLN  | C-N-CA | 9.21  | 138.28      | 121.70   |
| 1   | CP    | 257 | ILE  | N-CA-C | -9.20 | 96.75       | 108.89   |
| 5   | G     | 762 | LEU  | N-CA-C | -9.20 | 101.34      | 111.36   |
| 5   | 9     | 519 | GLN  | CA-C-N | 9.19  | 138.23      | 121.70   |
| 5   | 9     | 519 | GLN  | C-N-CA | 9.19  | 138.23      | 121.70   |
| 2   | k     | 351 | ILE  | N-CA-C | 9.18  | 128.43      | 109.34   |
| 2   | y     | 354 | GLU  | CA-C-O | -9.18 | 112.37      | 122.01   |
| 2   | q     | 115 | GLU  | N-CA-C | -9.16 | 100.23      | 111.40   |
| 1   | BD    | 288 | HIS  | N-CA-C | 9.16  | 116.29      | 108.78   |
| 3   | E     | 558 | VAL  | N-CA-C | 9.15  | 119.95      | 110.62   |
| 5   | R     | 292 | ASN  | CA-C-N | 9.14  | 130.08      | 119.47   |
| 5   | R     | 292 | ASN  | C-N-CA | 9.14  | 130.08      | 119.47   |
| 2   | z     | 354 | GLU  | CA-C-O | -9.14 | 112.42      | 122.01   |
| 5   | L     | 432 | LYS  | CA-C-N | -9.14 | 113.85      | 123.08   |
| 5   | L     | 432 | LYS  | C-N-CA | -9.14 | 113.85      | 123.08   |
| 5   | AE    | 622 | ILE  | N-CA-C | -9.12 | 97.40       | 108.53   |
| 5   | L     | 519 | GLN  | CA-C-N | 9.09  | 138.07      | 121.70   |
| 5   | L     | 519 | GLN  | C-N-CA | 9.09  | 138.07      | 121.70   |
| 16  | CI    | 154 | THR  | N-CA-C | -9.09 | 98.92       | 110.19   |
| 5   | M     | 235 | PHE  | N-CA-C | 9.05  | 122.64      | 108.79   |
| 16  | CB    | 113 | SER  | N-CA-C | -9.05 | 98.33       | 110.55   |
| 5   | AO    | 329 | ARG  | N-CA-C | -9.05 | 102.75      | 113.88   |
| 1   | C     | 234 | THR  | N-CA-C | -9.04 | 95.59       | 109.41   |
| 1   | i     | 398 | LEU  | CA-C-N | 9.03  | 128.88      | 120.21   |
| 1   | i     | 398 | LEU  | C-N-CA | 9.03  | 128.88      | 120.21   |
| 5   | AO    | 191 | SER  | CA-C-O | -9.02 | 111.59      | 121.33   |
| 2   | CW    | 120 | LYS  | N-CA-C | -9.02 | 100.60      | 111.69   |
| 7   | O     | 58  | LYS  | N-CA-C | -9.01 | 102.69      | 114.31   |
| 5   | L     | 928 | ARG  | N-CA-C | -8.99 | 100.90      | 112.23   |
| 3   | 7     | 206 | ILE  | N-CA-C | -8.99 | 103.09      | 111.45   |
| 5   | Bf    | 622 | ILE  | N-CA-C | -8.99 | 95.68       | 108.80   |
| 7   | AM    | 328 | TYR  | CA-C-N | 8.98  | 137.32      | 120.97   |
| 7   | AM    | 328 | TYR  | C-N-CA | 8.98  | 137.32      | 120.97   |
| 5   | G     | 519 | GLN  | CA-C-N | 8.98  | 137.87      | 121.70   |
| 5   | G     | 519 | GLN  | C-N-CA | 8.98  | 137.87      | 121.70   |
| 16  | A7    | 154 | THR  | CA-C-O | -8.98 | 111.61      | 121.94   |
| 3   | 1     | 660 | ILE  | N-CA-C | -8.98 | 95.16       | 108.45   |
| 5   | v     | 545 | HIS  | CA-C-N | 8.96  | 129.61      | 120.38   |
| 5   | v     | 545 | HIS  | C-N-CA | 8.96  | 129.61      | 120.38   |
| 3   | 7     | 527 | LEU  | N-CA-C | -8.96 | 101.88      | 113.17   |
| 3   | BY    | 660 | ILE  | N-CA-C | -8.93 | 95.23       | 108.45   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | An    | 113 | SER  | N-CA-C | -8.92 | 98.51       | 110.55   |
| 2   | k     | 269 | ASN  | CA-C-N | 8.92  | 137.75      | 121.70   |
| 2   | k     | 269 | ASN  | C-N-CA | 8.92  | 137.75      | 121.70   |
| 16  | CI    | 54  | PRO  | N-CA-C | -8.88 | 97.35       | 111.03   |
| 3   | E     | 601 | THR  | N-CA-C | -8.88 | 102.86      | 114.31   |
| 7   | J     | 48  | ASP  | CA-C-O | -8.87 | 111.82      | 121.31   |
| 2   | CW    | 269 | ASN  | CA-C-N | 8.85  | 137.63      | 121.70   |
| 2   | CW    | 269 | ASN  | C-N-CA | 8.85  | 137.63      | 121.70   |
| 2   | CW    | 269 | ASN  | N-CA-C | 8.84  | 121.65      | 109.54   |
| 2   | Ch    | 269 | ASN  | CA-C-N | 8.84  | 137.60      | 121.70   |
| 2   | Ch    | 269 | ASN  | C-N-CA | 8.84  | 137.60      | 121.70   |
| 2   | Cd    | 54  | ASN  | N-CA-C | -8.83 | 101.33      | 112.90   |
| 5   | AE    | 519 | GLN  | CA-C-N | 8.83  | 137.59      | 121.70   |
| 5   | AE    | 519 | GLN  | C-N-CA | 8.83  | 137.59      | 121.70   |
| 16  | CT    | 156 | LYS  | N-CA-C | -8.82 | 97.46       | 110.52   |
| 3   | 1     | 558 | VAL  | N-CA-C | 8.82  | 119.61      | 110.62   |
| 5   | G     | 484 | GLN  | N-CA-C | -8.81 | 101.13      | 112.23   |
| 16  | Z     | 131 | VAL  | N-CA-C | -8.81 | 98.29       | 109.30   |
| 3   | E     | 512 | GLN  | CA-C-N | 8.81  | 137.55      | 121.70   |
| 3   | E     | 512 | GLN  | C-N-CA | 8.81  | 137.55      | 121.70   |
| 5   | M     | 282 | LYS  | N-CA-C | 8.80  | 122.71      | 108.63   |
| 5   | Bf    | 484 | GLN  | N-CA-C | -8.80 | 101.14      | 112.23   |
| 3   | BY    | 881 | ASP  | N-CA-C | -8.80 | 101.38      | 112.90   |
| 5   | Bt    | 72  | SER  | CA-C-N | 8.79  | 128.74      | 120.03   |
| 5   | Bt    | 72  | SER  | C-N-CA | 8.79  | 128.74      | 120.03   |
| 3   | 1     | 256 | GLN  | N-CA-C | -8.79 | 103.14      | 114.04   |
| 7   | Bm    | 328 | TYR  | CA-C-N | 8.79  | 136.97      | 120.97   |
| 7   | Bm    | 328 | TYR  | C-N-CA | 8.79  | 136.97      | 120.97   |
| 5   | v     | 562 | ASP  | CA-C-N | 8.78  | 128.43      | 119.82   |
| 5   | v     | 562 | ASP  | C-N-CA | 8.78  | 128.43      | 119.82   |
| 16  | c     | 154 | THR  | N-CA-C | -8.77 | 99.31       | 110.19   |
| 3   | E     | 475 | HIS  | CA-C-N | 8.76  | 128.49      | 119.56   |
| 3   | E     | 475 | HIS  | C-N-CA | 8.76  | 128.49      | 119.56   |
| 3   | 1     | 507 | CYS  | CA-C-N | 8.76  | 128.40      | 119.82   |
| 3   | 1     | 507 | CYS  | C-N-CA | 8.76  | 128.40      | 119.82   |
| 2   | BR    | 314 | GLU  | N-CA-C | -8.76 | 101.43      | 112.90   |
| 5   | G     | 622 | ILE  | N-CA-C | -8.75 | 94.52       | 108.95   |
| 5   | AE    | 641 | PHE  | CA-C-N | 8.75  | 137.45      | 121.70   |
| 5   | AE    | 641 | PHE  | C-N-CA | 8.75  | 137.45      | 121.70   |
| 5   | v     | 576 | PHE  | N-CA-C | -8.74 | 98.98       | 110.43   |
| 3   | BY    | 256 | GLN  | N-CA-C | -8.73 | 103.21      | 114.04   |
| 5   | L     | 750 | ARG  | N-CA-C | -8.73 | 102.41      | 113.23   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | 4     | 48  | ASP  | CA-C-O  | -8.73 | 111.97      | 121.31   |
| 7   | AG    | 208 | VAL  | N-CA-C  | -8.72 | 101.49      | 111.00   |
| 5   | Bt    | 134 | GLN  | N-CA-C  | 8.71  | 120.75      | 108.74   |
| 5   | AO    | 158 | THR  | N-CA-C  | 8.70  | 119.41      | 108.45   |
| 2   | f     | 295 | ASN  | N-CA-C  | -8.68 | 101.76      | 111.14   |
| 7   | AG    | 48  | ASP  | CA-C-O  | -8.67 | 112.03      | 121.31   |
| 3   | I     | 601 | THR  | N-CA-C  | -8.67 | 103.13      | 114.31   |
| 5   | AE    | 622 | ILE  | CB-CA-C | 8.67  | 123.57      | 110.91   |
| 2   | BR    | 29  | ILE  | CA-C-O  | -8.66 | 111.43      | 121.05   |
| 3   | 1     | 512 | GLN  | CA-C-N  | 8.66  | 137.29      | 121.70   |
| 3   | 1     | 512 | GLN  | C-N-CA  | 8.66  | 137.29      | 121.70   |
| 1   | A     | 288 | HIS  | N-CA-C  | 8.65  | 115.87      | 108.78   |
| 1   | Ca    | 234 | THR  | N-CA-C  | -8.64 | 97.46       | 110.07   |
| 7   | 4     | 328 | TYR  | CA-C-N  | 8.63  | 136.68      | 120.97   |
| 7   | 4     | 328 | TYR  | C-N-CA  | 8.63  | 136.68      | 120.97   |
| 3   | BY    | 559 | SER  | CA-C-N  | 8.63  | 137.23      | 121.70   |
| 3   | BY    | 559 | SER  | C-N-CA  | 8.63  | 137.23      | 121.70   |
| 5   | Bf    | 749 | ILE  | CA-C-O  | -8.62 | 111.16      | 120.47   |
| 7   | O     | 48  | ASP  | CA-C-O  | -8.61 | 112.02      | 121.23   |
| 5   | AU    | 292 | ASN  | CA-C-N  | 8.61  | 129.46      | 119.47   |
| 5   | AU    | 292 | ASN  | C-N-CA  | 8.61  | 129.46      | 119.47   |
| 3   | 7     | 558 | VAL  | N-CA-C  | 8.60  | 119.41      | 110.72   |
| 2   | k     | 103 | ASN  | N-CA-C  | -8.58 | 102.01      | 111.36   |
| 2   | BK    | 120 | LYS  | N-CA-C  | -8.57 | 101.14      | 111.69   |
| 3   | I     | 527 | LEU  | N-CA-C  | -8.56 | 102.39      | 112.92   |
| 5   | AE    | 646 | ASN  | CA-C-N  | 8.56  | 128.21      | 119.56   |
| 5   | AE    | 646 | ASN  | C-N-CA  | 8.56  | 128.21      | 119.56   |
| 7   | AG    | 211 | TYR  | N-CA-C  | -8.56 | 95.35       | 108.96   |
| 3   | BY    | 746 | GLU  | N-CA-C  | -8.55 | 98.55       | 110.35   |
| 2   | k     | 39  | LEU  | N-CA-C  | -8.54 | 101.97      | 111.28   |
| 5   | AE    | 762 | LEU  | N-CA-C  | -8.54 | 102.05      | 111.36   |
| 5   | AE    | 877 | GLN  | N-CA-C  | -8.54 | 101.47      | 112.23   |
| 2   | BR    | 54  | ASN  | N-CA-C  | -8.54 | 101.71      | 112.90   |
| 2   | BR    | 118 | ASP  | N-CA-C  | -8.54 | 101.47      | 112.23   |
| 5   | M     | 163 | PRO  | N-CA-C  | 8.54  | 124.53      | 113.86   |
| 2   | Cd    | 87  | LEU  | N-CA-C  | -8.54 | 101.47      | 112.23   |
| 16  | Az    | 113 | SER  | N-CA-C  | -8.53 | 99.03       | 110.55   |
| 7   | Bm    | 151 | ASP  | N-CA-C  | 8.53  | 123.24      | 113.01   |
| 3   | 7     | 703 | TYR  | CA-C-N  | 8.52  | 130.49      | 119.84   |
| 3   | 7     | 703 | TYR  | C-N-CA  | 8.52  | 130.49      | 119.84   |
| 16  | Z     | 123 | PHE  | N-CA-C  | -8.52 | 101.01      | 111.40   |
| 5   | L     | 562 | ASP  | CA-C-N  | 8.51  | 128.24      | 119.56   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 562 | ASP  | C-N-CA  | 8.51  | 128.24      | 119.56   |
| 3   | BY    | 175 | THR  | CA-C-N  | 8.50  | 128.23      | 119.56   |
| 3   | BY    | 175 | THR  | C-N-CA  | 8.50  | 128.23      | 119.56   |
| 5   | v     | 484 | GLN  | N-CA-C  | -8.50 | 101.53      | 112.23   |
| 5   | L     | 653 | ILE  | N-CA-C  | -8.49 | 102.58      | 111.58   |
| 3   | n     | 475 | HIS  | CA-C-N  | 8.49  | 128.22      | 119.56   |
| 3   | n     | 475 | HIS  | C-N-CA  | 8.49  | 128.22      | 119.56   |
| 5   | L     | 546 | PRO  | N-CA-C  | 8.49  | 121.06      | 110.70   |
| 2   | Ch    | 120 | LYS  | N-CA-C  | -8.47 | 101.56      | 112.23   |
| 2   | q     | 269 | ASN  | CA-C-N  | 8.46  | 136.92      | 121.70   |
| 2   | q     | 269 | ASN  | C-N-CA  | 8.46  | 136.92      | 121.70   |
| 3   | 7     | 205 | GLU  | N-CA-C  | 8.46  | 120.41      | 108.74   |
| 3   | E     | 574 | GLN  | N-CA-C  | -8.45 | 101.94      | 113.18   |
| 5   | M     | 72  | SER  | CA-C-N  | 8.44  | 128.39      | 120.03   |
| 5   | M     | 72  | SER  | C-N-CA  | 8.44  | 128.39      | 120.03   |
| 16  | An    | 168 | ILE  | CB-CA-C | -8.43 | 103.07      | 111.08   |
| 5   | AU    | 298 | ILE  | N-CA-C  | 8.42  | 119.90      | 108.11   |
| 3   | I     | 475 | HIS  | CA-C-N  | 8.41  | 128.14      | 119.56   |
| 3   | I     | 475 | HIS  | C-N-CA  | 8.41  | 128.14      | 119.56   |
| 2   | D     | 269 | ASN  | CA-C-N  | 8.41  | 136.83      | 121.70   |
| 2   | D     | 269 | ASN  | C-N-CA  | 8.41  | 136.83      | 121.70   |
| 3   | E     | 53  | LYS  | N-CA-C  | -8.39 | 102.48      | 112.89   |
| 3   | I     | 660 | ILE  | CA-C-N  | 8.39  | 136.80      | 121.70   |
| 3   | I     | 660 | ILE  | C-N-CA  | 8.39  | 136.80      | 121.70   |
| 16  | Z     | 139 | LYS  | CA-C-N  | -8.38 | 108.79      | 122.11   |
| 16  | Z     | 139 | LYS  | C-N-CA  | -8.38 | 108.79      | 122.11   |
| 5   | AU    | 158 | THR  | N-CA-C  | 8.38  | 119.30      | 108.24   |
| 3   | 7     | 175 | THR  | CA-C-N  | 8.37  | 128.10      | 119.56   |
| 3   | 7     | 175 | THR  | C-N-CA  | 8.37  | 128.10      | 119.56   |
| 16  | CI    | 40  | GLN  | CA-C-O  | -8.37 | 112.21      | 121.00   |
| 5   | G     | 611 | PRO  | N-CA-C  | 8.37  | 124.78      | 113.98   |
| 5   | v     | 503 | SER  | CA-C-O  | -8.36 | 112.45      | 121.56   |
| 5   | M     | 329 | ARG  | N-CA-C  | -8.36 | 103.60      | 113.88   |
| 7   | 4     | 192 | SER  | N-CA-C  | 8.35  | 119.27      | 108.24   |
| 16  | CT    | 49  | VAL  | N-CA-C  | -8.35 | 102.29      | 110.72   |
| 3   | 1     | 667 | GLN  | N-CA-C  | -8.34 | 101.97      | 112.90   |
| 5   | 9     | 484 | GLN  | N-CA-C  | -8.34 | 102.14      | 111.82   |
| 5   | Bt    | 253 | ASN  | CA-C-N  | -8.34 | 109.22      | 122.73   |
| 5   | Bt    | 253 | ASN  | C-N-CA  | -8.34 | 109.22      | 122.73   |
| 5   | M     | 292 | ASN  | CA-C-N  | 8.34  | 129.14      | 119.47   |
| 5   | M     | 292 | ASN  | C-N-CA  | 8.34  | 129.14      | 119.47   |
| 2   | Ch    | 13  | LEU  | N-CA-C  | -8.33 | 101.99      | 112.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | BY    | 512 | GLN  | CA-C-N | 8.33  | 136.69      | 121.70   |
| 3   | BY    | 512 | GLN  | C-N-CA | 8.33  | 136.69      | 121.70   |
| 5   | AE    | 484 | GLN  | N-CA-C | -8.32 | 101.74      | 112.23   |
| 16  | CM    | 127 | LYS  | N-CA-C | -8.32 | 99.31       | 110.55   |
| 3   | BY    | 475 | HIS  | CA-C-N | 8.32  | 128.05      | 119.56   |
| 3   | BY    | 475 | HIS  | C-N-CA | 8.32  | 128.05      | 119.56   |
| 3   | 1     | 479 | LEU  | N-CA-C | 8.30  | 122.69      | 112.23   |
| 3   | 1     | 622 | LYS  | CA-C-N | 8.29  | 128.02      | 119.56   |
| 3   | 1     | 622 | LYS  | C-N-CA | 8.29  | 128.02      | 119.56   |
| 5   | AO    | 191 | SER  | N-CA-C | -8.29 | 96.47       | 109.07   |
| 2   | CW    | 246 | GLN  | CA-C-N | 8.29  | 136.62      | 121.70   |
| 2   | CW    | 246 | GLN  | C-N-CA | 8.29  | 136.62      | 121.70   |
| 2   | y     | 43  | LEU  | N-CA-C | -8.28 | 103.30      | 113.41   |
| 16  | CI    | 61  | VAL  | N-CA-C | -8.28 | 105.84      | 113.71   |
| 7   | 4     | 329 | PHE  | N-CA-C | 8.28  | 121.46      | 110.53   |
| 2   | Cd    | 331 | ASN  | N-CA-C | -8.28 | 102.62      | 114.12   |
| 2   | z     | 43  | LEU  | N-CA-C | -8.27 | 103.32      | 113.41   |
| 7   | J     | 328 | TYR  | CA-C-N | 8.26  | 137.53      | 121.66   |
| 7   | J     | 328 | TYR  | C-N-CA | 8.26  | 137.53      | 121.66   |
| 3   | n     | 175 | THR  | CA-C-N | 8.26  | 127.98      | 119.56   |
| 3   | n     | 175 | THR  | C-N-CA | 8.26  | 127.98      | 119.56   |
| 5   | Bt    | 310 | TYR  | N-CA-C | -8.26 | 96.66       | 108.96   |
| 16  | c     | 49  | VAL  | N-CA-C | -8.25 | 102.38      | 110.72   |
| 2   | D     | 103 | ASN  | N-CA-C | -8.25 | 102.37      | 111.36   |
| 2   | f     | 46  | SER  | CA-C-N | 8.24  | 132.42      | 120.38   |
| 2   | f     | 46  | SER  | C-N-CA | 8.24  | 132.42      | 120.38   |
| 2   | z     | 290 | ASN  | CA-C-N | 8.23  | 136.51      | 121.70   |
| 2   | z     | 290 | ASN  | C-N-CA | 8.23  | 136.51      | 121.70   |
| 7   | J     | 143 | GLY  | N-CA-C | -8.23 | 103.63      | 115.64   |
| 5   | L     | 484 | GLN  | N-CA-C | -8.23 | 101.86      | 112.23   |
| 5   | v     | 442 | ILE  | N-CA-C | -8.23 | 104.48      | 111.56   |
| 2   | y     | 290 | ASN  | CA-C-N | 8.22  | 136.50      | 121.70   |
| 2   | y     | 290 | ASN  | C-N-CA | 8.22  | 136.50      | 121.70   |
| 2   | CW    | 87  | LEU  | N-CA-C | -8.22 | 101.02      | 112.45   |
| 2   | Cd    | 329 | GLN  | CA-C-N | 8.21  | 137.22      | 121.54   |
| 2   | Cd    | 329 | GLN  | C-N-CA | 8.21  | 137.22      | 121.54   |
| 2   | D     | 246 | GLN  | CA-C-N | 8.20  | 136.46      | 121.70   |
| 2   | D     | 246 | GLN  | C-N-CA | 8.20  | 136.46      | 121.70   |
| 3   | I     | 512 | GLN  | CA-C-N | 8.20  | 136.46      | 121.70   |
| 3   | I     | 512 | GLN  | C-N-CA | 8.20  | 136.46      | 121.70   |
| 5   | G     | 610 | THR  | CA-C-N | 8.20  | 127.86      | 119.82   |
| 5   | G     | 610 | THR  | C-N-CA | 8.20  | 127.86      | 119.82   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | Aq    | 146 | GLN  | CA-C-N  | -8.20 | 106.75      | 120.68   |
| 16  | Aq    | 146 | GLN  | C-N-CA  | -8.20 | 106.75      | 120.68   |
| 2   | CW    | 318 | ILE  | CA-C-O  | -8.19 | 110.54      | 120.78   |
| 2   | Cd    | 348 | THR  | N-CA-C  | -8.18 | 101.92      | 112.23   |
| 3   | 7     | 475 | HIS  | CA-C-N  | 8.18  | 127.90      | 119.56   |
| 3   | 7     | 475 | HIS  | C-N-CA  | 8.18  | 127.90      | 119.56   |
| 5   | Bt    | 261 | ASN  | N-CA-C  | -8.18 | 100.27      | 113.19   |
| 5   | Bt    | 289 | PHE  | N-CA-C  | 8.17  | 121.29      | 108.79   |
| 16  | CB    | 168 | ILE  | CB-CA-C | -8.16 | 103.32      | 111.08   |
| 3   | I     | 826 | ARG  | CA-C-O  | -8.16 | 111.77      | 120.42   |
| 3   | BY    | 792 | GLN  | CA-C-O  | -8.16 | 110.59      | 119.97   |
| 2   | CW    | 267 | GLU  | N-CA-C  | -8.16 | 103.92      | 114.04   |
| 16  | Aq    | 158 | HIS  | N-CA-C  | -8.16 | 98.41       | 110.48   |
| 2   | f     | 54  | ASN  | N-CA-C  | -8.16 | 102.22      | 112.90   |
| 2   | BK    | 269 | ASN  | CA-C-N  | 8.14  | 136.35      | 121.70   |
| 2   | BK    | 269 | ASN  | C-N-CA  | 8.14  | 136.35      | 121.70   |
| 3   | n     | 256 | GLN  | N-CA-C  | -8.14 | 103.95      | 114.04   |
| 3   | 1     | 660 | ILE  | CA-C-N  | 8.13  | 136.34      | 121.70   |
| 3   | 1     | 660 | ILE  | C-N-CA  | 8.13  | 136.34      | 121.70   |
| 2   | z     | 87  | LEU  | N-CA-C  | -8.13 | 103.50      | 113.50   |
| 2   | y     | 87  | LEU  | N-CA-C  | -8.12 | 103.51      | 113.50   |
| 2   | k     | 350 | GLU  | CA-C-N  | 8.12  | 136.59      | 121.97   |
| 2   | k     | 350 | GLU  | C-N-CA  | 8.12  | 136.59      | 121.97   |
| 3   | 7     | 808 | GLU  | CA-C-O  | -8.12 | 111.94      | 120.55   |
| 7   | Bm    | 278 | ILE  | N-CA-C  | 8.12  | 119.08      | 107.88   |
| 5   | v     | 653 | ILE  | N-CA-C  | -8.11 | 102.98      | 111.58   |
| 5   | AB    | 162 | THR  | CA-C-N  | 8.10  | 129.97      | 119.84   |
| 5   | AB    | 162 | THR  | C-N-CA  | 8.10  | 129.97      | 119.84   |
| 3   | E     | 507 | CYS  | CA-C-N  | 8.10  | 127.82      | 119.56   |
| 3   | E     | 507 | CYS  | C-N-CA  | 8.10  | 127.82      | 119.56   |
| 16  | Z     | 34  | PHE  | N-CA-C  | -8.09 | 102.46      | 111.28   |
| 5   | G     | 597 | TRP  | CA-C-O  | -8.08 | 110.67      | 119.97   |
| 7   | J     | 192 | SER  | N-CA-C  | 8.08  | 119.27      | 107.88   |
| 2   | k     | 13  | LEU  | N-CA-C  | -8.07 | 102.32      | 112.90   |
| 5   | Bf    | 562 | ASP  | CA-C-N  | 8.07  | 127.80      | 119.56   |
| 5   | Bf    | 562 | ASP  | C-N-CA  | 8.07  | 127.80      | 119.56   |
| 3   | 7     | 793 | MET  | N-CA-C  | -8.07 | 102.06      | 112.23   |
| 7   | 4     | 534 | GLU  | N-CA-C  | -8.07 | 103.26      | 113.43   |
| 2   | k     | 26  | PRO  | N-CA-C  | 8.06  | 123.87      | 112.26   |
| 2   | z     | 295 | ASN  | N-CA-C  | -8.06 | 102.43      | 111.14   |
| 5   | M     | 39  | SER  | N-CA-C  | 8.06  | 121.32      | 109.07   |
| 2   | Ch    | 246 | GLN  | CA-C-N  | 8.05  | 136.19      | 121.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Ch    | 246 | GLN  | C-N-CA  | 8.05  | 136.19      | 121.70   |
| 2   | q     | 103 | ASN  | N-CA-C  | -8.05 | 102.58      | 111.36   |
| 1   | Ca    | 398 | LEU  | CA-C-N  | 8.05  | 127.94      | 120.21   |
| 1   | Ca    | 398 | LEU  | C-N-CA  | 8.05  | 127.94      | 120.21   |
| 5   | v     | 433 | VAL  | N-CA-CB | -8.05 | 103.60      | 111.57   |
| 5   | L     | 893 | LYS  | CA-C-O  | -8.04 | 112.03      | 120.55   |
| 1   | i     | 349 | VAL  | CA-C-O  | -8.04 | 112.15      | 120.27   |
| 2   | y     | 54  | ASN  | N-CA-C  | -8.04 | 102.37      | 112.90   |
| 2   | y     | 295 | ASN  | N-CA-C  | -8.04 | 102.46      | 111.14   |
| 5   | AE    | 928 | ARG  | N-CA-C  | -8.04 | 102.10      | 112.23   |
| 2   | BR    | 265 | ASP  | CA-C-O  | -8.04 | 112.03      | 120.55   |
| 5   | AB    | 312 | LEU  | N-CA-C  | -8.03 | 102.11      | 112.23   |
| 3   | E     | 264 | ILE  | N-CA-C  | 8.01  | 119.33      | 108.11   |
| 5   | M     | 308 | PHE  | CA-C-N  | 8.01  | 136.12      | 121.70   |
| 5   | M     | 308 | PHE  | C-N-CA  | 8.01  | 136.12      | 121.70   |
| 2   | q     | 120 | LYS  | N-CA-C  | -8.01 | 101.84      | 111.69   |
| 5   | AE    | 728 | GLN  | CA-C-O  | -8.01 | 111.93      | 120.42   |
| 16  | Ai    | 131 | VAL  | N-CA-C  | -8.01 | 99.29       | 109.30   |
| 5   | 9     | 622 | ILE  | N-CA-C  | -8.01 | 97.11       | 108.80   |
| 7   | O     | 77  | LYS  | CA-C-N  | 8.00  | 129.84      | 119.84   |
| 7   | O     | 77  | LYS  | C-N-CA  | 8.00  | 129.84      | 119.84   |
| 2   | BK    | 85  | ASN  | N-CA-C  | -8.00 | 102.15      | 112.23   |
| 16  | CI    | 156 | LYS  | N-CA-C  | -8.00 | 97.56       | 110.20   |
| 2   | z     | 54  | ASN  | N-CA-C  | -8.00 | 102.43      | 112.90   |
| 7   | J     | 202 | LEU  | N-CA-C  | 7.99  | 121.09      | 111.82   |
| 2   | z     | 266 | GLY  | N-CA-C  | -7.99 | 101.87      | 113.86   |
| 5   | AO    | 292 | ASN  | CA-C-N  | 7.99  | 128.74      | 119.47   |
| 5   | AO    | 292 | ASN  | C-N-CA  | 7.99  | 128.74      | 119.47   |
| 2   | k     | 120 | LYS  | N-CA-C  | -7.99 | 101.87      | 111.69   |
| 3   | I     | 205 | GLU  | N-CA-C  | 7.98  | 120.25      | 108.60   |
| 7   | O     | 70  | ILE  | N-CA-C  | 7.98  | 120.26      | 108.45   |
| 3   | n     | 512 | GLN  | CA-C-N  | 7.98  | 136.06      | 121.70   |
| 3   | n     | 512 | GLN  | C-N-CA  | 7.98  | 136.06      | 121.70   |
| 5   | G     | 562 | ASP  | CA-C-N  | 7.97  | 128.72      | 119.47   |
| 5   | G     | 562 | ASP  | C-N-CA  | 7.97  | 128.72      | 119.47   |
| 2   | y     | 266 | GLY  | N-CA-C  | -7.97 | 101.91      | 113.86   |
| 5   | AE    | 893 | LYS  | CA-C-O  | -7.97 | 112.11      | 120.55   |
| 5   | L     | 475 | TYR  | CA-C-N  | 7.96  | 129.34      | 120.66   |
| 5   | L     | 475 | TYR  | C-N-CA  | 7.96  | 129.34      | 120.66   |
| 5   | L     | 920 | GLU  | N-CA-C  | -7.96 | 102.20      | 112.23   |
| 7   | J     | 328 | TYR  | N-CA-C  | 7.96  | 120.08      | 108.86   |
| 3   | BY    | 660 | ILE  | CA-C-N  | 7.96  | 136.03      | 121.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | BY    | 660 | ILE  | C-N-CA  | 7.96  | 136.03      | 121.70   |
| 3   | n     | 622 | LYS  | CA-C-N  | 7.96  | 129.79      | 119.84   |
| 3   | n     | 622 | LYS  | C-N-CA  | 7.96  | 129.79      | 119.84   |
| 5   | Bf    | 859 | ASP  | N-CA-C  | -7.96 | 102.21      | 112.23   |
| 2   | z     | 33  | GLU  | N-CA-C  | -7.96 | 102.20      | 112.23   |
| 16  | Av    | 61  | VAL  | N-CA-C  | -7.96 | 106.15      | 113.71   |
| 2   | y     | 33  | GLU  | N-CA-C  | -7.95 | 102.21      | 112.23   |
| 3   | BY    | 631 | VAL  | CA-C-O  | -7.93 | 112.44      | 120.85   |
| 3   | 7     | 601 | THR  | N-CA-C  | -7.93 | 104.08      | 114.31   |
| 1   | BD    | 349 | VAL  | CA-C-O  | -7.93 | 112.27      | 120.27   |
| 3   | BY    | 745 | LEU  | N-CA-C  | -7.92 | 101.74      | 111.40   |
| 16  | CM    | 139 | LYS  | CA-C-N  | -7.91 | 109.53      | 122.11   |
| 16  | CM    | 139 | LYS  | C-N-CA  | -7.91 | 109.53      | 122.11   |
| 5   | L     | 622 | ILE  | CB-CA-C | 7.91  | 122.42      | 111.34   |
| 5   | M     | 321 | ASN  | N-CA-C  | -7.91 | 102.27      | 112.23   |
| 2   | Cd    | 290 | ASN  | CA-C-N  | 7.90  | 135.93      | 121.70   |
| 2   | Cd    | 290 | ASN  | C-N-CA  | 7.90  | 135.93      | 121.70   |
| 1   | A     | 349 | VAL  | CA-C-O  | -7.90 | 112.18      | 120.39   |
| 3   | 1     | 85  | SER  | N-CA-C  | 7.90  | 121.21      | 110.55   |
| 3   | BY    | 805 | GLN  | N-CA-C  | -7.89 | 103.11      | 112.89   |
| 5   | R     | 329 | ARG  | N-CA-C  | -7.88 | 104.19      | 113.88   |
| 7   | O     | 151 | ASP  | N-CA-C  | 7.87  | 122.45      | 113.01   |
| 5   | AE    | 475 | TYR  | CA-C-N  | 7.87  | 129.24      | 120.66   |
| 5   | AE    | 475 | TYR  | C-N-CA  | 7.87  | 129.24      | 120.66   |
| 16  | An    | 139 | LYS  | CA-C-N  | -7.87 | 109.60      | 122.11   |
| 16  | An    | 139 | LYS  | C-N-CA  | -7.87 | 109.60      | 122.11   |
| 3   | BY    | 206 | ILE  | N-CA-C  | -7.87 | 105.04      | 111.81   |
| 5   | L     | 909 | LYS  | N-CA-C  | -7.87 | 102.31      | 112.23   |
| 5   | AB    | 39  | SER  | CA-C-N  | 7.87  | 133.91      | 121.17   |
| 5   | AB    | 39  | SER  | C-N-CA  | 7.87  | 133.91      | 121.17   |
| 5   | G     | 432 | LYS  | CA-C-N  | -7.86 | 115.03      | 122.66   |
| 5   | G     | 432 | LYS  | C-N-CA  | -7.86 | 115.03      | 122.66   |
| 5   | Bf    | 462 | LYS  | CA-C-N  | -7.86 | 109.10      | 120.97   |
| 5   | Bf    | 462 | LYS  | C-N-CA  | -7.86 | 109.10      | 120.97   |
| 3   | n     | 507 | CYS  | CA-C-N  | 7.86  | 127.58      | 119.56   |
| 3   | n     | 507 | CYS  | C-N-CA  | 7.86  | 127.58      | 119.56   |
| 2   | q     | 269 | ASN  | N-CA-C  | 7.86  | 120.31      | 109.54   |
| 7   | AM    | 522 | PHE  | CA-C-O  | -7.86 | 112.57      | 120.82   |
| 5   | AU    | 4   | ILE  | N-CA-C  | 7.86  | 119.60      | 108.36   |
| 3   | 1     | 264 | ILE  | N-CA-C  | 7.86  | 119.11      | 108.11   |
| 5   | L     | 875 | ILE  | N-CA-C  | -7.86 | 103.14      | 110.53   |
| 7   | AG    | 77  | LYS  | CA-C-N  | 7.86  | 129.66      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | AG    | 77  | LYS  | C-N-CA | 7.86  | 129.66      | 119.84   |
| 2   | BR    | 29  | ILE  | O-C-N  | -7.86 | 113.73      | 121.90   |
| 5   | L     | 859 | ASP  | N-CA-C | -7.85 | 102.61      | 112.90   |
| 3   | I     | 558 | VAL  | N-CA-C | 7.85  | 118.62      | 110.62   |
| 5   | Bf    | 475 | TYR  | CA-C-N | 7.84  | 129.21      | 120.66   |
| 5   | Bf    | 475 | TYR  | C-N-CA | 7.84  | 129.21      | 120.66   |
| 5   | 9     | 492 | CYS  | CA-C-O | -7.84 | 112.24      | 120.55   |
| 1   | Ca    | 382 | SER  | N-CA-C | 7.83  | 122.94      | 113.23   |
| 16  | Ai    | 141 | LYS  | CA-C-N | 7.83  | 135.79      | 121.70   |
| 16  | Ai    | 141 | LYS  | C-N-CA | 7.83  | 135.79      | 121.70   |
| 5   | M     | 320 | MET  | CA-C-O | -7.83 | 110.97      | 119.97   |
| 1   | C     | 349 | VAL  | CA-C-O | -7.82 | 112.37      | 120.27   |
| 3   | 7     | 454 | ASN  | N-CA-C | -7.81 | 102.38      | 112.23   |
| 2   | BR    | 92  | ILE  | N-CA-C | -7.81 | 102.66      | 110.62   |
| 5   | 9     | 475 | TYR  | CA-C-N | 7.80  | 129.17      | 120.66   |
| 5   | 9     | 475 | TYR  | C-N-CA | 7.80  | 129.17      | 120.66   |
| 2   | f     | 136 | GLU  | CA-C-O | -7.80 | 112.28      | 120.55   |
| 3   | 7     | 264 | ILE  | N-CA-C | 7.80  | 119.03      | 108.11   |
| 7   | AG    | 274 | GLN  | N-CA-C | -7.80 | 102.78      | 111.28   |
| 3   | I     | 264 | ILE  | N-CA-C | 7.79  | 119.02      | 108.11   |
| 3   | E     | 660 | ILE  | N-CA-C | -7.79 | 96.91       | 108.12   |
| 5   | AE    | 767 | LYS  | N-CA-C | -7.78 | 102.80      | 111.28   |
| 7   | 4     | 202 | LEU  | N-CA-C | 7.78  | 122.88      | 113.23   |
| 3   | 1     | 631 | VAL  | CA-C-O | -7.78 | 112.86      | 120.95   |
| 5   | Bf    | 503 | SER  | CA-C-O | -7.77 | 112.53      | 121.47   |
| 3   | n     | 766 | ILE  | CA-C-N | 7.77  | 133.92      | 121.34   |
| 3   | n     | 766 | ILE  | C-N-CA | 7.77  | 133.92      | 121.34   |
| 3   | 7     | 512 | GLN  | CA-C-N | 7.76  | 135.67      | 121.70   |
| 3   | 7     | 512 | GLN  | C-N-CA | 7.76  | 135.67      | 121.70   |
| 3   | n     | 660 | ILE  | CA-C-N | 7.75  | 135.66      | 121.70   |
| 3   | n     | 660 | ILE  | C-N-CA | 7.75  | 135.66      | 121.70   |
| 5   | AU    | 308 | PHE  | CA-C-N | 7.75  | 135.66      | 121.70   |
| 5   | AU    | 308 | PHE  | C-N-CA | 7.75  | 135.66      | 121.70   |
| 5   | L     | 462 | LYS  | CA-C-N | -7.75 | 109.27      | 120.97   |
| 5   | L     | 462 | LYS  | C-N-CA | -7.75 | 109.27      | 120.97   |
| 2   | k     | 246 | GLN  | CA-C-N | 7.75  | 135.65      | 121.70   |
| 2   | k     | 246 | GLN  | C-N-CA | 7.75  | 135.65      | 121.70   |
| 5   | G     | 734 | GLN  | N-CA-C | -7.75 | 103.63      | 113.23   |
| 5   | AE    | 876 | GLN  | CA-C-O | -7.75 | 112.21      | 120.42   |
| 2   | Ch    | 238 | GLU  | N-CA-C | -7.74 | 102.17      | 111.69   |
| 5   | 9     | 653 | ILE  | N-CA-C | -7.74 | 103.37      | 111.58   |
| 3   | E     | 85  | SER  | N-CA-C | 7.73  | 120.99      | 110.55   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | Cd    | 136 | GLU  | CA-C-O | -7.73 | 112.35      | 120.55   |
| 1   | Ca    | 349 | VAL  | CA-C-O | -7.73 | 112.46      | 120.27   |
| 7   | AG    | 328 | TYR  | CA-C-N | 7.73  | 136.50      | 121.66   |
| 7   | AG    | 328 | TYR  | C-N-CA | 7.73  | 136.50      | 121.66   |
| 5   | AE    | 432 | LYS  | CA-C-N | -7.72 | 115.28      | 123.08   |
| 5   | AE    | 432 | LYS  | C-N-CA | -7.72 | 115.28      | 123.08   |
| 5   | AE    | 562 | ASP  | CA-C-N | 7.72  | 127.44      | 119.56   |
| 5   | AE    | 562 | ASP  | C-N-CA | 7.72  | 127.44      | 119.56   |
| 3   | 7     | 441 | PHE  | N-CA-C | -7.72 | 102.80      | 111.14   |
| 7   | AM    | 553 | TYR  | N-CA-C | -7.72 | 103.47      | 113.12   |
| 16  | Aq    | 61  | VAL  | N-CA-C | -7.72 | 106.38      | 113.71   |
| 3   | n     | 631 | VAL  | CA-C-O | -7.71 | 112.67      | 120.85   |
| 3   | 1     | 175 | THR  | CA-C-N | 7.71  | 127.43      | 119.56   |
| 3   | 1     | 175 | THR  | C-N-CA | 7.71  | 127.43      | 119.56   |
| 5   | AO    | 52  | SER  | N-CA-C | -7.71 | 102.81      | 112.90   |
| 2   | f     | 348 | THR  | N-CA-C | -7.70 | 103.68      | 113.23   |
| 2   | q     | 318 | ILE  | CA-C-O | -7.70 | 111.85      | 120.32   |
| 2   | z     | 347 | LYS  | N-CA-C | -7.70 | 102.81      | 112.90   |
| 7   | AM    | 542 | GLN  | N-CA-C | -7.70 | 103.89      | 113.28   |
| 3   | I     | 685 | VAL  | N-CA-C | -7.69 | 98.74       | 108.89   |
| 5   | M     | 158 | THR  | N-CA-C | 7.69  | 118.39      | 108.24   |
| 3   | I     | 175 | THR  | CA-C-N | 7.68  | 127.40      | 119.56   |
| 3   | I     | 175 | THR  | C-N-CA | 7.68  | 127.40      | 119.56   |
| 2   | BR    | 241 | ARG  | N-CA-C | -7.68 | 101.77      | 112.45   |
| 16  | CT    | 61  | VAL  | N-CA-C | -7.68 | 106.41      | 113.71   |
| 7   | J     | 322 | PHE  | N-CA-C | 7.68  | 121.84      | 110.48   |
| 2   | y     | 347 | LYS  | N-CA-C | -7.68 | 102.84      | 112.90   |
| 16  | Az    | 139 | LYS  | CA-C-N | -7.67 | 110.18      | 122.53   |
| 16  | Az    | 139 | LYS  | C-N-CA | -7.67 | 110.18      | 122.53   |
| 7   | J     | 77  | LYS  | CA-C-N | 7.67  | 129.43      | 119.84   |
| 7   | J     | 77  | LYS  | C-N-CA | 7.67  | 129.43      | 119.84   |
| 5   | AE    | 783 | ILE  | N-CA-C | -7.66 | 101.55      | 112.35   |
| 2   | BR    | 295 | ASN  | N-CA-C | -7.66 | 102.88      | 111.07   |
| 3   | 7     | 868 | SER  | N-CA-C | -7.66 | 99.70       | 110.50   |
| 3   | BY    | 264 | ILE  | N-CA-C | 7.66  | 118.83      | 108.11   |
| 2   | q     | 12  | LEU  | CA-C-O | -7.65 | 112.44      | 120.55   |
| 2   | BK    | 280 | ILE  | CA-C-N | 7.65  | 135.46      | 121.70   |
| 2   | BK    | 280 | ILE  | C-N-CA | 7.65  | 135.46      | 121.70   |
| 7   | J     | 274 | GLN  | N-CA-C | -7.64 | 102.95      | 111.28   |
| 5   | Bf    | 653 | ILE  | N-CA-C | -7.64 | 103.48      | 111.58   |
| 2   | s     | 240 | LEU  | N-CA-C | -7.63 | 101.84      | 112.45   |
| 5   | 9     | 462 | LYS  | CA-C-N | -7.63 | 109.45      | 120.97   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 9     | 462 | LYS  | C-N-CA | -7.63 | 109.45      | 120.97   |
| 5   | AO    | 251 | HIS  | N-CA-C | 7.63  | 119.59      | 111.28   |
| 3   | E     | 803 | ALA  | N-CA-C | -7.63 | 103.56      | 113.17   |
| 2   | k     | 32  | ALA  | N-CA-C | 7.62  | 121.51      | 109.39   |
| 7   | Bm    | 98  | SER  | CA-C-N | 7.61  | 127.24      | 119.56   |
| 7   | Bm    | 98  | SER  | C-N-CA | 7.61  | 127.24      | 119.56   |
| 7   | AM    | 274 | GLN  | N-CA-C | -7.61 | 102.99      | 111.28   |
| 5   | AO    | 72  | SER  | CA-C-N | 7.60  | 127.76      | 120.31   |
| 5   | AO    | 72  | SER  | C-N-CA | 7.60  | 127.76      | 120.31   |
| 2   | Cd    | 330 | ALA  | N-CA-C | -7.59 | 94.63       | 110.80   |
| 3   | E     | 36  | LYS  | CA-C-O | -7.59 | 112.51      | 120.55   |
| 5   | AU    | 253 | ASN  | CA-C-O | -7.59 | 112.84      | 122.63   |
| 5   | M     | 253 | ASN  | CA-C-O | -7.58 | 112.84      | 122.63   |
| 3   | I     | 833 | ILE  | CA-C-O | -7.58 | 113.38      | 121.27   |
| 3   | n     | 527 | LEU  | N-CA-C | -7.58 | 103.83      | 113.23   |
| 5   | AO    | 190 | LYS  | N-CA-C | 7.57  | 120.67      | 109.24   |
| 7   | Bm    | 145 | TYR  | N-CA-C | 7.57  | 121.25      | 109.52   |
| 16  | Ai    | 147 | LYS  | N-CA-C | -7.57 | 104.05      | 113.28   |
| 3   | E     | 205 | GLU  | N-CA-C | 7.56  | 119.64      | 108.60   |
| 3   | E     | 175 | THR  | CA-C-N | 7.56  | 127.27      | 119.56   |
| 3   | E     | 175 | THR  | C-N-CA | 7.56  | 127.27      | 119.56   |
| 5   | L     | 527 | ILE  | N-CA-C | -7.56 | 103.09      | 110.72   |
| 16  | Ai    | 43  | LYS  | N-CA-C | -7.56 | 102.98      | 111.14   |
| 2   | Cd    | 25  | GLN  | CA-C-N | 7.55  | 127.51      | 120.03   |
| 2   | Cd    | 25  | GLN  | C-N-CA | 7.55  | 127.51      | 120.03   |
| 3   | n     | 251 | LEU  | CA-C-N | 7.55  | 127.51      | 120.03   |
| 3   | n     | 251 | LEU  | C-N-CA | 7.55  | 127.51      | 120.03   |
| 3   | BY    | 36  | LYS  | CA-C-O | -7.55 | 112.55      | 120.55   |
| 2   | Cd    | 265 | ASP  | CA-C-O | -7.54 | 112.55      | 120.55   |
| 7   | J     | 142 | ASP  | N-CA-C | -7.54 | 103.14      | 111.36   |
| 3   | BY    | 445 | PRO  | CA-C-O | -7.54 | 112.47      | 121.67   |
| 5   | v     | 462 | LYS  | CA-C-N | -7.54 | 109.59      | 120.97   |
| 5   | v     | 462 | LYS  | C-N-CA | -7.54 | 109.59      | 120.97   |
| 2   | f     | 38  | LEU  | N-CA-C | -7.53 | 103.03      | 112.90   |
| 7   | O     | 46  | HIS  | N-CA-C | -7.53 | 102.10      | 110.91   |
| 3   | I     | 622 | LYS  | CA-C-N | 7.53  | 128.20      | 119.47   |
| 3   | I     | 622 | LYS  | C-N-CA | 7.53  | 128.20      | 119.47   |
| 2   | f     | 316 | ASP  | N-CA-C | -7.52 | 103.16      | 111.36   |
| 2   | D     | 12  | LEU  | CA-C-O | -7.51 | 112.45      | 120.42   |
| 5   | v     | 749 | ILE  | CA-C-O | -7.51 | 112.88      | 120.85   |
| 5   | AE    | 857 | ARG  | CA-C-O | -7.51 | 111.61      | 120.10   |
| 7   | O     | 328 | TYR  | N-CA-C | 7.51  | 121.18      | 110.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 7     | 453 | TRP  | CA-C-O | -7.51 | 111.34      | 119.97   |
| 2   | BK    | 246 | GLN  | CA-C-N | 7.51  | 135.21      | 121.70   |
| 2   | BK    | 246 | GLN  | C-N-CA | 7.51  | 135.21      | 121.70   |
| 3   | 7     | 622 | LYS  | CA-C-N | 7.50  | 128.18      | 119.47   |
| 3   | 7     | 622 | LYS  | C-N-CA | 7.50  | 128.18      | 119.47   |
| 1   | CP    | 349 | VAL  | CA-C-O | -7.50 | 112.58      | 120.39   |
| 16  | CM    | 34  | PHE  | N-CA-C | -7.50 | 103.12      | 111.82   |
| 2   | D     | 120 | LYS  | N-CA-C | -7.50 | 102.47      | 111.69   |
| 16  | Aq    | 156 | LYS  | N-CA-C | -7.50 | 97.90       | 109.52   |
| 2   | BR    | 136 | GLU  | CA-C-O | -7.50 | 112.47      | 120.42   |
| 5   | G     | 642 | ILE  | N-CA-C | 7.49  | 118.29      | 110.72   |
| 7   | AM    | 250 | PHE  | N-CA-C | -7.49 | 103.94      | 113.23   |
| 3   | BY    | 133 | VAL  | N-CA-C | 7.49  | 118.91      | 108.12   |
| 3   | E     | 746 | GLU  | N-CA-C | -7.49 | 100.91      | 110.19   |
| 7   | AM    | 329 | PHE  | N-CA-C | 7.48  | 120.40      | 110.53   |
| 3   | 1     | 527 | LEU  | N-CA-C | -7.47 | 103.11      | 112.90   |
| 7   | AG    | 70  | ILE  | N-CA-C | 7.47  | 118.21      | 108.35   |
| 3   | I     | 663 | GLN  | N-CA-C | -7.47 | 102.82      | 112.23   |
| 3   | 7     | 524 | VAL  | N-CA-C | -7.47 | 103.00      | 110.62   |
| 5   | AE    | 462 | LYS  | CA-C-N | -7.47 | 109.69      | 120.97   |
| 5   | AE    | 462 | LYS  | C-N-CA | -7.47 | 109.69      | 120.97   |
| 7   | AG    | 294 | SER  | CA-C-N | 7.47  | 135.14      | 121.70   |
| 7   | AG    | 294 | SER  | C-N-CA | 7.47  | 135.14      | 121.70   |
| 5   | 9     | 442 | ILE  | N-CA-C | -7.46 | 104.58      | 111.67   |
| 2   | Cd    | 32  | ALA  | CA-C-O | -7.46 | 112.57      | 120.63   |
| 5   | AB    | 280 | LEU  | CA-C-N | 7.46  | 129.16      | 119.84   |
| 5   | AB    | 280 | LEU  | C-N-CA | 7.46  | 129.16      | 119.84   |
| 3   | 7     | 85  | SER  | N-CA-C | 7.45  | 120.61      | 110.55   |
| 7   | AM    | 70  | ILE  | N-CA-C | 7.45  | 119.48      | 108.45   |
| 16  | CB    | 176 | ILE  | N-CA-C | -7.45 | 101.45      | 111.44   |
| 5   | AU    | 236 | ALA  | CA-C-O | -7.45 | 112.93      | 121.72   |
| 5   | G     | 462 | LYS  | CA-C-N | -7.44 | 109.73      | 120.97   |
| 5   | G     | 462 | LYS  | C-N-CA | -7.44 | 109.73      | 120.97   |
| 7   | Bm    | 274 | GLN  | N-CA-C | -7.44 | 103.17      | 111.28   |
| 2   | D     | 268 | ILE  | N-CA-C | 7.44  | 118.23      | 110.72   |
| 7   | 4     | 187 | LEU  | N-CA-C | 7.44  | 121.78      | 109.95   |
| 5   | AB    | 292 | ASN  | CA-C-N | 7.44  | 129.14      | 119.84   |
| 5   | AB    | 292 | ASN  | C-N-CA | 7.44  | 129.14      | 119.84   |
| 2   | k     | 115 | GLU  | N-CA-C | -7.43 | 103.11      | 111.14   |
| 16  | CB    | 35  | TYR  | CA-C-O | 7.43  | 123.01      | 118.33   |
| 5   | v     | 597 | TRP  | CA-C-O | -7.43 | 113.02      | 120.82   |
| 5   | L     | 749 | ILE  | CA-C-O | -7.42 | 112.45      | 120.47   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | Cd    | 38  | LEU  | N-CA-C | -7.42 | 104.03      | 113.23   |
| 3   | I     | 36  | LYS  | CA-C-O | -7.42 | 112.56      | 120.42   |
| 3   | BY    | 610 | LEU  | N-CA-C | -7.42 | 103.69      | 112.89   |
| 3   | I     | 631 | VAL  | CA-C-O | -7.42 | 113.24      | 120.95   |
| 16  | Az    | 171 | PHE  | CA-C-N | 7.41  | 135.04      | 121.70   |
| 16  | Az    | 171 | PHE  | C-N-CA | 7.41  | 135.04      | 121.70   |
| 7   | 4     | 151 | ASP  | N-CA-C | 7.41  | 122.14      | 113.18   |
| 5   | L     | 622 | ILE  | N-CA-C | -7.40 | 99.79       | 108.82   |
| 5   | v     | 492 | CYS  | CA-C-O | -7.40 | 112.71      | 120.55   |
| 3   | 1     | 205 | GLU  | N-CA-C | 7.40  | 119.40      | 108.60   |
| 3   | 7     | 36  | LYS  | CA-C-O | -7.40 | 112.70      | 120.55   |
| 5   | AE    | 503 | SER  | CA-C-O | -7.40 | 112.80      | 121.16   |
| 3   | E     | 622 | LYS  | CA-C-N | 7.40  | 128.05      | 119.47   |
| 3   | E     | 622 | LYS  | C-N-CA | 7.40  | 128.05      | 119.47   |
| 1   | CP    | 259 | THR  | N-CA-C | 7.40  | 119.81      | 108.42   |
| 7   | AM    | 77  | LYS  | CA-C-N | 7.39  | 129.08      | 119.84   |
| 7   | AM    | 77  | LYS  | C-N-CA | 7.39  | 129.08      | 119.84   |
| 3   | I     | 786 | ARG  | N-CA-C | -7.38 | 102.61      | 111.69   |
| 3   | n     | 36  | LYS  | CA-C-O | -7.38 | 112.72      | 120.55   |
| 2   | BR    | 290 | ASN  | CA-C-N | 7.38  | 134.99      | 121.70   |
| 2   | BR    | 290 | ASN  | C-N-CA | 7.38  | 134.99      | 121.70   |
| 5   | G     | 749 | ILE  | CA-C-O | -7.38 | 112.81      | 120.71   |
| 5   | AE    | 492 | CYS  | CA-C-O | -7.38 | 112.73      | 120.55   |
| 5   | G     | 492 | CYS  | CA-C-O | -7.38 | 112.73      | 120.55   |
| 3   | n     | 85  | SER  | N-CA-C | 7.38  | 120.51      | 110.55   |
| 5   | AU    | 142 | SER  | N-CA-C | 7.38  | 121.70      | 111.74   |
| 5   | M     | 40  | ASP  | N-CA-C | 7.37  | 122.47      | 109.58   |
| 16  | CM    | 169 | PRO  | N-CA-C | -7.35 | 99.64       | 111.19   |
| 3   | I     | 785 | VAL  | CA-C-O | -7.35 | 112.79      | 120.14   |
| 5   | L     | 762 | LEU  | N-CA-C | -7.35 | 103.35      | 111.36   |
| 5   | Bf    | 642 | ILE  | N-CA-C | 7.35  | 119.37      | 111.58   |
| 2   | k     | 267 | GLU  | N-CA-C | -7.34 | 104.85      | 113.88   |
| 2   | BK    | 12  | LEU  | CA-C-O | -7.34 | 112.77      | 120.55   |
| 2   | CW    | 124 | GLN  | N-CA-C | -7.33 | 103.30      | 112.90   |
| 5   | G     | 503 | SER  | CA-C-O | -7.33 | 112.70      | 121.05   |
| 2   | CW    | 317 | SER  | N-CA-C | -7.32 | 100.39      | 110.35   |
| 16  | CM    | 125 | ALA  | CA-C-O | -7.32 | 112.66      | 120.42   |
| 1   | i     | 288 | HIS  | N-CA-C | 7.32  | 115.78      | 108.75   |
| 3   | 7     | 445 | PRO  | CA-C-O | -7.32 | 113.05      | 122.12   |
| 2   | Ch    | 343 | GLU  | N-CA-C | -7.32 | 102.69      | 111.69   |
| 5   | AU    | 72  | SER  | CA-C-N | 7.31  | 127.47      | 120.31   |
| 5   | AU    | 72  | SER  | C-N-CA | 7.31  | 127.47      | 120.31   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | Bm    | 77  | LYS  | CA-C-N | 7.31  | 128.98      | 119.84   |
| 7   | Bm    | 77  | LYS  | C-N-CA | 7.31  | 128.98      | 119.84   |
| 3   | BY    | 733 | LYS  | N-CA-C | -7.31 | 104.39      | 112.72   |
| 2   | z     | 348 | THR  | N-CA-C | -7.31 | 103.33      | 112.90   |
| 3   | I     | 85  | SER  | N-CA-C | 7.30  | 120.41      | 110.55   |
| 2   | f     | 265 | ASP  | CA-C-O | -7.30 | 111.85      | 120.10   |
| 7   | Bm    | 329 | PHE  | N-CA-C | 7.30  | 120.17      | 110.53   |
| 2   | y     | 348 | THR  | N-CA-C | -7.30 | 103.34      | 112.90   |
| 3   | E     | 527 | LEU  | N-CA-C | -7.30 | 104.38      | 113.28   |
| 1   | i     | 100 | ALA  | CA-C-N | 7.30  | 128.96      | 119.84   |
| 1   | i     | 100 | ALA  | C-N-CA | 7.30  | 128.96      | 119.84   |
| 7   | Bm    | 533 | THR  | CA-C-N | -7.29 | 109.81      | 122.79   |
| 7   | Bm    | 533 | THR  | C-N-CA | -7.29 | 109.81      | 122.79   |
| 2   | y     | 83  | GLU  | N-CA-C | -7.29 | 103.34      | 111.28   |
| 7   | Bm    | 154 | THR  | N-CA-C | -7.28 | 99.69       | 110.46   |
| 2   | z     | 83  | GLU  | N-CA-C | -7.28 | 103.34      | 111.28   |
| 7   | 4     | 541 | GLN  | CA-C-N | -7.28 | 110.53      | 122.54   |
| 7   | 4     | 541 | GLN  | C-N-CA | -7.28 | 110.53      | 122.54   |
| 7   | 4     | 182 | SER  | CA-C-N | 7.27  | 127.20      | 119.85   |
| 7   | 4     | 182 | SER  | C-N-CA | 7.27  | 127.20      | 119.85   |
| 2   | s     | 29  | ILE  | CA-C-O | -7.27 | 111.96      | 120.83   |
| 2   | Ch    | 12  | LEU  | CA-C-O | -7.27 | 112.85      | 120.55   |
| 5   | L     | 919 | THR  | CA-C-O | -7.26 | 112.85      | 120.55   |
| 2   | Cd    | 86  | ASN  | CA-C-O | -7.26 | 112.18      | 120.24   |
| 16  | Av    | 38  | LYS  | N-CA-C | -7.26 | 103.08      | 112.23   |
| 5   | AU    | 283 | ASN  | CA-C-N | 7.26  | 134.77      | 121.70   |
| 5   | AU    | 283 | ASN  | C-N-CA | 7.26  | 134.77      | 121.70   |
| 16  | CB    | 175 | GLY  | CA-C-O | -7.26 | 112.96      | 120.66   |
| 3   | BY    | 622 | LYS  | CA-C-N | 7.25  | 127.88      | 119.47   |
| 3   | BY    | 622 | LYS  | C-N-CA | 7.25  | 127.88      | 119.47   |
| 3   | E     | 206 | ILE  | N-CA-C | -7.25 | 104.71      | 111.45   |
| 3   | I     | 125 | THR  | N-CA-C | -7.25 | 98.39       | 109.41   |
| 5   | AE    | 919 | THR  | CA-C-O | -7.25 | 112.86      | 120.55   |
| 5   | Bt    | 158 | THR  | N-CA-C | 7.25  | 117.44      | 107.73   |
| 7   | AG    | 76  | PHE  | CA-C-O | -7.24 | 112.86      | 120.89   |
| 16  | Aq    | 90  | SER  | N-CA-C | 7.24  | 126.21      | 110.80   |
| 3   | n     | 205 | GLU  | N-CA-C | 7.24  | 119.16      | 108.60   |
| 2   | BK    | 83  | GLU  | N-CA-C | -7.24 | 103.42      | 112.90   |
| 3   | 1     | 441 | PHE  | N-CA-C | -7.23 | 103.33      | 111.14   |
| 16  | Ai    | 171 | PHE  | CA-C-N | 7.23  | 134.71      | 121.70   |
| 16  | Ai    | 171 | PHE  | C-N-CA | 7.23  | 134.71      | 121.70   |
| 3   | I     | 803 | ALA  | N-CA-C | -7.21 | 104.45      | 113.18   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | f     | 266 | GLY  | N-CA-C | -7.21 | 103.05      | 113.86   |
| 2   | q     | 86  | ASN  | N-CA-C | -7.21 | 102.43      | 112.45   |
| 7   | AG    | 328 | TYR  | N-CA-C | 7.21  | 119.42      | 109.18   |
| 16  | Aq    | 146 | GLN  | CA-C-O | -7.21 | 112.78      | 120.42   |
| 3   | E     | 703 | TYR  | CA-C-N | 7.21  | 128.85      | 119.84   |
| 3   | E     | 703 | TYR  | C-N-CA | 7.21  | 128.85      | 119.84   |
| 5   | M     | 289 | PHE  | N-CA-C | 7.20  | 119.80      | 108.79   |
| 2   | s     | 266 | GLY  | N-CA-C | -7.19 | 103.08      | 113.86   |
| 5   | Bf    | 432 | LYS  | CA-C-N | -7.18 | 114.08      | 122.63   |
| 5   | Bf    | 432 | LYS  | C-N-CA | -7.18 | 114.08      | 122.63   |
| 5   | v     | 475 | TYR  | CA-C-N | 7.18  | 128.49      | 120.66   |
| 5   | v     | 475 | TYR  | C-N-CA | 7.18  | 128.49      | 120.66   |
| 5   | AB    | 236 | ALA  | CA-C-O | -7.18 | 113.25      | 121.72   |
| 16  | Ai    | 34  | PHE  | N-CA-C | -7.18 | 103.45      | 111.71   |
| 1   | BD    | 401 | TYR  | N-CA-C | -7.18 | 99.04       | 109.59   |
| 5   | L     | 597 | TRP  | CA-C-O | -7.17 | 111.73      | 119.97   |
| 2   | CW    | 13  | LEU  | N-CA-C | -7.17 | 103.55      | 111.36   |
| 2   | s     | 136 | GLU  | CA-C-O | -7.17 | 112.95      | 120.55   |
| 3   | 7     | 251 | LEU  | CA-C-N | 7.17  | 127.12      | 120.03   |
| 3   | 7     | 251 | LEU  | C-N-CA | 7.17  | 127.12      | 120.03   |
| 7   | AM    | 76  | PHE  | CA-C-O | -7.16 | 112.94      | 120.89   |
| 2   | y     | 89  | SER  | N-CA-C | -7.16 | 103.56      | 111.36   |
| 5   | M     | 236 | ALA  | CA-C-O | -7.16 | 113.28      | 121.72   |
| 5   | R     | 42  | ASP  | N-CA-C | -7.16 | 104.43      | 113.02   |
| 5   | AO    | 236 | ALA  | CA-C-O | -7.16 | 113.37      | 121.81   |
| 2   | z     | 89  | SER  | N-CA-C | -7.15 | 103.56      | 111.36   |
| 3   | E     | 445 | PRO  | CA-C-O | -7.15 | 112.94      | 121.67   |
| 5   | R     | 308 | PHE  | CA-C-N | 7.15  | 134.58      | 121.70   |
| 5   | R     | 308 | PHE  | C-N-CA | 7.15  | 134.58      | 121.70   |
| 5   | AE    | 920 | GLU  | N-CA-C | -7.15 | 103.57      | 111.36   |
| 1   | A     | 100 | ALA  | CA-C-N | 7.15  | 128.77      | 119.84   |
| 1   | A     | 100 | ALA  | C-N-CA | 7.15  | 128.77      | 119.84   |
| 2   | CW    | 123 | LEU  | CA-C-O | -7.15 | 112.97      | 120.55   |
| 3   | 1     | 676 | THR  | CA-C-N | 7.14  | 124.80      | 119.66   |
| 3   | 1     | 676 | THR  | C-N-CA | 7.14  | 124.80      | 119.66   |
| 2   | Ch    | 342 | LEU  | CA-C-O | -7.13 | 111.77      | 119.97   |
| 2   | q     | 357 | ARG  | CA-C-O | -7.13 | 111.76      | 122.38   |
| 2   | k     | 269 | ASN  | N-CA-C | 7.12  | 119.30      | 109.54   |
| 3   | BY    | 533 | PHE  | CA-C-O | -7.12 | 113.34      | 120.82   |
| 5   | G     | 475 | TYR  | CA-C-N | 7.12  | 128.42      | 120.66   |
| 5   | G     | 475 | TYR  | C-N-CA | 7.12  | 128.42      | 120.66   |
| 3   | I     | 660 | ILE  | N-CA-C | -7.12 | 97.91       | 108.45   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 398 | LEU  | N-CA-C  | -7.11 | 101.15      | 110.39   |
| 5   | G     | 609 | ASP  | N-CA-C  | -7.10 | 101.86      | 111.87   |
| 1   | A     | 155 | ASP  | CA-C-O  | -7.09 | 113.31      | 121.54   |
| 3   | E     | 125 | THR  | N-CA-C  | -7.09 | 98.63       | 109.41   |
| 3   | BY    | 85  | SER  | N-CA-C  | 7.09  | 120.12      | 110.55   |
| 2   | k     | 29  | ILE  | N-CA-C  | 7.09  | 118.09      | 108.17   |
| 7   | O     | 506 | GLN  | CA-C-N  | 7.09  | 126.79      | 119.56   |
| 7   | O     | 506 | GLN  | C-N-CA  | 7.09  | 126.79      | 119.56   |
| 5   | AB    | 114 | LYS  | N-CA-C  | -7.09 | 104.26      | 113.12   |
| 5   | AE    | 546 | PRO  | CA-C-N  | 7.09  | 128.70      | 119.84   |
| 5   | AE    | 546 | PRO  | C-N-CA  | 7.09  | 128.70      | 119.84   |
| 2   | Ch    | 280 | ILE  | CB-CA-C | 7.09  | 122.91      | 111.29   |
| 2   | BR    | 89  | SER  | N-CA-C  | -7.08 | 103.64      | 111.36   |
| 1   | BD    | 398 | LEU  | CA-C-N  | 7.08  | 128.69      | 119.84   |
| 1   | BD    | 398 | LEU  | C-N-CA  | 7.08  | 128.69      | 119.84   |
| 16  | CB    | 139 | LYS  | CA-C-N  | -7.08 | 110.86      | 122.11   |
| 16  | CB    | 139 | LYS  | C-N-CA  | -7.08 | 110.86      | 122.11   |
| 7   | O     | 110 | ASP  | N-CA-C  | 7.08  | 122.04      | 113.41   |
| 5   | v     | 611 | PRO  | CA-C-N  | 7.08  | 134.44      | 121.70   |
| 5   | v     | 611 | PRO  | C-N-CA  | 7.08  | 134.44      | 121.70   |
| 7   | 4     | 522 | PHE  | CA-C-O  | -7.08 | 113.39      | 120.82   |
| 2   | CW    | 102 | TYR  | N-CA-C  | -7.07 | 103.63      | 112.90   |
| 2   | Cd    | 354 | GLU  | CA-C-O  | -7.07 | 114.24      | 122.37   |
| 16  | An    | 34  | PHE  | N-CA-C  | -7.07 | 103.58      | 111.71   |
| 3   | 7     | 803 | ALA  | N-CA-C  | -7.06 | 104.27      | 113.17   |
| 7   | AM    | 98  | SER  | CA-C-N  | 7.06  | 126.74      | 119.82   |
| 7   | AM    | 98  | SER  | C-N-CA  | 7.06  | 126.74      | 119.82   |
| 16  | Z     | 171 | PHE  | CA-C-N  | 7.06  | 134.40      | 121.70   |
| 16  | Z     | 171 | PHE  | C-N-CA  | 7.06  | 134.40      | 121.70   |
| 1   | Ca    | 131 | ASN  | CA-C-N  | 7.06  | 127.47      | 119.92   |
| 1   | Ca    | 131 | ASN  | C-N-CA  | 7.06  | 127.47      | 119.92   |
| 2   | k     | 85  | ASN  | N-CA-C  | -7.06 | 103.34      | 112.23   |
| 5   | 9     | 562 | ASP  | CA-C-N  | 7.05  | 127.20      | 119.87   |
| 5   | 9     | 562 | ASP  | C-N-CA  | 7.05  | 127.20      | 119.87   |
| 7   | AG    | 182 | SER  | CA-C-N  | 7.05  | 126.97      | 119.85   |
| 7   | AG    | 182 | SER  | C-N-CA  | 7.05  | 126.97      | 119.85   |
| 2   | BR    | 29  | ILE  | CA-C-N  | 7.05  | 135.00      | 121.54   |
| 2   | BR    | 29  | ILE  | C-N-CA  | 7.05  | 135.00      | 121.54   |
| 2   | s     | 314 | GLU  | CA-C-O  | -7.04 | 113.08      | 120.55   |
| 2   | Cd    | 322 | LYS  | CA-C-N  | 7.04  | 126.72      | 119.82   |
| 2   | Cd    | 322 | LYS  | C-N-CA  | 7.04  | 126.72      | 119.82   |
| 7   | AM    | 333 | GLY  | CA-C-N  | 7.04  | 131.01      | 120.31   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AM    | 333 | GLY  | C-N-CA  | 7.04  | 131.01      | 120.31   |
| 1   | i     | 155 | ASP  | CA-C-O  | -7.03 | 113.38      | 121.54   |
| 3   | n     | 677 | PRO  | CA-C-N  | 7.03  | 127.18      | 119.87   |
| 3   | n     | 677 | PRO  | C-N-CA  | 7.03  | 127.18      | 119.87   |
| 5   | AB    | 284 | LYS  | CA-C-N  | 7.03  | 131.59      | 121.54   |
| 5   | AB    | 284 | LYS  | C-N-CA  | 7.03  | 131.59      | 121.54   |
| 2   | k     | 280 | ILE  | CB-CA-C | 7.03  | 122.81      | 111.29   |
| 2   | CW    | 12  | LEU  | CA-C-O  | -7.03 | 112.16      | 120.10   |
| 5   | Bt    | 236 | ALA  | CA-C-O  | -7.02 | 113.52      | 121.81   |
| 2   | k     | 99  | GLN  | N-CA-C  | -7.02 | 103.38      | 112.23   |
| 1   | Ca    | 155 | ASP  | CA-C-O  | -7.02 | 113.40      | 121.54   |
| 1   | Ca    | 349 | VAL  | O-C-N   | -7.02 | 115.88      | 123.18   |
| 5   | v     | 467 | SER  | N-CA-C  | -7.02 | 103.78      | 114.16   |
| 5   | Bt    | 308 | PHE  | CA-C-N  | 7.01  | 134.32      | 121.70   |
| 5   | Bt    | 308 | PHE  | C-N-CA  | 7.01  | 134.32      | 121.70   |
| 3   | I     | 827 | ALA  | N-CA-C  | -7.01 | 103.39      | 112.23   |
| 3   | n     | 264 | ILE  | N-CA-C  | 7.01  | 117.93      | 108.11   |
| 5   | G     | 545 | HIS  | CA-C-N  | 7.00  | 127.59      | 120.38   |
| 5   | G     | 545 | HIS  | C-N-CA  | 7.00  | 127.59      | 120.38   |
| 7   | J     | 294 | SER  | CA-C-O  | -7.00 | 111.94      | 122.38   |
| 5   | v     | 646 | ASN  | CA-C-N  | 7.00  | 126.70      | 119.56   |
| 5   | v     | 646 | ASN  | C-N-CA  | 7.00  | 126.70      | 119.56   |
| 5   | v     | 588 | PHE  | N-CA-C  | 7.00  | 125.71      | 110.80   |
| 2   | f     | 321 | SER  | N-CA-C  | 7.00  | 118.70      | 111.14   |
| 2   | k     | 355 | TYR  | CA-C-O  | -7.00 | 111.17      | 119.15   |
| 5   | Bt    | 292 | ASN  | CA-C-N  | 7.00  | 126.70      | 119.56   |
| 5   | Bt    | 292 | ASN  | C-N-CA  | 7.00  | 126.70      | 119.56   |
| 7   | 4     | 250 | PHE  | N-CA-C  | -7.00 | 103.70      | 111.82   |
| 3   | 7     | 881 | ASP  | N-CA-C  | -7.00 | 102.72      | 112.45   |
| 5   | 9     | 642 | ILE  | N-CA-C  | 7.00  | 118.63      | 111.00   |
| 7   | AG    | 553 | TYR  | N-CA-C  | -7.00 | 104.38      | 113.12   |
| 16  | A7    | 54  | PRO  | N-CA-C  | -6.99 | 100.23      | 111.14   |
| 1   | i     | 349 | VAL  | O-C-N   | -6.99 | 115.91      | 123.18   |
| 5   | L     | 599 | GLN  | CA-C-N  | 6.99  | 130.34      | 120.28   |
| 5   | L     | 599 | GLN  | C-N-CA  | 6.99  | 130.34      | 120.28   |
| 7   | O     | 194 | ASP  | N-CA-C  | -6.99 | 102.61      | 113.02   |
| 2   | Ch    | 296 | ASP  | N-CA-C  | -6.99 | 103.75      | 112.90   |
| 1   | A     | 398 | LEU  | CA-C-N  | 6.98  | 126.91      | 120.21   |
| 1   | A     | 398 | LEU  | C-N-CA  | 6.98  | 126.91      | 120.21   |
| 3   | 7     | 864 | GLN  | N-CA-C  | -6.97 | 104.90      | 113.41   |
| 7   | AM    | 204 | PHE  | N-CA-C  | -6.97 | 105.40      | 114.04   |
| 2   | Ch    | 65  | ILE  | N-CA-C  | -6.97 | 103.68      | 110.72   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | M     | 295 | ASN  | N-CA-C  | -6.96 | 103.30      | 114.09   |
| 2   | BK    | 103 | ASN  | N-CA-C  | -6.96 | 103.77      | 111.36   |
| 2   | Ch    | 82  | ARG  | CA-C-O  | -6.96 | 111.50      | 120.00   |
| 5   | AB    | 351 | PHE  | N-CA-C  | 6.96  | 119.82      | 108.26   |
| 7   | AG    | 522 | PHE  | CA-C-O  | -6.96 | 113.51      | 120.82   |
| 5   | R     | 163 | PRO  | N-CA-C  | 6.96  | 122.89      | 113.84   |
| 2   | y     | 53  | LYS  | CA-C-O  | -6.96 | 113.17      | 120.55   |
| 5   | AE    | 576 | PHE  | N-CA-C  | -6.96 | 101.36      | 110.33   |
| 1   | CP    | 349 | VAL  | O-C-N   | -6.96 | 115.82      | 123.20   |
| 7   | O     | 250 | PHE  | N-CA-C  | -6.96 | 104.80      | 113.28   |
| 3   | 7     | 238 | LEU  | CA-C-N  | 6.95  | 134.22      | 121.70   |
| 3   | 7     | 238 | LEU  | C-N-CA  | 6.95  | 134.22      | 121.70   |
| 5   | 9     | 609 | ASP  | N-CA-C  | -6.94 | 101.98      | 111.56   |
| 7   | AG    | 68  | ASP  | N-CA-C  | 6.94  | 118.82      | 107.23   |
| 3   | E     | 791 | GLN  | CA-C-O  | -6.94 | 112.26      | 120.10   |
| 3   | 1     | 703 | TYR  | CA-C-N  | 6.94  | 128.51      | 119.84   |
| 3   | 1     | 703 | TYR  | C-N-CA  | 6.94  | 128.51      | 119.84   |
| 7   | AG    | 250 | PHE  | N-CA-C  | -6.94 | 103.77      | 111.82   |
| 5   | AU    | 40  | ASP  | CA-C-N  | 6.94  | 126.64      | 119.56   |
| 5   | AU    | 40  | ASP  | C-N-CA  | 6.94  | 126.64      | 119.56   |
| 5   | R     | 158 | THR  | N-CA-C  | 6.93  | 117.39      | 108.24   |
| 2   | z     | 53  | LYS  | CA-C-O  | -6.93 | 113.20      | 120.55   |
| 3   | n     | 660 | ILE  | N-CA-C  | -6.93 | 98.20       | 108.45   |
| 2   | Cd    | 266 | GLY  | N-CA-C  | -6.93 | 103.47      | 113.86   |
| 2   | f     | 86  | ASN  | CA-C-O  | -6.92 | 112.56      | 120.24   |
| 7   | J     | 553 | TYR  | N-CA-C  | -6.92 | 104.97      | 113.41   |
| 1   | Ca    | 100 | ALA  | CA-C-N  | 6.92  | 128.49      | 119.84   |
| 1   | Ca    | 100 | ALA  | C-N-CA  | 6.92  | 128.49      | 119.84   |
| 2   | Ch    | 319 | LEU  | N-CA-C  | -6.92 | 104.99      | 113.50   |
| 2   | s     | 265 | ASP  | CA-C-O  | -6.92 | 113.22      | 120.55   |
| 3   | BY    | 785 | VAL  | CA-C-O  | -6.92 | 113.36      | 119.38   |
| 3   | BY    | 793 | MET  | N-CA-C  | -6.91 | 103.53      | 112.23   |
| 7   | Bm    | 522 | PHE  | CA-C-O  | -6.90 | 113.58      | 120.82   |
| 2   | BR    | 117 | GLN  | CA-C-O  | -6.89 | 111.65      | 119.79   |
| 3   | E     | 441 | PHE  | N-CA-C  | -6.89 | 103.70      | 111.14   |
| 3   | E     | 785 | VAL  | N-CA-C  | -6.89 | 103.49      | 111.00   |
| 1   | BD    | 264 | LYS  | CB-CA-C | -6.89 | 108.62      | 116.54   |
| 5   | L     | 927 | MET  | CA-C-O  | -6.88 | 111.67      | 119.79   |
| 5   | L     | 646 | ASN  | CA-C-N  | 6.88  | 126.58      | 119.56   |
| 5   | L     | 646 | ASN  | C-N-CA  | 6.88  | 126.58      | 119.56   |
| 5   | R     | 59  | VAL  | O-C-N   | -6.88 | 115.91      | 123.20   |
| 3   | 7     | 792 | GLN  | CA-C-O  | -6.87 | 112.07      | 119.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | Bf    | 483 | TYR  | CA-C-O  | -6.87 | 113.82      | 120.90   |
| 2   | k     | 350 | GLU  | CB-CA-C | -6.87 | 102.34      | 111.82   |
| 7   | O     | 174 | ASN  | N-CA-C  | 6.87  | 124.32      | 114.16   |
| 2   | BR    | 266 | GLY  | N-CA-C  | -6.86 | 103.57      | 113.86   |
| 7   | AG    | 154 | THR  | N-CA-C  | 6.86  | 118.92      | 109.18   |
| 3   | I     | 441 | PHE  | N-CA-C  | -6.85 | 103.74      | 111.14   |
| 1   | BD    | 349 | VAL  | O-C-N   | -6.85 | 116.05      | 123.18   |
| 1   | A     | 349 | VAL  | O-C-N   | -6.84 | 115.94      | 123.20   |
| 1   | C     | 38  | GLU  | N-CA-C  | -6.84 | 100.18      | 110.24   |
| 3   | E     | 238 | LEU  | CA-C-N  | 6.84  | 134.02      | 121.70   |
| 3   | E     | 238 | LEU  | C-N-CA  | 6.84  | 134.02      | 121.70   |
| 2   | s     | 40  | ASN  | N-CA-C  | -6.84 | 103.61      | 112.23   |
| 1   | C     | 349 | VAL  | O-C-N   | -6.84 | 116.06      | 123.18   |
| 3   | n     | 155 | THR  | N-CA-C  | -6.84 | 104.61      | 114.12   |
| 16  | An    | 131 | VAL  | N-CA-C  | -6.84 | 100.75      | 109.30   |
| 16  | An    | 35  | TYR  | CA-C-N  | 6.83  | 133.99      | 121.70   |
| 16  | An    | 35  | TYR  | C-N-CA  | 6.83  | 133.99      | 121.70   |
| 3   | BY    | 559 | SER  | N-CA-C  | 6.82  | 122.13      | 109.24   |
| 3   | I     | 537 | VAL  | N-CA-C  | -6.81 | 103.84      | 110.72   |
| 2   | Cd    | 53  | LYS  | CA-C-O  | -6.81 | 113.33      | 120.55   |
| 3   | 1     | 610 | LEU  | N-CA-C  | -6.81 | 104.23      | 112.54   |
| 5   | AB    | 308 | PHE  | CA-C-N  | 6.81  | 133.96      | 121.70   |
| 5   | AB    | 308 | PHE  | C-N-CA  | 6.81  | 133.96      | 121.70   |
| 3   | 1     | 238 | LEU  | CA-C-N  | 6.81  | 133.95      | 121.70   |
| 3   | 1     | 238 | LEU  | C-N-CA  | 6.81  | 133.95      | 121.70   |
| 3   | BY    | 238 | LEU  | CA-C-N  | 6.80  | 133.95      | 121.70   |
| 3   | BY    | 238 | LEU  | C-N-CA  | 6.80  | 133.95      | 121.70   |
| 5   | G     | 519 | GLN  | N-CA-C  | 6.80  | 121.75      | 113.38   |
| 3   | n     | 768 | THR  | CA-C-N  | 6.80  | 130.07      | 120.28   |
| 3   | n     | 768 | THR  | C-N-CA  | 6.80  | 130.07      | 120.28   |
| 16  | Az    | 71  | SER  | N-CA-C  | -6.80 | 103.95      | 111.36   |
| 3   | E     | 631 | VAL  | CA-C-O  | -6.80 | 113.88      | 120.95   |
| 16  | CM    | 174 | GLU  | N-CA-C  | -6.79 | 91.97       | 111.00   |
| 5   | Bt    | 252 | GLY  | N-CA-C  | -6.79 | 100.59      | 112.55   |
| 2   | k     | 83  | GLU  | N-CA-C  | -6.79 | 104.01      | 112.90   |
| 1   | A     | 128 | LEU  | N-CA-C  | 6.79  | 120.30      | 109.24   |
| 3   | BY    | 880 | LEU  | CA-C-O  | -6.79 | 113.23      | 120.42   |
| 5   | AE    | 463 | GLY  | N-CA-C  | 6.79  | 120.66      | 110.75   |
| 7   | 4     | 246 | ILE  | N-CA-CB | -6.78 | 102.05      | 111.41   |
| 5   | AB    | 39  | SER  | N-CA-C  | 6.78  | 119.48      | 109.24   |
| 5   | R     | 72  | SER  | CA-C-N  | 6.78  | 126.70      | 119.85   |
| 5   | R     | 72  | SER  | C-N-CA  | 6.78  | 126.70      | 119.85   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | Bt    | 61  | LYS  | N-CA-C  | -6.78 | 105.95      | 114.56   |
| 5   | G     | 483 | TYR  | CA-C-O  | -6.78 | 113.92      | 120.90   |
| 5   | 9     | 687 | PHE  | N-CA-C  | -6.78 | 100.00      | 110.10   |
| 2   | Ch    | 267 | GLU  | N-CA-C  | -6.78 | 104.89      | 113.43   |
| 3   | E     | 51  | ASP  | N-CA-C  | 6.78  | 119.70      | 110.55   |
| 1   | C     | 26  | ASN  | N-CA-C  | -6.77 | 99.64       | 110.14   |
| 5   | L     | 858 | MET  | CA-C-O  | -6.77 | 112.18      | 119.97   |
| 1   | BD    | 100 | ALA  | CA-C-N  | 6.77  | 128.30      | 119.84   |
| 1   | BD    | 100 | ALA  | C-N-CA  | 6.77  | 128.30      | 119.84   |
| 3   | n     | 206 | ILE  | N-CA-C  | -6.77 | 105.16      | 111.45   |
| 3   | BY    | 677 | PRO  | CA-C-N  | 6.76  | 126.91      | 119.87   |
| 3   | BY    | 677 | PRO  | C-N-CA  | 6.76  | 126.91      | 119.87   |
| 5   | Bt    | 31  | ASN  | CA-C-O  | -6.76 | 114.60      | 122.37   |
| 2   | s     | 29  | ILE  | CA-C-N  | 6.76  | 133.86      | 121.70   |
| 2   | s     | 29  | ILE  | C-N-CA  | 6.76  | 133.86      | 121.70   |
| 3   | 7     | 453 | TRP  | CA-C-N  | -6.76 | 109.19      | 120.68   |
| 3   | 7     | 453 | TRP  | C-N-CA  | -6.76 | 109.19      | 120.68   |
| 3   | BY    | 428 | PHE  | CA-C-N  | 6.76  | 130.46      | 120.87   |
| 3   | BY    | 428 | PHE  | C-N-CA  | 6.76  | 130.46      | 120.87   |
| 5   | Bf    | 609 | ASP  | N-CA-C  | -6.76 | 103.63      | 112.41   |
| 3   | E     | 660 | ILE  | CA-C-N  | 6.75  | 133.86      | 121.70   |
| 3   | E     | 660 | ILE  | C-N-CA  | 6.75  | 133.86      | 121.70   |
| 2   | s     | 322 | LYS  | CA-C-N  | 6.75  | 126.43      | 119.82   |
| 2   | s     | 322 | LYS  | C-N-CA  | 6.75  | 126.43      | 119.82   |
| 5   | AU    | 175 | GLY  | N-CA-C  | -6.75 | 106.01      | 115.32   |
| 5   | Bt    | 337 | TYR  | CA-C-O  | -6.75 | 112.21      | 119.97   |
| 7   | Bm    | 182 | SER  | CA-C-N  | 6.75  | 126.66      | 119.85   |
| 7   | Bm    | 182 | SER  | C-N-CA  | 6.75  | 126.66      | 119.85   |
| 1   | C     | 100 | ALA  | CA-C-N  | 6.74  | 128.27      | 119.84   |
| 1   | C     | 100 | ALA  | C-N-CA  | 6.74  | 128.27      | 119.84   |
| 7   | Bm    | 166 | MET  | N-CA-CB | -6.74 | 100.63      | 110.47   |
| 2   | BR    | 38  | LEU  | N-CA-C  | -6.74 | 103.74      | 112.23   |
| 2   | D     | 65  | ILE  | N-CA-C  | -6.73 | 103.66      | 111.00   |
| 5   | G     | 575 | LYS  | N-CA-C  | 6.73  | 120.11      | 109.81   |
| 7   | O     | 90  | GLY  | N-CA-C  | -6.73 | 102.86      | 112.55   |
| 2   | BK    | 331 | ASN  | CA-C-O  | -6.73 | 111.10      | 119.38   |
| 5   | Bf    | 492 | CYS  | CA-C-O  | -6.73 | 113.29      | 120.42   |
| 16  | c     | 158 | HIS  | N-CA-C  | -6.73 | 101.02      | 110.50   |
| 3   | I     | 238 | LEU  | CA-C-N  | 6.72  | 133.80      | 121.70   |
| 3   | I     | 238 | LEU  | C-N-CA  | 6.72  | 133.80      | 121.70   |
| 5   | L     | 545 | HIS  | CA-C-N  | 6.71  | 127.30      | 120.38   |
| 5   | L     | 545 | HIS  | C-N-CA  | 6.71  | 127.30      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | AE    | 782 | LYS  | CA-C-O | -6.71 | 111.65      | 119.24   |
| 3   | E     | 444 | PHE  | CA-C-N | 6.71  | 126.63      | 119.85   |
| 3   | E     | 444 | PHE  | C-N-CA | 6.71  | 126.63      | 119.85   |
| 3   | 1     | 444 | PHE  | CA-C-N | 6.71  | 126.67      | 120.03   |
| 3   | 1     | 444 | PHE  | C-N-CA | 6.71  | 126.67      | 120.03   |
| 7   | AG    | 322 | PHE  | N-CA-C | 6.71  | 119.96      | 110.50   |
| 16  | Aq    | 54  | PRO  | N-CA-C | -6.71 | 100.54      | 111.21   |
| 5   | L     | 875 | ILE  | CA-C-O | -6.71 | 113.60      | 121.05   |
| 16  | Z     | 148 | LEU  | N-CA-C | -6.71 | 103.78      | 112.23   |
| 16  | CB    | 171 | PHE  | CA-C-N | 6.70  | 133.77      | 121.70   |
| 16  | CB    | 171 | PHE  | C-N-CA | 6.70  | 133.77      | 121.70   |
| 3   | I     | 471 | ARG  | CA-C-O | -6.70 | 112.20      | 122.32   |
| 3   | I     | 805 | GLN  | N-CA-C | -6.70 | 104.97      | 113.01   |
| 5   | M     | 351 | PHE  | N-CA-C | 6.70  | 119.38      | 108.26   |
| 5   | AU    | 351 | PHE  | N-CA-C | 6.69  | 119.37      | 108.26   |
| 1   | Ca    | 132 | PRO  | CA-C-O | -6.69 | 113.58      | 121.95   |
| 3   | n     | 238 | LEU  | CA-C-N | 6.69  | 133.74      | 121.70   |
| 3   | n     | 238 | LEU  | C-N-CA | 6.69  | 133.74      | 121.70   |
| 3   | BY    | 441 | PHE  | N-CA-C | -6.69 | 103.91      | 111.14   |
| 1   | Ca    | 214 | ILE  | N-CA-C | -6.69 | 105.32      | 111.67   |
| 5   | AO    | 31  | ASN  | CA-C-O | -6.68 | 114.68      | 122.37   |
| 3   | I     | 921 | LYS  | CA-C-O | -6.68 | 113.81      | 120.82   |
| 7   | J     | 38  | ALA  | N-CA-C | 6.67  | 120.45      | 111.24   |
| 16  | c     | 90  | SER  | N-CA-C | 6.67  | 125.00      | 110.80   |
| 2   | BR    | 37  | LYS  | CA-C-O | -6.67 | 113.48      | 120.55   |
| 5   | Bt    | 146 | ILE  | N-CA-C | -6.66 | 105.25      | 111.45   |
| 5   | L     | 585 | SER  | N-CA-C | -6.66 | 104.98      | 113.23   |
| 1   | CP    | 398 | LEU  | CA-C-N | 6.65  | 128.16      | 119.84   |
| 1   | CP    | 398 | LEU  | C-N-CA | 6.65  | 128.16      | 119.84   |
| 7   | J     | 126 | ILE  | N-CA-C | 6.65  | 118.41      | 108.23   |
| 16  | CB    | 53  | ALA  | CA-C-N | 6.65  | 126.57      | 119.85   |
| 16  | CB    | 53  | ALA  | C-N-CA | 6.65  | 126.57      | 119.85   |
| 5   | L     | 492 | CYS  | CA-C-O | -6.65 | 113.50      | 120.55   |
| 3   | I     | 733 | LYS  | N-CA-C | -6.65 | 105.16      | 113.20   |
| 5   | AU    | 213 | ILE  | N-CA-C | 6.65  | 117.47      | 108.17   |
| 5   | v     | 463 | GLY  | N-CA-C | 6.64  | 120.45      | 110.75   |
| 5   | R     | 236 | ALA  | CA-C-O | -6.64 | 113.69      | 121.46   |
| 16  | Ai    | 125 | ALA  | CA-C-O | -6.64 | 113.51      | 120.55   |
| 5   | L     | 483 | TYR  | CA-C-O | -6.63 | 114.07      | 120.90   |
| 3   | 7     | 312 | TYR  | N-CA-C | 6.63  | 119.75      | 109.07   |
| 16  | Av    | 127 | LYS  | CA-C-O | -6.63 | 113.98      | 121.81   |
| 7   | O     | 206 | LYS  | N-CA-C | 6.63  | 119.26      | 109.24   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | Bf    | 621 | PHE  | CA-C-N | 6.63  | 132.47      | 122.92   |
| 5   | Bf    | 621 | PHE  | C-N-CA | 6.63  | 132.47      | 122.92   |
| 2   | f     | 32  | ALA  | CA-C-O | -6.63 | 113.47      | 120.63   |
| 7   | AM    | 39  | LEU  | N-CA-C | -6.63 | 100.22      | 110.10   |
| 7   | AM    | 81  | ARG  | CA-C-N | 6.63  | 126.54      | 119.85   |
| 7   | AM    | 81  | ARG  | C-N-CA | 6.63  | 126.54      | 119.85   |
| 5   | R     | 253 | ASN  | CA-C-O | -6.62 | 112.51      | 122.38   |
| 3   | n     | 662 | ILE  | CA-C-O | -6.62 | 113.83      | 120.85   |
| 5   | Bt    | 150 | PHE  | N-CA-C | 6.62  | 120.31      | 109.72   |
| 5   | Bf    | 576 | PHE  | N-CA-C | -6.61 | 101.99      | 110.19   |
| 5   | L     | 463 | GLY  | N-CA-C | 6.61  | 120.40      | 110.75   |
| 7   | AG    | 533 | THR  | CA-C-N | -6.61 | 110.73      | 122.42   |
| 7   | AG    | 533 | THR  | C-N-CA | -6.61 | 110.73      | 122.42   |
| 7   | J     | 533 | THR  | CA-C-N | -6.60 | 111.01      | 122.36   |
| 7   | J     | 533 | THR  | C-N-CA | -6.60 | 111.01      | 122.36   |
| 2   | f     | 91  | ILE  | N-CA-C | -6.60 | 104.06      | 110.72   |
| 5   | L     | 642 | ILE  | N-CA-C | 6.59  | 118.19      | 111.00   |
| 5   | AE    | 585 | SER  | N-CA-C | -6.59 | 105.05      | 113.23   |
| 5   | Bf    | 646 | ASN  | CA-C-N | 6.59  | 126.22      | 119.56   |
| 5   | Bf    | 646 | ASN  | C-N-CA | 6.59  | 126.22      | 119.56   |
| 3   | I     | 459 | LEU  | CA-C-N | 6.58  | 126.29      | 119.64   |
| 3   | I     | 459 | LEU  | C-N-CA | 6.58  | 126.29      | 119.64   |
| 1   | CP    | 155 | ASP  | CA-C-O | -6.58 | 113.90      | 121.54   |
| 16  | Ai    | 57  | ARG  | N-CA-C | 6.58  | 120.25      | 109.72   |
| 1   | BD    | 417 | LYS  | N-CA-C | -6.58 | 105.88      | 114.04   |
| 2   | q     | 82  | ARG  | CA-C-O | -6.58 | 111.97      | 120.00   |
| 3   | BY    | 459 | LEU  | CA-C-N | 6.58  | 127.14      | 120.04   |
| 3   | BY    | 459 | LEU  | C-N-CA | 6.58  | 127.14      | 120.04   |
| 3   | n     | 663 | GLN  | N-CA-C | -6.58 | 103.94      | 112.23   |
| 5   | 9     | 463 | GLY  | N-CA-C | 6.57  | 120.35      | 110.75   |
| 7   | Bm    | 238 | PHE  | N-CA-C | 6.57  | 120.23      | 109.72   |
| 7   | Bm    | 541 | GLN  | CA-C-N | -6.57 | 111.70      | 122.54   |
| 7   | Bm    | 541 | GLN  | C-N-CA | -6.57 | 111.70      | 122.54   |
| 2   | BR    | 53  | LYS  | CA-C-O | -6.57 | 113.54      | 120.63   |
| 7   | AM    | 533 | THR  | CA-C-N | -6.56 | 110.81      | 122.42   |
| 7   | AM    | 533 | THR  | C-N-CA | -6.56 | 110.81      | 122.42   |
| 7   | Bm    | 187 | LEU  | N-CA-C | 6.56  | 120.21      | 109.72   |
| 2   | f     | 53  | LYS  | CA-C-O | -6.55 | 113.60      | 120.55   |
| 5   | v     | 483 | TYR  | CA-C-O | -6.55 | 114.15      | 120.90   |
| 1   | i     | 415 | ASN  | N-CA-C | -6.55 | 96.96       | 108.23   |
| 2   | s     | 37  | LYS  | CA-C-O | -6.55 | 112.14      | 119.67   |
| 7   | 4     | 126 | ILE  | N-CA-C | 6.55  | 117.56      | 107.99   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AO    | 39  | SER  | N-CA-C  | 6.55  | 119.18      | 110.53   |
| 5   | AE    | 483 | TYR  | CA-C-O  | -6.55 | 114.16      | 120.90   |
| 16  | Az    | 56  | GLU  | N-CA-C  | 6.55  | 120.53      | 112.54   |
| 5   | 9     | 585 | SER  | N-CA-C  | -6.54 | 105.45      | 113.50   |
| 2   | Ch    | 237 | GLN  | CA-C-O  | -6.54 | 112.45      | 119.97   |
| 5   | G     | 493 | LEU  | N-CA-C  | -6.53 | 104.00      | 112.23   |
| 5   | L     | 493 | LEU  | N-CA-C  | -6.53 | 104.00      | 112.23   |
| 1   | i     | 214 | ILE  | N-CA-C  | -6.53 | 105.46      | 111.67   |
| 7   | 4     | 130 | HIS  | N-CA-C  | 6.53  | 115.02      | 108.75   |
| 7   | AG    | 55  | PHE  | N-CA-C  | 6.53  | 120.15      | 109.24   |
| 16  | Ai    | 119 | ARG  | N-CA-C  | -6.53 | 104.92      | 114.39   |
| 5   | 9     | 611 | PRO  | N-CA-C  | 6.53  | 123.89      | 113.12   |
| 7   | AM    | 190 | SER  | N-CA-C  | 6.53  | 118.99      | 109.07   |
| 16  | CI    | 39  | HIS  | N-CA-C  | -6.53 | 97.88       | 108.52   |
| 7   | J     | 522 | PHE  | CA-C-O  | -6.53 | 113.00      | 120.24   |
| 7   | Bm    | 202 | LEU  | CA-C-N  | -6.53 | 110.41      | 122.09   |
| 7   | Bm    | 202 | LEU  | C-N-CA  | -6.53 | 110.41      | 122.09   |
| 5   | AO    | 304 | ASN  | N-CA-C  | -6.52 | 104.58      | 112.54   |
| 5   | 9     | 465 | TYR  | CA-C-N  | 6.52  | 126.21      | 119.82   |
| 5   | 9     | 465 | TYR  | C-N-CA  | 6.52  | 126.21      | 119.82   |
| 1   | Ca    | 240 | ILE  | CB-CA-C | -6.52 | 102.05      | 110.98   |
| 7   | Bm    | 113 | ILE  | CA-C-N  | -6.52 | 113.00      | 122.19   |
| 7   | Bm    | 113 | ILE  | C-N-CA  | -6.52 | 113.00      | 122.19   |
| 16  | CB    | 131 | VAL  | N-CA-C  | -6.52 | 101.16      | 109.30   |
| 5   | AO    | 293 | PRO  | N-CA-C  | 6.51  | 123.25      | 113.81   |
| 5   | 9     | 432 | LYS  | CA-C-N  | -6.51 | 116.35      | 122.66   |
| 5   | 9     | 432 | LYS  | C-N-CA  | -6.51 | 116.35      | 122.66   |
| 16  | Az    | 172 | ASP  | CA-C-N  | 6.51  | 131.29      | 120.62   |
| 16  | Az    | 172 | ASP  | C-N-CA  | 6.51  | 131.29      | 120.62   |
| 3   | I     | 112 | ILE  | CB-CA-C | -6.50 | 104.52      | 110.63   |
| 16  | Ai    | 56  | GLU  | N-CA-C  | 6.50  | 120.47      | 112.54   |
| 16  | An    | 56  | GLU  | N-CA-C  | 6.50  | 118.45      | 111.36   |
| 7   | Bm    | 47  | GLU  | N-CA-C  | 6.50  | 119.36      | 111.82   |
| 5   | G     | 669 | ILE  | N-CA-C  | 6.50  | 117.27      | 108.17   |
| 5   | AU    | 261 | ASN  | N-CA-C  | -6.50 | 104.92      | 112.92   |
| 5   | Bf    | 767 | LYS  | N-CA-C  | -6.50 | 104.23      | 111.71   |
| 5   | G     | 767 | LYS  | N-CA-C  | -6.50 | 104.24      | 111.71   |
| 5   | L     | 927 | MET  | N-CA-C  | -6.50 | 104.04      | 112.23   |
| 3   | I     | 703 | TYR  | CA-C-N  | 6.50  | 127.96      | 119.84   |
| 3   | I     | 703 | TYR  | C-N-CA  | 6.50  | 127.96      | 119.84   |
| 2   | z     | 239 | GLN  | CA-C-O  | -6.49 | 112.76      | 120.10   |
| 7   | J     | 182 | SER  | CA-C-N  | 6.49  | 126.41      | 119.85   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | J     | 182 | SER  | C-N-CA  | 6.49  | 126.41      | 119.85   |
| 2   | f     | 137 | ASN  | N-CA-C  | -6.49 | 104.29      | 111.36   |
| 7   | 4     | 98  | SER  | CA-C-N  | 6.49  | 127.95      | 119.84   |
| 7   | 4     | 98  | SER  | C-N-CA  | 6.49  | 127.95      | 119.84   |
| 2   | BR    | 95  | SER  | N-CA-C  | -6.48 | 104.06      | 112.23   |
| 5   | 9     | 503 | SER  | CA-C-O  | -6.48 | 113.90      | 121.16   |
| 2   | BR    | 239 | GLN  | CA-C-O  | -6.48 | 112.78      | 120.10   |
| 2   | k     | 318 | ILE  | CA-C-O  | -6.48 | 113.25      | 120.96   |
| 3   | n     | 709 | ASP  | N-CA-C  | 6.48  | 124.60      | 110.80   |
| 1   | i     | 126 | GLN  | N-CA-C  | 6.48  | 119.69      | 109.39   |
| 2   | y     | 239 | GLN  | CA-C-O  | -6.48 | 112.78      | 120.10   |
| 5   | v     | 504 | ASP  | N-CA-C  | -6.47 | 104.42      | 112.90   |
| 3   | 7     | 236 | GLY  | N-CA-C  | -6.47 | 101.31      | 112.06   |
| 5   | AU    | 293 | PRO  | N-CA-C  | 6.47  | 123.20      | 113.81   |
| 5   | Bf    | 584 | LEU  | CA-C-O  | -6.47 | 114.09      | 120.89   |
| 2   | BR    | 137 | ASN  | N-CA-C  | -6.47 | 103.73      | 111.69   |
| 3   | n     | 632 | ALA  | N-CA-C  | -6.47 | 104.31      | 111.82   |
| 5   | AB    | 121 | ASN  | CA-C-N  | 6.47  | 126.60      | 119.87   |
| 5   | AB    | 121 | ASN  | C-N-CA  | 6.47  | 126.60      | 119.87   |
| 3   | BY    | 114 | SER  | N-CA-C  | -6.47 | 104.53      | 112.88   |
| 5   | R     | 351 | PHE  | N-CA-C  | 6.47  | 118.99      | 108.26   |
| 5   | L     | 611 | PRO  | CA-C-O  | -6.46 | 116.40      | 121.38   |
| 5   | 9     | 519 | GLN  | N-CA-C  | 6.46  | 121.31      | 113.17   |
| 5   | AU    | 121 | ASN  | CA-C-N  | 6.46  | 126.59      | 119.87   |
| 5   | AU    | 121 | ASN  | C-N-CA  | 6.46  | 126.59      | 119.87   |
| 5   | Bt    | 4   | ILE  | N-CA-C  | 6.46  | 116.93      | 107.37   |
| 16  | An    | 35  | TYR  | CA-C-O  | -6.46 | 111.27      | 120.51   |
| 2   | BK    | 73  | LEU  | N-CA-C  | -6.46 | 104.09      | 112.23   |
| 7   | 4     | 542 | GLN  | N-CA-C  | -6.46 | 105.03      | 113.17   |
| 16  | A7    | 108 | LEU  | CB-CA-C | -6.46 | 102.09      | 111.91   |
| 5   | L     | 876 | GLN  | N-CA-C  | -6.46 | 104.44      | 112.90   |
| 2   | k     | 34  | LEU  | N-CA-CB | -6.45 | 101.06      | 110.47   |
| 5   | Bf    | 463 | GLY  | N-CA-C  | 6.45  | 120.16      | 110.75   |
| 16  | CT    | 90  | SER  | N-CA-C  | 6.44  | 124.53      | 110.80   |
| 5   | M     | 274 | ILE  | N-CA-C  | 6.44  | 118.07      | 108.54   |
| 5   | Bt    | 267 | ILE  | N-CA-C  | 6.44  | 117.12      | 108.11   |
| 7   | AM    | 278 | ILE  | N-CA-C  | 6.43  | 118.41      | 108.44   |
| 5   | Bt    | 59  | VAL  | O-C-N   | -6.43 | 116.38      | 123.20   |
| 5   | L     | 455 | ASN  | N-CA-C  | 6.43  | 119.28      | 111.82   |
| 7   | AM    | 68  | ASP  | N-CA-C  | 6.43  | 118.13      | 107.20   |
| 16  | Av    | 90  | SER  | N-CA-C  | 6.43  | 124.49      | 110.80   |
| 5   | M     | 346 | ASN  | N-CA-C  | 6.43  | 120.22      | 112.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AB    | 124 | THR  | CA-C-O  | -6.43 | 111.83      | 118.90   |
| 16  | A7    | 155 | ILE  | N-CA-C  | 6.42  | 118.64      | 108.87   |
| 5   | Bt    | 351 | PHE  | N-CA-C  | 6.42  | 118.92      | 108.26   |
| 7   | O     | 39  | LEU  | N-CA-C  | -6.42 | 100.53      | 110.10   |
| 7   | O     | 541 | GLN  | CA-C-N  | -6.42 | 111.95      | 122.54   |
| 7   | O     | 541 | GLN  | C-N-CA  | -6.42 | 111.95      | 122.54   |
| 1   | CP    | 398 | LEU  | N-CA-C  | -6.42 | 102.05      | 110.39   |
| 3   | I     | 662 | ILE  | CA-C-O  | -6.41 | 114.05      | 120.85   |
| 5   | L     | 761 | LYS  | N-CA-C  | -6.41 | 105.42      | 113.18   |
| 3   | 1     | 51  | ASP  | N-CA-C  | 6.41  | 119.20      | 110.55   |
| 5   | G     | 733 | GLU  | CA-C-O  | -6.41 | 113.76      | 120.55   |
| 3   | I     | 445 | PRO  | CA-C-O  | -6.41 | 113.85      | 121.67   |
| 5   | G     | 434 | TYR  | CA-C-N  | 6.41  | 126.75      | 119.83   |
| 5   | G     | 434 | TYR  | C-N-CA  | 6.41  | 126.75      | 119.83   |
| 5   | M     | 316 | PHE  | N-CA-C  | -6.41 | 104.22      | 111.14   |
| 5   | v     | 551 | LEU  | N-CA-C  | -6.40 | 104.30      | 111.28   |
| 3   | 1     | 36  | LYS  | CA-C-O  | -6.40 | 112.61      | 119.97   |
| 7   | Bm    | 553 | TYR  | N-CA-C  | -6.40 | 105.12      | 113.12   |
| 5   | AE    | 927 | MET  | CA-C-O  | -6.40 | 111.51      | 119.38   |
| 5   | AO    | 223 | CYS  | N-CA-C  | 6.40  | 120.47      | 110.17   |
| 5   | AO    | 4   | ILE  | N-CA-C  | 6.39  | 117.32      | 107.99   |
| 2   | q     | 13  | LEU  | N-CA-C  | -6.39 | 104.18      | 112.23   |
| 16  | CI    | 31  | LYS  | N-CA-C  | -6.39 | 106.02      | 113.88   |
| 5   | L     | 690 | TYR  | N-CA-C  | 6.39  | 121.95      | 112.94   |
| 16  | Av    | 127 | LYS  | O-C-N   | -6.39 | 115.57      | 122.85   |
| 1   | CP    | 100 | ALA  | CA-C-N  | 6.39  | 127.83      | 119.84   |
| 1   | CP    | 100 | ALA  | C-N-CA  | 6.39  | 127.83      | 119.84   |
| 5   | AB    | 31  | ASN  | CA-C-O  | -6.39 | 115.03      | 122.37   |
| 5   | Bt    | 40  | ASP  | CA-C-N  | 6.39  | 126.07      | 119.56   |
| 5   | Bt    | 40  | ASP  | C-N-CA  | 6.39  | 126.07      | 119.56   |
| 1   | CP    | 218 | GLN  | CA-C-N  | 6.38  | 126.57      | 120.31   |
| 1   | CP    | 218 | GLN  | C-N-CA  | 6.38  | 126.57      | 120.31   |
| 3   | I     | 331 | ILE  | CB-CA-C | -6.38 | 103.80      | 111.97   |
| 5   | AB    | 163 | PRO  | N-CA-C  | 6.38  | 125.62      | 112.47   |
| 16  | CT    | 54  | PRO  | N-CA-C  | -6.38 | 100.86      | 111.26   |
| 5   | v     | 664 | THR  | CA-C-N  | 6.38  | 126.35      | 119.78   |
| 5   | v     | 664 | THR  | C-N-CA  | 6.38  | 126.35      | 119.78   |
| 1   | Ca    | 70  | SER  | N-CA-C  | -6.38 | 104.94      | 114.64   |
| 5   | Bf    | 858 | MET  | CA-C-O  | -6.38 | 112.27      | 119.79   |
| 2   | Cd    | 37  | LYS  | CA-C-O  | -6.38 | 113.66      | 120.42   |
| 5   | AE    | 858 | MET  | N-CA-C  | -6.37 | 104.20      | 112.23   |
| 5   | Bt    | 253 | ASN  | CA-C-O  | -6.37 | 112.88      | 122.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | E     | 598 | VAL  | N-CA-C  | 6.37  | 122.59      | 109.34   |
| 7   | O     | 294 | SER  | CA-C-O  | -6.37 | 112.89      | 122.38   |
| 16  | c     | 155 | ILE  | N-CA-C  | 6.37  | 117.09      | 108.17   |
| 5   | AO    | 328 | GLU  | N-CA-C  | -6.37 | 105.47      | 113.18   |
| 16  | Ai    | 139 | LYS  | CA-C-N  | -6.37 | 113.21      | 122.44   |
| 16  | Ai    | 139 | LYS  | C-N-CA  | -6.37 | 113.21      | 122.44   |
| 5   | M     | 59  | VAL  | O-C-N   | -6.36 | 116.46      | 123.20   |
| 7   | AM    | 120 | VAL  | N-CA-C  | 6.36  | 117.98      | 108.96   |
| 2   | z     | 91  | ILE  | N-CA-C  | -6.36 | 104.30      | 110.72   |
| 5   | G     | 465 | TYR  | CA-C-N  | 6.35  | 126.04      | 119.56   |
| 5   | G     | 465 | TYR  | C-N-CA  | 6.35  | 126.04      | 119.56   |
| 16  | Z     | 125 | ALA  | CA-C-O  | -6.35 | 113.81      | 120.55   |
| 16  | CB    | 125 | ALA  | CA-C-O  | -6.35 | 113.82      | 120.55   |
| 3   | n     | 125 | THR  | N-CA-C  | -6.35 | 99.76       | 109.41   |
| 7   | 4     | 70  | ILE  | N-CA-C  | 6.35  | 117.92      | 108.46   |
| 2   | y     | 91  | ILE  | N-CA-C  | -6.35 | 104.31      | 110.72   |
| 7   | AM    | 306 | GLN  | N-CA-C  | -6.35 | 100.44      | 109.96   |
| 2   | D     | 85  | ASN  | N-CA-C  | -6.35 | 105.02      | 112.89   |
| 5   | 9     | 483 | TYR  | CA-C-O  | -6.34 | 114.14      | 120.80   |
| 3   | BY    | 507 | CYS  | CA-C-N  | 6.34  | 127.77      | 119.84   |
| 3   | BY    | 507 | CYS  | C-N-CA  | 6.34  | 127.77      | 119.84   |
| 2   | q     | 34  | LEU  | N-CA-C  | -6.34 | 104.29      | 111.14   |
| 16  | An    | 71  | SER  | N-CA-C  | -6.34 | 104.45      | 111.36   |
| 16  | Az    | 53  | ALA  | CA-C-N  | 6.34  | 126.30      | 120.03   |
| 16  | Az    | 53  | ALA  | C-N-CA  | 6.34  | 126.30      | 120.03   |
| 3   | 7     | 112 | ILE  | CB-CA-C | -6.33 | 104.68      | 110.63   |
| 3   | n     | 327 | PHE  | N-CA-C  | -6.33 | 103.65      | 112.45   |
| 7   | AG    | 187 | LEU  | N-CA-C  | 6.33  | 120.02      | 109.95   |
| 16  | CB    | 55  | ILE  | N-CA-C  | 6.33  | 119.87      | 113.47   |
| 1   | Ca    | 264 | LYS  | CB-CA-C | -6.33 | 109.26      | 116.54   |
| 5   | M     | 280 | LEU  | N-CA-C  | 6.33  | 120.45      | 109.82   |
| 5   | AU    | 320 | MET  | N-CA-C  | -6.33 | 97.32       | 110.80   |
| 16  | Ai    | 146 | GLN  | CA-C-O  | -6.33 | 113.80      | 120.63   |
| 3   | 7     | 507 | CYS  | CA-C-N  | 6.32  | 127.74      | 119.84   |
| 3   | 7     | 507 | CYS  | C-N-CA  | 6.32  | 127.74      | 119.84   |
| 1   | C     | 415 | ASN  | N-CA-C  | -6.32 | 97.36       | 108.23   |
| 3   | 1     | 459 | LEU  | CA-C-N  | 6.32  | 126.02      | 119.64   |
| 3   | 1     | 459 | LEU  | C-N-CA  | 6.32  | 126.02      | 119.64   |
| 5   | AU    | 31  | ASN  | CA-C-O  | -6.32 | 115.11      | 122.37   |
| 5   | Bf    | 750 | ARG  | N-CA-C  | -6.32 | 104.62      | 112.90   |
| 5   | Bt    | 274 | ILE  | N-CA-C  | 6.32  | 116.34      | 107.37   |
| 16  | An    | 125 | ALA  | CA-C-O  | -6.31 | 113.86      | 120.55   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 1     | 666 | LEU  | CA-C-O  | -6.31 | 113.73      | 120.42   |
| 2   | BK    | 298 | ILE  | N-CA-C  | -6.31 | 104.35      | 110.72   |
| 7   | AG    | 81  | ARG  | CA-C-N  | 6.31  | 126.22      | 119.85   |
| 7   | AG    | 81  | ARG  | C-N-CA  | 6.31  | 126.22      | 119.85   |
| 5   | M     | 328 | GLU  | N-CA-C  | -6.30 | 105.56      | 113.18   |
| 5   | M     | 337 | TYR  | CA-C-O  | -6.30 | 112.36      | 119.79   |
| 7   | 4     | 506 | GLN  | CA-C-N  | 6.30  | 126.78      | 119.47   |
| 7   | 4     | 506 | GLN  | C-N-CA  | 6.30  | 126.78      | 119.47   |
| 7   | AG    | 120 | VAL  | N-CA-C  | 6.30  | 117.90      | 108.96   |
| 5   | AU    | 162 | THR  | CA-C-N  | 6.30  | 127.71      | 119.84   |
| 5   | AU    | 162 | THR  | C-N-CA  | 6.30  | 127.71      | 119.84   |
| 7   | J     | 81  | ARG  | CA-C-N  | 6.29  | 126.21      | 119.85   |
| 7   | J     | 81  | ARG  | C-N-CA  | 6.29  | 126.21      | 119.85   |
| 16  | Ai    | 168 | ILE  | CB-CA-C | -6.29 | 105.10      | 111.08   |
| 5   | G     | 576 | PHE  | CB-CA-C | -6.29 | 97.90       | 110.42   |
| 5   | M     | 40  | ASP  | CA-C-N  | 6.29  | 125.98      | 119.56   |
| 5   | M     | 40  | ASP  | C-N-CA  | 6.29  | 125.98      | 119.56   |
| 2   | BK    | 25  | GLN  | N-CA-C  | 6.29  | 118.67      | 109.30   |
| 3   | I     | 922 | GLN  | N-CA-C  | -6.29 | 104.67      | 112.90   |
| 5   | L     | 611 | PRO  | N-CA-C  | 6.29  | 123.49      | 113.12   |
| 5   | AU    | 274 | ILE  | N-CA-C  | 6.29  | 117.85      | 108.23   |
| 1   | i     | 218 | GLN  | CA-C-N  | 6.28  | 126.47      | 120.31   |
| 1   | i     | 218 | GLN  | C-N-CA  | 6.28  | 126.47      | 120.31   |
| 3   | 1     | 529 | THR  | N-CA-C  | -6.28 | 104.49      | 111.71   |
| 5   | AU    | 212 | VAL  | N-CA-C  | 6.28  | 117.81      | 108.46   |
| 2   | z     | 73  | LEU  | N-CA-C  | -6.28 | 104.68      | 112.90   |
| 3   | 7     | 809 | ASN  | N-CA-C  | -6.27 | 104.68      | 112.90   |
| 7   | Bm    | 68  | ASP  | N-CA-C  | 6.27  | 117.86      | 107.20   |
| 7   | AG    | 192 | SER  | N-CA-C  | 6.27  | 117.75      | 108.60   |
| 3   | 7     | 805 | GLN  | N-CA-C  | -6.26 | 104.90      | 112.54   |
| 7   | Bm    | 70  | ILE  | N-CA-C  | 6.26  | 117.72      | 108.45   |
| 16  | An    | 35  | TYR  | O-C-N   | -6.26 | 114.26      | 122.59   |
| 5   | AE    | 519 | GLN  | N-CA-C  | 6.26  | 121.08      | 113.38   |
| 5   | M     | 75  | THR  | N-CA-C  | -6.25 | 104.71      | 112.90   |
| 7   | 4     | 81  | ARG  | CA-C-N  | 6.25  | 126.17      | 119.85   |
| 7   | 4     | 81  | ARG  | C-N-CA  | 6.25  | 126.17      | 119.85   |
| 2   | y     | 73  | LEU  | N-CA-C  | -6.25 | 104.71      | 112.90   |
| 2   | y     | 258 | LYS  | N-CA-C  | -6.25 | 104.47      | 111.28   |
| 5   | AO    | 171 | SER  | N-CA-C  | 6.25  | 119.44      | 108.75   |
| 1   | BD    | 95  | LEU  | N-CA-C  | -6.25 | 104.55      | 111.36   |
| 3   | 1     | 445 | PRO  | CA-C-O  | -6.25 | 114.08      | 122.08   |
| 5   | AU    | 75  | THR  | N-CA-C  | -6.25 | 103.77      | 112.45   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | AG    | 38  | ALA  | N-CA-C | 6.25  | 119.86      | 111.24   |
| 5   | R     | 31  | ASN  | CA-C-O | -6.24 | 115.19      | 122.37   |
| 7   | J     | 68  | ASP  | N-CA-C | 6.24  | 117.65      | 107.23   |
| 3   | 1     | 236 | GLY  | N-CA-C | -6.24 | 101.71      | 112.06   |
| 5   | v     | 609 | ASP  | N-CA-C | -6.24 | 104.30      | 112.41   |
| 5   | Bt    | 163 | PRO  | N-CA-C | 6.24  | 121.65      | 113.86   |
| 3   | n     | 445 | PRO  | CA-C-O | -6.23 | 113.52      | 122.31   |
| 7   | AG    | 98  | SER  | CA-C-N | 6.23  | 125.92      | 119.56   |
| 7   | AG    | 98  | SER  | C-N-CA | 6.23  | 125.92      | 119.56   |
| 7   | AG    | 306 | GLN  | N-CA-C | -6.23 | 101.71      | 110.50   |
| 5   | AE    | 609 | ASP  | N-CA-C | -6.23 | 103.08      | 111.87   |
| 7   | AM    | 144 | GLY  | N-CA-C | -6.23 | 105.08      | 113.24   |
| 1   | BD    | 203 | LYS  | N-CA-C | 6.23  | 118.89      | 109.23   |
| 5   | R     | 44  | HIS  | N-CA-C | 6.23  | 118.15      | 111.36   |
| 16  | An    | 171 | PHE  | CA-C-N | 6.23  | 132.91      | 121.70   |
| 16  | An    | 171 | PHE  | C-N-CA | 6.23  | 132.91      | 121.70   |
| 5   | Bt    | 327 | LEU  | N-CA-C | -6.23 | 104.38      | 112.23   |
| 1   | C     | 218 | GLN  | CA-C-N | 6.22  | 126.41      | 120.31   |
| 1   | C     | 218 | GLN  | C-N-CA | 6.22  | 126.41      | 120.31   |
| 3   | I     | 680 | ILE  | N-CA-C | 6.22  | 114.05      | 107.76   |
| 7   | Bm    | 143 | GLY  | N-CA-C | 6.22  | 124.81      | 114.48   |
| 2   | k     | 12  | LEU  | CA-C-O | -6.22 | 113.95      | 120.55   |
| 5   | AU    | 59  | VAL  | CA-C-O | -6.22 | 113.87      | 120.53   |
| 5   | M     | 252 | GLY  | CA-C-N | -6.22 | 112.85      | 122.05   |
| 5   | M     | 252 | GLY  | C-N-CA | -6.22 | 112.85      | 122.05   |
| 3   | n     | 703 | TYR  | CA-C-N | 6.22  | 127.61      | 119.84   |
| 3   | n     | 703 | TYR  | C-N-CA | 6.22  | 127.61      | 119.84   |
| 7   | AM    | 182 | SER  | CA-C-N | 6.22  | 126.13      | 119.85   |
| 7   | AM    | 182 | SER  | C-N-CA | 6.22  | 126.13      | 119.85   |
| 2   | z     | 258 | LYS  | N-CA-C | -6.21 | 104.51      | 111.28   |
| 7   | O     | 524 | PRO  | N-CA-C | -6.21 | 101.71      | 111.34   |
| 3   | n     | 459 | LEU  | CA-C-N | 6.21  | 126.75      | 120.04   |
| 3   | n     | 459 | LEU  | C-N-CA | 6.21  | 126.75      | 120.04   |
| 3   | I     | 327 | PHE  | N-CA-C | -6.21 | 103.81      | 112.45   |
| 7   | J     | 39  | LEU  | N-CA-C | -6.21 | 100.84      | 110.10   |
| 7   | J     | 70  | ILE  | N-CA-C | 6.21  | 117.64      | 108.45   |
| 3   | 1     | 291 | LEU  | N-CA-C | 6.21  | 119.36      | 108.75   |
| 5   | L     | 506 | PHE  | N-CA-C | -6.20 | 105.85      | 113.41   |
| 7   | 4     | 533 | THR  | CA-C-O | -6.20 | 114.52      | 120.90   |
| 3   | n     | 114 | SER  | N-CA-C | -6.20 | 104.89      | 112.88   |
| 5   | AO    | 147 | LYS  | N-CA-C | 6.20  | 117.96      | 108.42   |
| 3   | E     | 610 | LEU  | N-CA-C | -6.19 | 104.99      | 112.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 503 | SER  | CA-C-O  | -6.19 | 114.16      | 121.16   |
| 3   | 1     | 609 | TRP  | CA-C-O  | -6.18 | 111.01      | 119.05   |
| 1   | BD    | 126 | GLN  | N-CA-C  | 6.18  | 119.28      | 108.52   |
| 5   | Bf    | 611 | PRO  | N-CA-C  | 6.18  | 125.21      | 112.47   |
| 5   | Bt    | 286 | ILE  | N-CA-CB | 6.18  | 118.42      | 110.13   |
| 1   | Ca    | 95  | LEU  | N-CA-C  | -6.18 | 104.62      | 111.36   |
| 1   | BD    | 218 | GLN  | CA-C-N  | 6.18  | 126.37      | 120.31   |
| 1   | BD    | 218 | GLN  | C-N-CA  | 6.18  | 126.37      | 120.31   |
| 3   | E     | 327 | PHE  | N-CA-C  | -6.17 | 103.87      | 112.45   |
| 5   | M     | 31  | ASN  | CA-C-O  | -6.17 | 115.27      | 122.37   |
| 3   | 7     | 697 | TYR  | CA-C-N  | 6.17  | 126.14      | 120.03   |
| 3   | 7     | 697 | TYR  | C-N-CA  | 6.17  | 126.14      | 120.03   |
| 1   | BD    | 288 | HIS  | CA-C-O  | 6.17  | 121.52      | 117.94   |
| 2   | y     | 25  | GLN  | CA-C-N  | 6.17  | 126.08      | 119.85   |
| 2   | y     | 25  | GLN  | C-N-CA  | 6.17  | 126.08      | 119.85   |
| 3   | 1     | 680 | ILE  | N-CA-C  | 6.17  | 113.99      | 107.76   |
| 3   | BY    | 117 | LEU  | N-CA-C  | -6.17 | 97.13       | 107.99   |
| 16  | Ai    | 142 | ASN  | N-CA-CB | 6.17  | 120.98      | 110.50   |
| 2   | z     | 25  | GLN  | CA-C-N  | 6.17  | 126.08      | 119.85   |
| 2   | z     | 25  | GLN  | C-N-CA  | 6.17  | 126.08      | 119.85   |
| 5   | AU    | 134 | GLN  | N-CA-C  | 6.17  | 118.55      | 109.24   |
| 5   | AU    | 303 | GLY  | N-CA-C  | -6.17 | 107.24      | 115.32   |
| 16  | CM    | 61  | VAL  | CB-CA-C | -6.17 | 104.53      | 111.80   |
| 3   | 7     | 152 | ASN  | CA-C-N  | 6.16  | 128.90      | 120.46   |
| 3   | 7     | 152 | ASN  | C-N-CA  | 6.16  | 128.90      | 120.46   |
| 2   | k     | 82  | ARG  | CA-C-O  | -6.16 | 112.28      | 119.24   |
| 5   | Bf    | 762 | LEU  | N-CA-C  | -6.16 | 105.25      | 112.89   |
| 3   | 7     | 880 | LEU  | CA-C-O  | -6.16 | 113.89      | 120.42   |
| 5   | AO    | 75  | THR  | N-CA-C  | -6.16 | 104.12      | 111.69   |
| 1   | CP    | 203 | LYS  | N-CA-C  | 6.16  | 119.23      | 109.50   |
| 7   | 4     | 255 | LYS  | CA-C-N  | -6.16 | 115.11      | 123.12   |
| 7   | 4     | 255 | LYS  | C-N-CA  | -6.16 | 115.11      | 123.12   |
| 3   | BY    | 837 | MET  | CA-C-O  | -6.16 | 114.69      | 121.28   |
| 3   | n     | 93  | LYS  | CA-C-N  | 6.15  | 125.84      | 119.56   |
| 3   | n     | 93  | LYS  | C-N-CA  | 6.15  | 125.84      | 119.56   |
| 5   | G     | 577 | VAL  | CA-C-N  | 6.15  | 128.84      | 120.54   |
| 5   | G     | 577 | VAL  | C-N-CA  | 6.15  | 128.84      | 120.54   |
| 7   | J     | 541 | GLN  | CA-C-N  | -6.15 | 112.39      | 122.54   |
| 7   | J     | 541 | GLN  | C-N-CA  | -6.15 | 112.39      | 122.54   |
| 2   | s     | 315 | MET  | N-CA-C  | -6.15 | 105.60      | 113.23   |
| 2   | s     | 32  | ALA  | CA-C-O  | -6.15 | 113.99      | 120.63   |
| 7   | 4     | 169 | PHE  | N-CA-C  | 6.15  | 118.51      | 108.55   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AO    | 298 | ILE  | N-CA-C  | 6.15  | 116.72      | 108.11   |
| 7   | AG    | 150 | SER  | N-CA-C  | 6.15  | 119.62      | 110.52   |
| 16  | CM    | 71  | SER  | N-CA-C  | -6.15 | 104.66      | 111.36   |
| 2   | q     | 246 | GLN  | CA-C-N  | 6.14  | 132.76      | 121.70   |
| 2   | q     | 246 | GLN  | C-N-CA  | 6.14  | 132.76      | 121.70   |
| 5   | 9     | 456 | PHE  | N-CA-C  | -6.14 | 104.67      | 111.36   |
| 2   | s     | 83  | GLU  | N-CA-C  | -6.14 | 104.59      | 111.28   |
| 3   | 7     | 133 | VAL  | N-CA-C  | 6.14  | 116.96      | 108.12   |
| 3   | 7     | 64  | GLY  | N-CA-C  | -6.14 | 106.85      | 115.32   |
| 2   | s     | 310 | LYS  | N-CA-C  | -6.13 | 105.08      | 113.30   |
| 2   | BK    | 13  | LEU  | N-CA-C  | -6.13 | 105.62      | 113.23   |
| 5   | Bt    | 295 | ASN  | N-CA-C  | -6.13 | 105.08      | 114.16   |
| 7   | J     | 98  | SER  | N-CA-C  | -6.13 | 101.32      | 109.84   |
| 7   | AM    | 47  | GLU  | N-CA-C  | 6.13  | 117.96      | 111.28   |
| 16  | CB    | 119 | ARG  | N-CA-C  | -6.13 | 105.50      | 114.39   |
| 16  | CT    | 155 | ILE  | N-CA-C  | 6.13  | 118.19      | 108.87   |
| 1   | A     | 371 | HIS  | N-CA-C  | -6.12 | 101.87      | 110.50   |
| 7   | J     | 202 | LEU  | CA-C-O  | -6.12 | 112.93      | 119.97   |
| 1   | Ca    | 218 | GLN  | CA-C-N  | 6.12  | 126.31      | 120.31   |
| 1   | Ca    | 218 | GLN  | C-N-CA  | 6.12  | 126.31      | 120.31   |
| 5   | AO    | 164 | ASN  | CA-C-N  | 6.12  | 129.07      | 120.57   |
| 5   | AO    | 164 | ASN  | C-N-CA  | 6.12  | 129.07      | 120.57   |
| 2   | Ch    | 158 | LYS  | N-CA-C  | -6.12 | 103.94      | 111.40   |
| 3   | E     | 251 | LEU  | CA-C-N  | 6.11  | 126.08      | 120.03   |
| 3   | E     | 251 | LEU  | C-N-CA  | 6.11  | 126.08      | 120.03   |
| 3   | 7     | 327 | PHE  | N-CA-C  | -6.11 | 103.95      | 112.45   |
| 3   | n     | 480 | ASN  | N-CA-CB | 6.11  | 120.89      | 110.50   |
| 5   | AB    | 59  | VAL  | O-C-N   | -6.11 | 116.45      | 122.99   |
| 5   | AO    | 257 | ILE  | N-CA-C  | 6.11  | 116.67      | 108.11   |
| 5   | AB    | 102 | GLY  | N-CA-C  | -6.11 | 104.34      | 114.48   |
| 5   | Bf    | 503 | SER  | O-C-N   | -6.11 | 116.06      | 122.96   |
| 3   | n     | 444 | PHE  | CA-C-N  | 6.11  | 126.07      | 120.21   |
| 3   | n     | 444 | PHE  | C-N-CA  | 6.11  | 126.07      | 120.21   |
| 5   | G     | 597 | TRP  | N-CA-C  | -6.10 | 104.74      | 111.82   |
| 5   | AU    | 124 | THR  | CA-C-O  | -6.10 | 112.19      | 118.90   |
| 16  | CT    | 132 | GLN  | CA-C-O  | -6.10 | 111.78      | 120.51   |
| 16  | c     | 109 | ARG  | N-CA-C  | 6.10  | 118.69      | 109.23   |
| 3   | n     | 676 | THR  | CA-C-N  | 6.10  | 124.05      | 119.66   |
| 3   | n     | 676 | THR  | C-N-CA  | 6.10  | 124.05      | 119.66   |
| 3   | 1     | 152 | ASN  | CA-C-N  | 6.10  | 129.13      | 120.53   |
| 3   | 1     | 152 | ASN  | C-N-CA  | 6.10  | 129.13      | 120.53   |
| 7   | 4     | 510 | VAL  | N-CA-C  | -6.10 | 105.12      | 111.58   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | I     | 834 | ALA  | N-CA-C  | -6.10 | 104.55      | 112.23   |
| 2   | k     | 274 | ARG  | N-CA-C  | -6.10 | 104.75      | 111.82   |
| 2   | f     | 290 | ASN  | CA-C-N  | 6.09  | 132.66      | 121.70   |
| 2   | f     | 290 | ASN  | C-N-CA  | 6.09  | 132.66      | 121.70   |
| 2   | s     | 38  | LEU  | N-CA-C  | -6.09 | 105.68      | 113.23   |
| 16  | An    | 119 | ARG  | N-CA-C  | -6.09 | 105.56      | 114.39   |
| 7   | Bm    | 285 | TYR  | CA-C-N  | -6.09 | 113.36      | 122.74   |
| 7   | Bm    | 285 | TYR  | C-N-CA  | -6.09 | 113.36      | 122.74   |
| 1   | Ca    | 415 | ASN  | N-CA-C  | -6.09 | 96.91       | 108.17   |
| 2   | Cd    | 347 | LYS  | CA-C-O  | -6.09 | 114.10      | 120.55   |
| 2   | f     | 89  | SER  | N-CA-C  | -6.08 | 104.56      | 112.23   |
| 2   | BR    | 25  | GLN  | CA-C-N  | 6.08  | 126.05      | 119.78   |
| 2   | BR    | 25  | GLN  | C-N-CA  | 6.08  | 126.05      | 119.78   |
| 2   | Cd    | 291 | TYR  | CA-C-N  | -6.08 | 111.06      | 120.31   |
| 2   | Cd    | 291 | TYR  | C-N-CA  | -6.08 | 111.06      | 120.31   |
| 7   | AM    | 510 | VAL  | N-CA-C  | -6.08 | 105.13      | 111.58   |
| 1   | BD    | 26  | ASN  | N-CA-C  | -6.08 | 100.71      | 110.14   |
| 5   | v     | 764 | ARG  | N-CA-C  | -6.08 | 104.73      | 111.36   |
| 7   | Bm    | 39  | LEU  | N-CA-C  | -6.08 | 101.04      | 110.10   |
| 2   | Ch    | 280 | ILE  | N-CA-C  | -6.08 | 96.70       | 109.34   |
| 5   | R     | 274 | ILE  | N-CA-C  | 6.08  | 116.86      | 107.99   |
| 5   | L     | 858 | MET  | CA-C-N  | -6.07 | 110.34      | 121.52   |
| 5   | L     | 858 | MET  | C-N-CA  | -6.07 | 110.34      | 121.52   |
| 2   | f     | 347 | LYS  | CA-C-O  | -6.07 | 114.11      | 120.55   |
| 16  | Az    | 168 | ILE  | CB-CA-C | -6.07 | 105.31      | 111.08   |
| 2   | f     | 333 | LYS  | N-CA-C  | -6.07 | 104.75      | 111.36   |
| 3   | BY    | 444 | PHE  | CA-C-N  | 6.07  | 125.98      | 119.85   |
| 3   | BY    | 444 | PHE  | C-N-CA  | 6.07  | 125.98      | 119.85   |
| 7   | 4     | 166 | MET  | N-CA-CB | -6.07 | 101.51      | 110.49   |
| 3   | 7     | 53  | LYS  | N-CA-C  | -6.07 | 105.37      | 112.89   |
| 3   | BY    | 327 | PHE  | N-CA-C  | -6.07 | 104.02      | 112.45   |
| 5   | 9     | 624 | TYR  | N-CA-C  | -6.06 | 105.84      | 113.18   |
| 5   | G     | 584 | LEU  | CA-C-O  | -6.06 | 114.53      | 120.89   |
| 3   | 1     | 481 | LEU  | N-CA-C  | 6.06  | 118.68      | 111.71   |
| 3   | BY    | 527 | LEU  | N-CA-C  | -6.06 | 105.89      | 113.28   |
| 5   | Bf    | 749 | ILE  | CA-C-N  | -6.06 | 110.37      | 121.52   |
| 5   | Bf    | 749 | ILE  | C-N-CA  | -6.06 | 110.37      | 121.52   |
| 7   | Bm    | 212 | SER  | N-CA-C  | 6.06  | 117.35      | 108.14   |
| 1   | BD    | 208 | HIS  | N-CA-C  | -6.06 | 102.42      | 109.93   |
| 5   | AE    | 496 | PHE  | N-CA-C  | -6.05 | 104.01      | 111.40   |
| 5   | Bt    | 38  | VAL  | CB-CA-C | 6.05  | 119.85      | 110.83   |
| 7   | 4     | 68  | ASP  | N-CA-C  | 6.05  | 117.34      | 107.23   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AM    | 55  | PHE  | N-CA-C  | 6.05  | 118.61      | 109.23   |
| 7   | 4     | 39  | LEU  | N-CA-C  | -6.05 | 101.09      | 110.10   |
| 5   | AE    | 894 | GLN  | N-CA-C  | -6.05 | 104.61      | 112.23   |
| 1   | BD    | 401 | TYR  | CB-CA-C | -6.05 | 101.19      | 110.26   |
| 7   | J     | 190 | SER  | N-CA-C  | 6.05  | 118.26      | 109.07   |
| 2   | s     | 272 | LYS  | CA-C-N  | 6.04  | 130.81      | 120.72   |
| 2   | s     | 272 | LYS  | C-N-CA  | 6.04  | 130.81      | 120.72   |
| 3   | 7     | 51  | ASP  | N-CA-C  | 6.04  | 118.71      | 110.55   |
| 1   | A     | 288 | HIS  | CA-C-O  | 6.04  | 121.44      | 117.94   |
| 16  | Az    | 119 | ARG  | N-CA-C  | -6.03 | 105.47      | 114.64   |
| 3   | BY    | 480 | ASN  | N-CA-CB | 6.03  | 120.75      | 110.50   |
| 3   | BY    | 534 | CYS  | N-CA-C  | -6.03 | 104.63      | 112.23   |
| 16  | CM    | 119 | ARG  | N-CA-C  | -6.03 | 105.65      | 114.39   |
| 3   | I     | 479 | LEU  | N-CA-C  | 6.03  | 120.76      | 113.41   |
| 1   | i     | 371 | HIS  | N-CA-C  | -6.02 | 101.56      | 110.48   |
| 7   | J     | 329 | PHE  | CB-CA-C | -6.02 | 98.28       | 111.71   |
| 16  | Az    | 34  | PHE  | N-CA-C  | -6.02 | 104.83      | 111.82   |
| 3   | 1     | 526 | LEU  | CA-C-O  | -6.02 | 114.09      | 120.71   |
| 5   | AB    | 61  | LYS  | N-CA-C  | -6.02 | 106.55      | 114.31   |
| 5   | AU    | 325 | ARG  | N-CA-C  | -6.02 | 104.28      | 111.69   |
| 16  | Aq    | 31  | LYS  | N-CA-C  | -6.02 | 106.07      | 113.41   |
| 7   | O     | 265 | ILE  | N-CA-C  | 6.02  | 117.96      | 111.58   |
| 1   | BD    | 155 | ASP  | CA-C-O  | -6.02 | 113.56      | 121.08   |
| 3   | 1     | 64  | GLY  | N-CA-C  | -6.01 | 107.02      | 115.32   |
| 5   | AE    | 456 | PHE  | N-CA-C  | -6.01 | 104.80      | 111.36   |
| 2   | k     | 278 | GLY  | N-CA-C  | 6.01  | 119.91      | 111.19   |
| 5   | AO    | 212 | VAL  | N-CA-C  | 6.01  | 118.65      | 108.86   |
| 3   | 1     | 327 | PHE  | N-CA-C  | -6.01 | 104.10      | 112.45   |
| 7   | AG    | 202 | LEU  | CA-C-N  | -6.01 | 111.18      | 120.31   |
| 7   | AG    | 202 | LEU  | C-N-CA  | -6.01 | 111.18      | 120.31   |
| 1   | BD    | 415 | ASN  | N-CA-C  | -6.01 | 97.06       | 108.17   |
| 1   | CP    | 415 | ASN  | N-CA-C  | -6.01 | 97.06       | 108.17   |
| 3   | I     | 235 | ILE  | N-CA-C  | 6.00  | 116.52      | 108.11   |
| 7   | 4     | 274 | GLN  | N-CA-C  | -6.00 | 104.74      | 111.28   |
| 5   | v     | 521 | GLU  | N-CA-C  | 6.00  | 117.62      | 111.14   |
| 5   | Bf    | 581 | TRP  | N-CA-C  | 6.00  | 121.79      | 113.45   |
| 5   | AO    | 172 | PHE  | N-CA-C  | 6.00  | 118.65      | 110.55   |
| 2   | z     | 38  | LEU  | N-CA-C  | -6.00 | 105.05      | 112.90   |
| 7   | 4     | 202 | LEU  | CA-C-N  | -5.99 | 110.50      | 121.52   |
| 7   | 4     | 202 | LEU  | C-N-CA  | -5.99 | 110.50      | 121.52   |
| 16  | Z     | 53  | ALA  | CA-C-N  | 5.99  | 125.90      | 119.85   |
| 16  | Z     | 53  | ALA  | C-N-CA  | 5.99  | 125.90      | 119.85   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | i     | 208 | HIS  | N-CA-C | -5.99 | 102.50      | 109.93   |
| 3   | 7     | 680 | ILE  | N-CA-C | 5.99  | 115.12      | 108.05   |
| 2   | Cd    | 137 | ASN  | N-CA-C | -5.99 | 104.32      | 111.69   |
| 3   | I     | 53  | LYS  | N-CA-C | -5.99 | 105.47      | 112.89   |
| 2   | y     | 240 | LEU  | N-CA-C | -5.99 | 104.13      | 112.45   |
| 7   | AG    | 110 | ASP  | N-CA-C | 5.99  | 120.60      | 113.12   |
| 5   | G     | 576 | PHE  | N-CA-C | -5.99 | 98.05       | 110.80   |
| 5   | 9     | 464 | LEU  | CA-C-N | 5.99  | 132.47      | 121.70   |
| 5   | 9     | 464 | LEU  | C-N-CA | 5.99  | 132.47      | 121.70   |
| 7   | O     | 38  | ALA  | N-CA-C | 5.98  | 119.64      | 111.39   |
| 3   | 7     | 598 | VAL  | N-CA-C | 5.98  | 121.78      | 109.34   |
| 16  | Av    | 142 | ASN  | N-CA-C | -5.98 | 100.86      | 109.29   |
| 2   | Cd    | 329 | GLN  | O-C-N  | -5.98 | 114.64      | 122.59   |
| 2   | z     | 240 | LEU  | N-CA-C | -5.98 | 104.14      | 112.45   |
| 3   | E     | 774 | ARG  | N-CA-C | -5.98 | 104.85      | 111.36   |
| 2   | y     | 38  | LEU  | N-CA-C | -5.98 | 105.07      | 112.90   |
| 5   | G     | 463 | GLY  | N-CA-C | 5.97  | 119.47      | 110.75   |
| 5   | 9     | 646 | ASN  | CA-C-N | 5.97  | 126.08      | 119.87   |
| 5   | 9     | 646 | ASN  | C-N-CA | 5.97  | 126.08      | 119.87   |
| 16  | Ai    | 53  | ALA  | CA-C-N | 5.97  | 125.94      | 120.03   |
| 16  | Ai    | 53  | ALA  | C-N-CA | 5.97  | 125.94      | 120.03   |
| 3   | BY    | 748 | LEU  | N-CA-C | -5.97 | 104.89      | 111.82   |
| 5   | R     | 121 | ASN  | CA-C-N | 5.97  | 126.08      | 119.87   |
| 5   | R     | 121 | ASN  | C-N-CA | 5.97  | 126.08      | 119.87   |
| 2   | f     | 291 | TYR  | N-CA-C | 5.97  | 127.71      | 111.00   |
| 2   | k     | 331 | ASN  | CA-C-O | -5.97 | 112.04      | 119.38   |
| 3   | E     | 256 | GLN  | N-CA-C | -5.97 | 106.64      | 114.04   |
| 16  | Aq    | 143 | GLN  | CA-C-N | -5.97 | 117.12      | 122.97   |
| 16  | Aq    | 143 | GLN  | C-N-CA | -5.97 | 117.12      | 122.97   |
| 7   | AG    | 47  | GLU  | N-CA-C | 5.96  | 118.55      | 111.33   |
| 5   | AO    | 270 | SER  | CA-C-O | -5.96 | 113.11      | 119.97   |
| 5   | Bf    | 597 | TRP  | N-CA-C | -5.96 | 105.50      | 112.89   |
| 7   | O     | 98  | SER  | CA-C-N | 5.96  | 125.64      | 119.56   |
| 7   | O     | 98  | SER  | C-N-CA | 5.96  | 125.64      | 119.56   |
| 3   | n     | 43  | TRP  | N-CA-C | 5.96  | 117.59      | 108.12   |
| 3   | 7     | 863 | ASP  | CA-C-O | -5.96 | 113.37      | 120.10   |
| 5   | AE    | 782 | LYS  | CA-C-N | -5.95 | 111.59      | 120.82   |
| 5   | AE    | 782 | LYS  | C-N-CA | -5.95 | 111.59      | 120.82   |
| 3   | BY    | 703 | TYR  | CA-C-N | 5.95  | 127.28      | 119.84   |
| 3   | BY    | 703 | TYR  | C-N-CA | 5.95  | 127.28      | 119.84   |
| 1   | Ca    | 371 | HIS  | N-CA-C | -5.95 | 102.11      | 110.50   |
| 3   | 7     | 707 | SER  | N-CA-C | 5.95  | 119.95      | 109.96   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AG    | 169 | PHE  | N-CA-C  | 5.95  | 118.19      | 108.55   |
| 7   | AG    | 202 | LEU  | N-CA-C  | 5.95  | 120.69      | 112.90   |
| 16  | An    | 117 | GLU  | N-CA-C  | 5.95  | 119.63      | 111.54   |
| 16  | CI    | 109 | ARG  | N-CA-C  | 5.95  | 118.45      | 109.23   |
| 3   | I     | 737 | THR  | N-CA-C  | -5.95 | 105.98      | 113.18   |
| 16  | A7    | 94  | PRO  | CA-C-N  | 5.95  | 132.90      | 121.54   |
| 16  | A7    | 94  | PRO  | C-N-CA  | 5.95  | 132.90      | 121.54   |
| 5   | AB    | 312 | LEU  | N-CA-CB | 5.95  | 119.45      | 110.30   |
| 5   | AO    | 312 | LEU  | N-CA-CB | 5.95  | 119.46      | 110.30   |
| 5   | M     | 38  | VAL  | CA-C-N  | -5.94 | 111.47      | 121.75   |
| 5   | M     | 38  | VAL  | C-N-CA  | -5.94 | 111.47      | 121.75   |
| 5   | AB    | 42  | ASP  | N-CA-C  | -5.94 | 105.89      | 113.02   |
| 5   | L     | 749 | ILE  | CA-C-N  | -5.94 | 111.20      | 121.66   |
| 5   | L     | 749 | ILE  | C-N-CA  | -5.94 | 111.20      | 121.66   |
| 16  | c     | 132 | GLN  | N-CA-C  | -5.94 | 98.15       | 110.80   |
| 7   | AG    | 314 | ASP  | CB-CA-C | -5.94 | 103.44      | 112.11   |
| 1   | Ca    | 288 | HIS  | CA-C-O  | 5.94  | 121.38      | 117.94   |
| 2   | s     | 354 | GLU  | CA-C-O  | -5.93 | 112.02      | 120.51   |
| 7   | 4     | 332 | GLY  | N-CA-C  | -5.93 | 106.31      | 111.95   |
| 5   | AB    | 253 | ASN  | CA-C-O  | -5.93 | 113.54      | 122.38   |
| 16  | CM    | 142 | ASN  | N-CA-CB | 5.93  | 120.58      | 110.50   |
| 16  | Z     | 169 | PRO  | N-CA-C  | -5.93 | 101.91      | 111.03   |
| 2   | CW    | 24  | THR  | CA-C-N  | -5.93 | 116.01      | 122.59   |
| 2   | CW    | 24  | THR  | C-N-CA  | -5.93 | 116.01      | 122.59   |
| 2   | D     | 83  | GLU  | N-CA-C  | -5.92 | 104.40      | 111.69   |
| 3   | n     | 301 | ILE  | N-CA-C  | 5.92  | 116.83      | 108.36   |
| 7   | Bm    | 202 | LEU  | N-CA-C  | 5.92  | 120.51      | 113.16   |
| 16  | Av    | 37  | ILE  | CA-C-O  | -5.92 | 113.60      | 120.83   |
| 16  | Z     | 147 | LYS  | CA-C-O  | -5.92 | 114.27      | 120.55   |
| 5   | v     | 597 | TRP  | N-CA-C  | -5.92 | 104.73      | 111.07   |
| 3   | 7     | 256 | GLN  | N-CA-C  | -5.92 | 106.70      | 114.04   |
| 5   | AB    | 270 | SER  | CA-C-O  | -5.92 | 113.16      | 119.97   |
| 1   | A     | 95  | LEU  | N-CA-C  | -5.92 | 104.77      | 112.23   |
| 5   | R     | 40  | ASP  | CA-C-N  | 5.92  | 126.03      | 119.87   |
| 5   | R     | 40  | ASP  | C-N-CA  | 5.92  | 126.03      | 119.87   |
| 7   | 4     | 278 | ILE  | N-CA-C  | 5.92  | 118.73      | 108.90   |
| 7   | J     | 55  | PHE  | N-CA-C  | 5.92  | 119.12      | 109.24   |
| 7   | J     | 278 | ILE  | N-CA-C  | 5.92  | 116.88      | 108.42   |
| 7   | AG    | 541 | GLN  | CA-C-N  | -5.92 | 112.78      | 122.54   |
| 7   | AG    | 541 | GLN  | C-N-CA  | -5.92 | 112.78      | 122.54   |
| 16  | Az    | 115 | LYS  | N-CA-C  | -5.91 | 107.88      | 114.62   |
| 3   | I     | 256 | GLN  | N-CA-C  | -5.91 | 106.71      | 114.04   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | J     | 281 | HIS  | CA-C-N  | 5.91  | 127.23      | 119.84   |
| 7   | J     | 281 | HIS  | C-N-CA  | 5.91  | 127.23      | 119.84   |
| 16  | Z     | 36  | ALA  | CA-C-N  | 5.91  | 131.24      | 121.54   |
| 16  | Z     | 36  | ALA  | C-N-CA  | 5.91  | 131.24      | 121.54   |
| 3   | 7     | 480 | ASN  | N-CA-CB | 5.91  | 120.55      | 110.50   |
| 5   | 9     | 551 | LEU  | N-CA-C  | -5.91 | 104.96      | 111.82   |
| 5   | L     | 502 | GLU  | N-CA-C  | 5.91  | 120.77      | 113.50   |
| 3   | E     | 480 | ASN  | N-CA-CB | 5.91  | 120.54      | 110.50   |
| 3   | E     | 493 | TYR  | N-CA-C  | -5.91 | 104.97      | 111.82   |
| 5   | R     | 75  | THR  | N-CA-C  | -5.91 | 105.16      | 112.90   |
| 7   | AM    | 202 | LEU  | N-CA-C  | 5.91  | 119.74      | 112.54   |
| 16  | A7    | 90  | SER  | N-CA-C  | 5.91  | 123.38      | 110.80   |
| 3   | 7     | 837 | MET  | O-C-N   | -5.90 | 118.10      | 123.41   |
| 2   | BR    | 329 | GLN  | CA-C-O  | -5.90 | 115.02      | 122.63   |
| 16  | CB    | 56  | GLU  | N-CA-C  | 5.90  | 120.55      | 113.23   |
| 1   | C     | 288 | HIS  | N-CA-CB | -5.90 | 100.52      | 110.49   |
| 3   | I     | 251 | LEU  | CA-C-N  | 5.90  | 125.87      | 120.03   |
| 3   | I     | 251 | LEU  | C-N-CA  | 5.90  | 125.87      | 120.03   |
| 7   | O     | 182 | SER  | CA-C-N  | 5.90  | 125.81      | 119.85   |
| 7   | O     | 182 | SER  | C-N-CA  | 5.90  | 125.81      | 119.85   |
| 5   | v     | 496 | PHE  | N-CA-C  | -5.90 | 104.77      | 111.14   |
| 5   | AU    | 286 | ILE  | CB-CA-C | -5.90 | 102.04      | 110.83   |
| 2   | CW    | 101 | LYS  | CA-C-O  | -5.90 | 113.43      | 120.10   |
| 2   | z     | 304 | GLN  | N-CA-C  | -5.90 | 104.93      | 111.36   |
| 5   | AB    | 158 | THR  | N-CA-C  | 5.90  | 117.18      | 108.86   |
| 3   | BY    | 526 | LEU  | CA-C-O  | -5.90 | 114.70      | 120.89   |
| 7   | J     | 561 | VAL  | N-CA-C  | -5.90 | 104.76      | 110.72   |
| 7   | 4     | 281 | HIS  | CA-C-N  | 5.90  | 126.31      | 119.47   |
| 7   | 4     | 281 | HIS  | C-N-CA  | 5.90  | 126.31      | 119.47   |
| 1   | A     | 234 | THR  | N-CA-C  | -5.90 | 96.78       | 109.81   |
| 1   | C     | 361 | GLN  | N-CA-C  | -5.89 | 100.89      | 110.20   |
| 2   | f     | 82  | ARG  | N-CA-C  | -5.89 | 104.94      | 111.36   |
| 2   | k     | 280 | ILE  | N-CA-C  | -5.89 | 97.08       | 109.34   |
| 16  | Aq    | 186 | LEU  | N-CA-C  | -5.89 | 104.86      | 111.28   |
| 1   | Ca    | 202 | TYR  | CA-C-N  | -5.89 | 112.57      | 122.29   |
| 1   | Ca    | 202 | TYR  | C-N-CA  | -5.89 | 112.57      | 122.29   |
| 7   | O     | 542 | GLN  | N-CA-C  | -5.89 | 105.75      | 113.17   |
| 5   | Bf    | 546 | PRO  | N-CA-C  | 5.89  | 117.89      | 110.70   |
| 5   | M     | 270 | SER  | CA-C-O  | -5.89 | 113.20      | 119.97   |
| 5   | v     | 575 | LYS  | N-CA-C  | 5.89  | 118.36      | 109.41   |
| 2   | f     | 83  | GLU  | N-CA-C  | -5.88 | 104.87      | 111.28   |
| 5   | Bt    | 207 | ASP  | N-CA-C  | -5.88 | 96.03       | 107.62   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | M     | 42  | ASP  | CA-C-N  | 5.88  | 130.48      | 122.19   |
| 5   | M     | 42  | ASP  | C-N-CA  | 5.88  | 130.48      | 122.19   |
| 3   | BY    | 64  | GLY  | N-CA-C  | -5.88 | 107.20      | 115.32   |
| 3   | E     | 526 | LEU  | CA-C-O  | -5.88 | 114.25      | 120.71   |
| 5   | R     | 61  | LYS  | N-CA-C  | -5.88 | 106.73      | 114.31   |
| 3   | n     | 747 | LYS  | CB-CA-C | -5.88 | 98.73       | 110.42   |
| 5   | AE    | 597 | TRP  | N-CA-C  | -5.88 | 105.77      | 113.17   |
| 7   | AG    | 329 | PHE  | CB-CA-C | -5.88 | 98.61       | 111.71   |
| 3   | E     | 479 | LEU  | N-CA-C  | 5.87  | 120.59      | 112.90   |
| 5   | AO    | 191 | SER  | CA-C-N  | 5.87  | 132.27      | 121.70   |
| 5   | AO    | 191 | SER  | C-N-CA  | 5.87  | 132.27      | 121.70   |
| 5   | Bt    | 270 | SER  | CA-C-O  | -5.87 | 113.22      | 119.97   |
| 7   | J     | 333 | GLY  | CA-C-N  | 5.87  | 130.52      | 120.72   |
| 7   | J     | 333 | GLY  | C-N-CA  | 5.87  | 130.52      | 120.72   |
| 2   | f     | 37  | LYS  | CA-C-O  | -5.87 | 114.33      | 120.55   |
| 2   | s     | 73  | LEU  | N-CA-C  | -5.87 | 104.29      | 112.45   |
| 3   | BY    | 558 | VAL  | N-CA-C  | -5.87 | 107.15      | 111.90   |
| 1   | C     | 3   | PHE  | N-CA-C  | 5.87  | 118.10      | 109.24   |
| 2   | y     | 304 | GLN  | N-CA-C  | -5.87 | 104.97      | 111.36   |
| 5   | AO    | 261 | ASN  | N-CA-C  | -5.87 | 105.89      | 113.16   |
| 2   | BK    | 115 | GLU  | N-CA-C  | -5.87 | 104.97      | 111.36   |
| 3   | 7     | 689 | ASN  | N-CA-C  | -5.86 | 104.33      | 112.30   |
| 1   | CP    | 6   | ILE  | N-CA-C  | -5.86 | 99.26       | 108.23   |
| 5   | L     | 609 | ASP  | CA-C-N  | 5.86  | 132.40      | 123.96   |
| 5   | L     | 609 | ASP  | C-N-CA  | 5.86  | 132.40      | 123.96   |
| 5   | Bt    | 75  | THR  | N-CA-C  | -5.86 | 105.22      | 112.90   |
| 16  | Z     | 118 | HIS  | N-CA-C  | 5.86  | 123.27      | 110.80   |
| 5   | v     | 714 | GLU  | N-CA-C  | -5.86 | 105.03      | 111.82   |
| 7   | AM    | 90  | GLY  | N-CA-C  | -5.86 | 104.12      | 112.55   |
| 7   | Bm    | 266 | GLN  | CA-C-N  | 5.86  | 131.71      | 122.34   |
| 7   | Bm    | 266 | GLN  | C-N-CA  | 5.86  | 131.71      | 122.34   |
| 3   | 1     | 469 | LEU  | N-CA-C  | -5.85 | 104.32      | 112.45   |
| 2   | BR    | 291 | TYR  | N-CA-C  | 5.85  | 127.38      | 111.00   |
| 5   | AB    | 337 | TYR  | CA-C-O  | -5.85 | 112.89      | 119.79   |
| 7   | AG    | 205 | GLN  | N-CA-C  | 5.85  | 119.63      | 111.74   |
| 7   | J     | 201 | ASP  | CA-C-N  | 5.85  | 129.20      | 120.31   |
| 7   | J     | 201 | ASP  | C-N-CA  | 5.85  | 129.20      | 120.31   |
| 16  | Z     | 101 | PHE  | CB-CA-C | -5.84 | 101.09      | 110.79   |
| 16  | CI    | 90  | SER  | N-CA-C  | 5.84  | 123.24      | 110.80   |
| 1   | CP    | 250 | VAL  | N-CA-C  | 5.84  | 116.29      | 108.11   |
| 7   | Bm    | 76  | PHE  | CA-C-O  | -5.84 | 113.08      | 120.84   |
| 7   | Bm    | 200 | TRP  | CA-C-N  | 5.84  | 129.65      | 121.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | Bm    | 200 | TRP  | C-N-CA  | 5.84  | 129.65      | 121.24   |
| 5   | AU    | 186 | GLU  | CA-C-N  | -5.84 | 115.07      | 122.37   |
| 5   | AU    | 186 | GLU  | C-N-CA  | -5.84 | 115.07      | 122.37   |
| 7   | J     | 251 | ASP  | N-CA-C  | -5.83 | 99.63       | 108.67   |
| 5   | 9     | 621 | PHE  | CA-C-N  | 5.83  | 131.32      | 122.92   |
| 5   | 9     | 621 | PHE  | C-N-CA  | 5.83  | 131.32      | 122.92   |
| 16  | A7    | 158 | HIS  | N-CA-C  | -5.83 | 101.65      | 110.28   |
| 1   | CP    | 371 | HIS  | N-CA-C  | -5.83 | 102.28      | 110.50   |
| 1   | Ca    | 132 | PRO  | CA-C-N  | -5.83 | 111.65      | 122.09   |
| 1   | Ca    | 132 | PRO  | C-N-CA  | -5.83 | 111.65      | 122.09   |
| 16  | An    | 53  | ALA  | CA-C-N  | 5.83  | 125.74      | 119.85   |
| 16  | An    | 53  | ALA  | C-N-CA  | 5.83  | 125.74      | 119.85   |
| 1   | A     | 218 | GLN  | CA-C-N  | 5.83  | 126.02      | 120.31   |
| 1   | A     | 218 | GLN  | C-N-CA  | 5.83  | 126.02      | 120.31   |
| 16  | Az    | 131 | VAL  | N-CA-C  | -5.83 | 102.02      | 109.30   |
| 3   | BY    | 205 | GLU  | N-CA-C  | 5.83  | 117.11      | 108.60   |
| 5   | 9     | 493 | LEU  | N-CA-C  | -5.82 | 104.89      | 112.23   |
| 7   | 4     | 55  | PHE  | N-CA-C  | 5.82  | 118.96      | 109.24   |
| 5   | G     | 625 | PHE  | CA-C-O  | -5.82 | 113.96      | 121.17   |
| 3   | E     | 459 | LEU  | CA-C-N  | 5.82  | 126.32      | 120.04   |
| 3   | E     | 459 | LEU  | C-N-CA  | 5.82  | 126.32      | 120.04   |
| 2   | BK    | 280 | ILE  | N-CA-C  | 5.82  | 121.44      | 109.34   |
| 16  | CM    | 57  | ARG  | N-CA-C  | 5.82  | 118.69      | 109.50   |
| 3   | n     | 232 | TYR  | N-CA-C  | 5.81  | 118.24      | 109.23   |
| 16  | CM    | 126 | LEU  | N-CA-C  | -5.81 | 105.86      | 113.12   |
| 3   | I     | 152 | ASN  | CA-C-N  | 5.81  | 128.41      | 120.46   |
| 3   | I     | 152 | ASN  | C-N-CA  | 5.81  | 128.41      | 120.46   |
| 7   | J     | 315 | LYS  | N-CA-C  | 5.81  | 119.39      | 107.37   |
| 2   | s     | 321 | SER  | N-CA-C  | 5.81  | 120.43      | 113.23   |
| 5   | AB    | 298 | ILE  | N-CA-C  | 5.81  | 116.24      | 108.11   |
| 5   | 9     | 597 | TRP  | CA-C-O  | -5.81 | 112.11      | 119.31   |
| 5   | L     | 456 | PHE  | N-CA-C  | -5.80 | 104.87      | 111.14   |
| 5   | M     | 212 | VAL  | N-CA-C  | 5.80  | 116.48      | 108.12   |
| 7   | Bm    | 250 | PHE  | N-CA-C  | -5.80 | 105.09      | 111.82   |
| 3   | n     | 53  | LYS  | N-CA-C  | -5.80 | 105.69      | 112.89   |
| 5   | v     | 503 | SER  | O-C-N   | -5.80 | 116.01      | 122.86   |
| 1   | Ca    | 203 | LYS  | N-CA-C  | 5.80  | 118.22      | 109.23   |
| 1   | C     | 131 | ASN  | CA-C-N  | 5.80  | 125.73      | 119.76   |
| 1   | C     | 131 | ASN  | C-N-CA  | 5.80  | 125.73      | 119.76   |
| 5   | v     | 622 | ILE  | CB-CA-C | 5.80  | 117.97      | 111.59   |
| 5   | AO    | 39  | SER  | CA-C-N  | 5.80  | 129.32      | 121.20   |
| 5   | AO    | 39  | SER  | C-N-CA  | 5.80  | 129.32      | 121.20   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | Bm    | 141 | ALA  | N-CA-C  | 5.80  | 117.60      | 111.28   |
| 7   | O     | 171 | GLY  | N-CA-C  | -5.80 | 105.71      | 115.80   |
| 3   | n     | 598 | VAL  | O-C-N   | -5.80 | 116.82      | 121.98   |
| 7   | 4     | 202 | LEU  | CA-C-O  | -5.80 | 112.49      | 119.27   |
| 3   | 7     | 43  | TRP  | N-CA-C  | 5.80  | 117.34      | 108.12   |
| 3   | 7     | 610 | LEU  | N-CA-C  | -5.80 | 105.70      | 112.89   |
| 7   | AG    | 521 | ASN  | CA-C-N  | 5.80  | 127.97      | 120.44   |
| 7   | AG    | 521 | ASN  | C-N-CA  | 5.80  | 127.97      | 120.44   |
| 5   | R     | 285 | GLY  | CA-C-N  | -5.79 | 114.89      | 122.37   |
| 5   | R     | 285 | GLY  | C-N-CA  | -5.79 | 114.89      | 122.37   |
| 3   | n     | 155 | THR  | CA-C-N  | 5.79  | 130.40      | 122.34   |
| 3   | n     | 155 | THR  | C-N-CA  | 5.79  | 130.40      | 122.34   |
| 3   | n     | 526 | LEU  | CA-C-O  | -5.79 | 114.34      | 120.71   |
| 7   | 4     | 547 | LEU  | N-CA-C  | -5.79 | 104.32      | 111.33   |
| 16  | Av    | 108 | LEU  | CB-CA-C | -5.79 | 103.11      | 111.91   |
| 5   | AO    | 207 | ASP  | N-CA-C  | -5.79 | 97.71       | 108.02   |
| 1   | A     | 415 | ASN  | N-CA-C  | -5.79 | 97.46       | 108.17   |
| 2   | z     | 86  | ASN  | CA-C-O  | -5.79 | 113.81      | 120.24   |
| 5   | AE    | 621 | PHE  | CA-C-N  | 5.79  | 131.39      | 123.46   |
| 5   | AE    | 621 | PHE  | C-N-CA  | 5.79  | 131.39      | 123.46   |
| 16  | An    | 139 | LYS  | CA-C-O  | -5.79 | 112.98      | 119.98   |
| 7   | Bm    | 55  | PHE  | N-CA-C  | 5.79  | 118.20      | 109.23   |
| 5   | Bt    | 310 | TYR  | CA-C-N  | -5.79 | 113.22      | 122.53   |
| 5   | Bt    | 310 | TYR  | C-N-CA  | -5.79 | 113.22      | 122.53   |
| 1   | i     | 26  | ASN  | N-CA-C  | -5.78 | 101.17      | 110.14   |
| 7   | Bm    | 81  | ARG  | CA-C-N  | 5.78  | 125.69      | 119.85   |
| 7   | Bm    | 81  | ARG  | C-N-CA  | 5.78  | 125.69      | 119.85   |
| 1   | C     | 144 | ASP  | N-CA-C  | -5.78 | 105.33      | 112.90   |
| 7   | O     | 522 | PHE  | N-CA-C  | -5.78 | 104.42      | 112.45   |
| 5   | L     | 908 | GLU  | CA-C-O  | -5.78 | 112.27      | 119.38   |
| 1   | C     | 37  | GLN  | N-CA-C  | -5.78 | 100.57      | 109.52   |
| 2   | k     | 15  | ARG  | N-CA-C  | -5.78 | 105.12      | 111.82   |
| 16  | Av    | 132 | GLN  | CA-C-O  | -5.77 | 112.25      | 120.51   |
| 3   | n     | 609 | TRP  | CA-C-O  | -5.77 | 111.55      | 119.05   |
| 3   | I     | 480 | ASN  | N-CA-CB | 5.77  | 120.30      | 110.50   |
| 3   | 7     | 93  | LYS  | CA-C-N  | 5.77  | 125.44      | 119.56   |
| 3   | 7     | 93  | LYS  | C-N-CA  | 5.77  | 125.44      | 119.56   |
| 5   | AU    | 252 | GLY  | CA-C-N  | -5.77 | 113.52      | 122.05   |
| 5   | AU    | 252 | GLY  | C-N-CA  | -5.77 | 113.52      | 122.05   |
| 3   | BY    | 471 | ARG  | CA-C-O  | -5.77 | 112.50      | 120.52   |
| 7   | O     | 274 | GLN  | N-CA-C  | -5.76 | 104.90      | 111.07   |
| 2   | BK    | 82  | ARG  | CA-C-O  | -5.76 | 112.73      | 119.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | O     | 68  | ASP  | N-CA-C  | 5.76  | 116.86      | 107.23   |
| 2   | D     | 267 | GLU  | N-CA-C  | -5.76 | 106.79      | 113.88   |
| 5   | v     | 499 | LEU  | CB-CA-C | -5.76 | 101.18      | 110.74   |
| 5   | 9     | 512 | PRO  | CA-C-N  | -5.76 | 112.11      | 120.29   |
| 5   | 9     | 512 | PRO  | C-N-CA  | -5.76 | 112.11      | 120.29   |
| 5   | Bf    | 546 | PRO  | CA-C-N  | 5.76  | 127.04      | 119.84   |
| 5   | Bf    | 546 | PRO  | C-N-CA  | 5.76  | 127.04      | 119.84   |
| 3   | I     | 908 | ARG  | N-CA-C  | -5.76 | 105.08      | 111.36   |
| 2   | y     | 272 | LYS  | CA-C-N  | 5.76  | 129.06      | 120.31   |
| 2   | y     | 272 | LYS  | C-N-CA  | 5.76  | 129.06      | 120.31   |
| 5   | AO    | 163 | PRO  | N-CA-C  | 5.76  | 122.18      | 114.18   |
| 2   | z     | 272 | LYS  | CA-C-N  | 5.76  | 129.06      | 120.31   |
| 2   | z     | 272 | LYS  | C-N-CA  | 5.76  | 129.06      | 120.31   |
| 2   | k     | 32  | ALA  | CB-CA-C | -5.75 | 102.73      | 112.00   |
| 16  | CI    | 49  | VAL  | N-CA-C  | -5.75 | 104.91      | 110.72   |
| 2   | y     | 86  | ASN  | CA-C-O  | -5.75 | 113.85      | 120.24   |
| 5   | AB    | 257 | ILE  | N-CA-C  | 5.75  | 116.41      | 108.12   |
| 16  | A7    | 168 | ILE  | CA-C-N  | 5.75  | 125.71      | 119.78   |
| 16  | A7    | 168 | ILE  | C-N-CA  | 5.75  | 125.71      | 119.78   |
| 5   | Bt    | 341 | LYS  | CA-C-N  | 5.75  | 125.69      | 119.76   |
| 5   | Bt    | 341 | LYS  | C-N-CA  | 5.75  | 125.69      | 119.76   |
| 1   | C     | 406 | SER  | N-CA-C  | 5.75  | 117.63      | 111.36   |
| 5   | AB    | 69  | LYS  | N-CA-C  | 5.75  | 122.52      | 109.81   |
| 16  | CI    | 108 | LEU  | CB-CA-C | -5.75 | 103.18      | 111.91   |
| 2   | CW    | 123 | LEU  | CA-C-N  | -5.75 | 110.95      | 121.52   |
| 2   | CW    | 123 | LEU  | C-N-CA  | -5.75 | 110.95      | 121.52   |
| 5   | v     | 506 | PHE  | N-CA-C  | -5.75 | 106.40      | 113.41   |
| 3   | 7     | 795 | LYS  | N-CA-C  | -5.75 | 105.16      | 111.82   |
| 1   | Ca    | 258 | ILE  | N-CA-C  | -5.74 | 105.49      | 111.58   |
| 5   | AU    | 52  | SER  | N-CA-C  | -5.74 | 103.78      | 112.04   |
| 16  | A7    | 132 | GLN  | CA-C-O  | -5.74 | 112.30      | 120.51   |
| 3   | I     | 291 | LEU  | N-CA-C  | 5.74  | 118.81      | 109.06   |
| 5   | R     | 328 | GLU  | N-CA-C  | -5.74 | 106.24      | 113.18   |
| 5   | AO    | 138 | TRP  | N-CA-C  | 5.74  | 117.79      | 109.07   |
| 1   | A     | 417 | LYS  | N-CA-C  | -5.74 | 106.20      | 113.43   |
| 5   | AU    | 194 | GLU  | CA-C-N  | -5.74 | 113.98      | 122.41   |
| 5   | AU    | 194 | GLU  | C-N-CA  | -5.74 | 113.98      | 122.41   |
| 3   | BY    | 816 | ASP  | N-CA-C  | -5.74 | 105.17      | 111.82   |
| 7   | J     | 545 | SER  | N-CA-C  | -5.73 | 105.03      | 111.28   |
| 1   | A     | 281 | SER  | N-CA-C  | 5.73  | 115.67      | 108.45   |
| 2   | D     | 357 | ARG  | CA-C-O  | -5.73 | 112.31      | 120.51   |
| 5   | G     | 611 | PRO  | CA-C-N  | 5.73  | 132.01      | 121.70   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | G     | 611 | PRO  | C-N-CA  | 5.73  | 132.01      | 121.70   |
| 5   | L     | 602 | ASP  | N-CA-C  | -5.73 | 105.96      | 113.12   |
| 16  | Z     | 142 | ASN  | N-CA-CB | 5.73  | 120.24      | 110.50   |
| 2   | z     | 265 | ASP  | CA-C-O  | -5.73 | 113.38      | 119.97   |
| 7   | AG    | 202 | LEU  | CA-C-O  | -5.73 | 112.90      | 119.60   |
| 3   | I     | 133 | VAL  | N-CA-C  | 5.72  | 116.36      | 108.12   |
| 7   | AG    | 333 | GLY  | CA-C-N  | 5.72  | 130.28      | 120.72   |
| 7   | AG    | 333 | GLY  | C-N-CA  | 5.72  | 130.28      | 120.72   |
| 16  | CT    | 158 | HIS  | N-CA-C  | -5.72 | 101.81      | 110.28   |
| 1   | Ca    | 160 | ILE  | N-CA-C  | 5.72  | 116.09      | 107.80   |
| 16  | Ai    | 140 | ASP  | N-CA-C  | 5.71  | 117.69      | 107.80   |
| 3   | BY    | 488 | GLN  | N-CA-C  | 5.71  | 118.47      | 109.39   |
| 1   | CP    | 131 | ASN  | CA-C-N  | 5.71  | 125.67      | 119.78   |
| 1   | CP    | 131 | ASN  | C-N-CA  | 5.71  | 125.67      | 119.78   |
| 16  | CT    | 73  | LEU  | CA-C-N  | -5.71 | 112.63      | 120.46   |
| 16  | CT    | 73  | LEU  | C-N-CA  | -5.71 | 112.63      | 120.46   |
| 16  | Z     | 97  | ILE  | N-CA-C  | -5.71 | 105.28      | 110.82   |
| 3   | 7     | 481 | LEU  | N-CA-C  | 5.71  | 117.50      | 111.28   |
| 3   | 7     | 97  | TYR  | N-CA-C  | -5.71 | 103.36      | 111.24   |
| 3   | 7     | 769 | TYR  | CB-CA-C | -5.71 | 100.97      | 110.68   |
| 7   | AM    | 558 | GLU  | N-CA-C  | -5.71 | 105.96      | 114.64   |
| 5   | AO    | 351 | PHE  | N-CA-CB | -5.71 | 102.17      | 110.84   |
| 7   | O     | 192 | SER  | N-CA-C  | 5.71  | 115.64      | 108.45   |
| 7   | AM    | 281 | HIS  | CA-C-N  | 5.71  | 126.09      | 119.47   |
| 7   | AM    | 281 | HIS  | C-N-CA  | 5.71  | 126.09      | 119.47   |
| 2   | z     | 333 | LYS  | N-CA-C  | -5.71 | 105.14      | 111.36   |
| 2   | D     | 331 | ASN  | CA-C-N  | -5.70 | 111.42      | 120.55   |
| 2   | D     | 331 | ASN  | C-N-CA  | -5.70 | 111.42      | 120.55   |
| 2   | y     | 333 | LYS  | N-CA-C  | -5.70 | 105.14      | 111.36   |
| 5   | AE    | 664 | THR  | CA-C-N  | 5.70  | 125.65      | 119.78   |
| 5   | AE    | 664 | THR  | C-N-CA  | 5.70  | 125.65      | 119.78   |
| 2   | y     | 265 | ASP  | CA-C-O  | -5.70 | 113.42      | 119.97   |
| 3   | 7     | 526 | LEU  | O-C-N   | -5.70 | 115.50      | 122.11   |
| 16  | Aq    | 112 | CYS  | N-CA-C  | 5.70  | 118.92      | 110.48   |
| 1   | BD    | 281 | SER  | N-CA-C  | 5.70  | 115.63      | 108.45   |
| 7   | Bm    | 295 | LYS  | N-CA-C  | 5.70  | 118.53      | 110.50   |
| 7   | AG    | 39  | LEU  | N-CA-C  | -5.69 | 101.62      | 110.10   |
| 7   | AG    | 331 | THR  | N-CA-C  | 5.69  | 117.26      | 109.18   |
| 3   | BY    | 291 | LEU  | N-CA-C  | 5.69  | 118.74      | 109.06   |
| 5   | R     | 38  | VAL  | CA-C-N  | -5.69 | 111.91      | 121.75   |
| 5   | R     | 38  | VAL  | C-N-CA  | -5.69 | 111.91      | 121.75   |
| 1   | BD    | 250 | VAL  | N-CA-C  | 5.69  | 116.08      | 108.11   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | CW    | 82  | ARG  | CA-C-O  | -5.69 | 112.81      | 119.24   |
| 3   | E     | 291 | LEU  | N-CA-C  | 5.69  | 118.47      | 108.75   |
| 2   | k     | 25  | GLN  | CA-C-N  | 5.69  | 128.98      | 120.96   |
| 2   | k     | 25  | GLN  | C-N-CA  | 5.69  | 128.98      | 120.96   |
| 5   | v     | 584 | LEU  | CA-C-O  | -5.69 | 114.46      | 120.71   |
| 2   | BR    | 46  | SER  | CA-C-N  | 5.69  | 129.70      | 120.60   |
| 2   | BR    | 46  | SER  | C-N-CA  | 5.69  | 129.70      | 120.60   |
| 5   | AB    | 295 | ASN  | N-CA-C  | -5.68 | 104.21      | 113.19   |
| 5   | L     | 608 | ASN  | O-C-N   | -5.68 | 115.24      | 122.34   |
| 3   | BY    | 847 | LEU  | CA-C-O  | -5.68 | 112.70      | 119.35   |
| 3   | n     | 610 | LEU  | N-CA-C  | -5.68 | 105.85      | 112.89   |
| 3   | I     | 481 | LEU  | N-CA-C  | 5.68  | 118.24      | 111.71   |
| 5   | AB    | 290 | ASP  | CB-CA-C | -5.68 | 102.33      | 110.62   |
| 3   | l     | 153 | ILE  | CB-CA-C | -5.68 | 104.60      | 112.04   |
| 1   | A     | 342 | ASN  | CA-C-N  | -5.68 | 112.92      | 122.29   |
| 1   | A     | 342 | ASN  | C-N-CA  | -5.68 | 112.92      | 122.29   |
| 5   | G     | 587 | PHE  | CA-C-N  | 5.68  | 128.67      | 120.38   |
| 5   | G     | 587 | PHE  | C-N-CA  | 5.68  | 128.67      | 120.38   |
| 3   | n     | 73  | LYS  | N-CA-C  | -5.68 | 106.19      | 113.23   |
| 2   | y     | 291 | TYR  | N-CA-C  | 5.68  | 126.89      | 111.00   |
| 16  | A7    | 60  | GLU  | N-CA-C  | 5.68  | 118.92      | 110.52   |
| 3   | BY    | 110 | TYR  | N-CA-CB | -5.67 | 101.29      | 110.71   |
| 1   | CP    | 59  | ASP  | CA-C-N  | 5.67  | 130.19      | 122.19   |
| 1   | CP    | 59  | ASP  | C-N-CA  | 5.67  | 130.19      | 122.19   |
| 7   | AG    | 160 | LEU  | CA-C-N  | 5.67  | 129.27      | 121.33   |
| 7   | AG    | 160 | LEU  | C-N-CA  | 5.67  | 129.27      | 121.33   |
| 16  | CI    | 158 | HIS  | N-CA-C  | -5.67 | 101.89      | 110.28   |
| 2   | z     | 291 | TYR  | N-CA-C  | 5.67  | 126.88      | 111.00   |
| 3   | n     | 110 | TYR  | N-CA-CB | -5.67 | 101.30      | 110.71   |
| 5   | Bf    | 588 | PHE  | N-CA-C  | 5.67  | 119.81      | 113.01   |
| 5   | Bf    | 597 | TRP  | CA-C-O  | -5.67 | 112.29      | 119.31   |
| 7   | J     | 324 | GLN  | CA-C-N  | 5.66  | 132.36      | 121.54   |
| 7   | J     | 324 | GLN  | C-N-CA  | 5.66  | 132.36      | 121.54   |
| 3   | 7     | 125 | THR  | N-CA-C  | -5.66 | 100.74      | 109.52   |
| 5   | G     | 511 | PHE  | CA-C-N  | 5.66  | 125.28      | 119.56   |
| 5   | G     | 511 | PHE  | C-N-CA  | 5.66  | 125.28      | 119.56   |
| 7   | AM    | 48  | ASP  | CA-C-O  | -5.66 | 112.41      | 120.51   |
| 5   | G     | 765 | GLN  | CA-C-O  | -5.66 | 111.86      | 119.11   |
| 3   | I     | 496 | THR  | CA-C-N  | 5.66  | 127.86      | 120.28   |
| 3   | I     | 496 | THR  | C-N-CA  | 5.66  | 127.86      | 120.28   |
| 3   | n     | 64  | GLY  | N-CA-C  | -5.66 | 107.51      | 115.32   |
| 2   | s     | 239 | GLN  | CA-C-O  | -5.66 | 113.46      | 119.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | CT    | 129 | LEU  | N-CA-C  | 5.66  | 117.53      | 111.36   |
| 16  | Aq    | 108 | LEU  | CB-CA-C | -5.66 | 103.31      | 111.91   |
| 5   | AE    | 623 | ILE  | CA-C-N  | 5.66  | 128.13      | 120.38   |
| 5   | AE    | 623 | ILE  | C-N-CA  | 5.66  | 128.13      | 120.38   |
| 7   | AG    | 513 | ASN  | N-CA-C  | 5.65  | 118.91      | 111.28   |
| 3   | I     | 526 | LEU  | O-C-N   | -5.65 | 115.82      | 122.32   |
| 7   | J     | 265 | ILE  | N-CA-C  | 5.65  | 116.67      | 111.81   |
| 7   | J     | 306 | GLN  | N-CA-C  | -5.65 | 101.91      | 110.28   |
| 5   | M     | 208 | SER  | N-CA-C  | 5.65  | 119.46      | 110.70   |
| 3   | 1     | 480 | ASN  | N-CA-CB | 5.65  | 120.11      | 110.50   |
| 5   | Bt    | 257 | ILE  | N-CA-C  | 5.65  | 116.08      | 108.17   |
| 5   | M     | 181 | ASN  | N-CA-C  | -5.65 | 98.04       | 107.99   |
| 3   | 1     | 73  | LYS  | N-CA-C  | -5.65 | 106.22      | 113.23   |
| 2   | BR    | 73  | LEU  | N-CA-C  | -5.65 | 104.59      | 112.45   |
| 7   | Bm    | 332 | GLY  | N-CA-C  | -5.65 | 105.96      | 112.29   |
| 16  | CT    | 167 | ASN  | N-CA-C  | 5.65  | 119.36      | 111.56   |
| 5   | L     | 609 | ASP  | N-CA-C  | -5.65 | 103.91      | 111.87   |
| 3   | 1     | 331 | ILE  | CB-CA-C | -5.65 | 104.74      | 111.97   |
| 7   | 4     | 113 | ILE  | CA-C-N  | -5.65 | 115.26      | 122.77   |
| 7   | 4     | 113 | ILE  | C-N-CA  | -5.65 | 115.26      | 122.77   |
| 5   | Bt    | 121 | ASN  | CA-C-N  | 5.65  | 125.74      | 119.87   |
| 5   | Bt    | 121 | ASN  | C-N-CA  | 5.65  | 125.74      | 119.87   |
| 1   | i     | 179 | MET  | N-CA-C  | -5.64 | 104.60      | 112.45   |
| 3   | 7     | 313 | LEU  | CA-C-N  | -5.64 | 115.75      | 123.14   |
| 3   | 7     | 313 | LEU  | C-N-CA  | -5.64 | 115.75      | 123.14   |
| 5   | M     | 298 | ILE  | N-CA-C  | 5.64  | 116.01      | 108.11   |
| 5   | AB    | 4   | ILE  | N-CA-C  | 5.64  | 116.89      | 108.54   |
| 5   | AU    | 40  | ASP  | N-CA-C  | 5.64  | 119.45      | 109.58   |
| 1   | C     | 371 | HIS  | N-CA-C  | -5.64 | 102.55      | 110.50   |
| 5   | v     | 493 | LEU  | N-CA-C  | -5.64 | 104.75      | 111.69   |
| 5   | AU    | 209 | SER  | N-CA-C  | -5.64 | 106.24      | 113.23   |
| 5   | AB    | 257 | ILE  | CA-C-N  | -5.64 | 116.20      | 123.19   |
| 5   | AB    | 257 | ILE  | C-N-CA  | -5.64 | 116.20      | 123.19   |
| 1   | A     | 258 | ILE  | N-CA-C  | -5.63 | 106.21      | 111.45   |
| 1   | C     | 318 | GLN  | N-CA-C  | -5.63 | 100.95      | 109.85   |
| 3   | I     | 555 | ASN  | N-CA-C  | -5.63 | 100.79      | 109.41   |
| 7   | J     | 544 | TYR  | N-CA-C  | -5.63 | 106.57      | 113.50   |
| 2   | Cd    | 82  | ARG  | N-CA-C  | -5.63 | 104.76      | 111.69   |
| 3   | I     | 491 | LYS  | N-CA-C  | -5.63 | 106.95      | 113.88   |
| 7   | O     | 522 | PHE  | CA-C-O  | -5.63 | 113.13      | 120.00   |
| 2   | s     | 313 | THR  | N-CA-C  | -5.63 | 105.14      | 111.28   |
| 5   | AB    | 118 | LEU  | N-CA-C  | 5.63  | 118.73      | 109.72   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AB    | 212 | VAL  | N-CA-C  | 5.63  | 115.78      | 108.35   |
| 7   | AM    | 534 | GLU  | N-CA-C  | -5.63 | 107.06      | 114.04   |
| 16  | CB    | 40  | GLN  | N-CA-C  | 5.63  | 115.82      | 107.88   |
| 2   | CW    | 85  | ASN  | N-CA-C  | -5.63 | 105.91      | 112.89   |
| 3   | I     | 780 | ASP  | N-CA-C  | -5.63 | 105.22      | 111.36   |
| 2   | s     | 137 | ASN  | N-CA-C  | -5.63 | 104.77      | 111.69   |
| 7   | J     | 510 | VAL  | N-CA-C  | -5.63 | 105.62      | 111.58   |
| 5   | L     | 543 | PHE  | N-CA-C  | 5.62  | 115.37      | 108.11   |
| 16  | c     | 167 | ASN  | N-CA-C  | 5.62  | 119.80      | 111.87   |
| 7   | 4     | 38  | ALA  | N-CA-C  | 5.62  | 119.00      | 111.24   |
| 16  | CM    | 53  | ALA  | CA-C-N  | 5.62  | 125.60      | 120.03   |
| 16  | CM    | 53  | ALA  | C-N-CA  | 5.62  | 125.60      | 120.03   |
| 5   | v     | 669 | ILE  | CA-C-N  | 5.62  | 127.75      | 120.44   |
| 5   | v     | 669 | ILE  | C-N-CA  | 5.62  | 127.75      | 120.44   |
| 16  | Ai    | 169 | PRO  | N-CA-C  | -5.62 | 102.37      | 111.14   |
| 2   | D     | 25  | GLN  | N-CA-C  | 5.62  | 118.83      | 108.94   |
| 2   | Ch    | 331 | ASN  | CA-C-O  | -5.62 | 112.46      | 119.38   |
| 3   | I     | 153 | ILE  | N-CA-C  | 5.62  | 116.35      | 110.62   |
| 3   | E     | 662 | ILE  | CA-C-O  | -5.62 | 114.28      | 120.96   |
| 3   | I     | 670 | LEU  | CA-C-N  | -5.62 | 110.98      | 120.58   |
| 3   | I     | 670 | LEU  | C-N-CA  | -5.62 | 110.98      | 120.58   |
| 16  | c     | 29  | LEU  | N-CA-C  | -5.62 | 105.31      | 111.82   |
| 3   | BY    | 155 | THR  | N-CA-C  | -5.62 | 107.43      | 114.56   |
| 1   | A     | 217 | ILE  | N-CA-C  | -5.61 | 99.64       | 108.23   |
| 2   | D     | 331 | ASN  | CA-C-O  | -5.61 | 112.48      | 119.38   |
| 2   | k     | 21  | LEU  | N-CA-C  | -5.61 | 106.02      | 112.92   |
| 5   | AE    | 888 | ARG  | N-CA-C  | -5.61 | 105.16      | 111.28   |
| 1   | BD    | 42  | ARG  | N-CA-C  | -5.61 | 106.48      | 113.55   |
| 7   | Bm    | 333 | GLY  | CA-C-N  | 5.61  | 130.09      | 120.72   |
| 7   | Bm    | 333 | GLY  | C-N-CA  | 5.61  | 130.09      | 120.72   |
| 7   | Bm    | 542 | GLN  | N-CA-C  | -5.61 | 106.10      | 113.17   |
| 2   | Cd    | 21  | LEU  | CA-C-N  | 5.61  | 130.10      | 122.19   |
| 2   | Cd    | 21  | LEU  | C-N-CA  | 5.61  | 130.10      | 122.19   |
| 3   | E     | 64  | GLY  | N-CA-C  | -5.61 | 107.58      | 115.32   |
| 2   | f     | 21  | LEU  | CA-C-N  | 5.61  | 130.10      | 122.19   |
| 2   | f     | 21  | LEU  | C-N-CA  | 5.61  | 130.10      | 122.19   |
| 5   | 9     | 468 | PHE  | N-CA-C  | 5.61  | 118.79      | 108.58   |
| 5   | AE    | 493 | LEU  | N-CA-C  | -5.61 | 105.16      | 112.23   |
| 5   | L     | 577 | VAL  | CB-CA-C | -5.61 | 102.09      | 111.29   |
| 3   | BY    | 792 | GLN  | O-C-N   | -5.61 | 115.38      | 122.27   |
| 7   | O     | 202 | LEU  | CA-C-O  | -5.60 | 113.11      | 119.78   |
| 2   | k     | 11  | TYR  | N-CA-C  | -5.60 | 105.17      | 111.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AG    | 314 | ASP  | CA-C-N  | -5.60 | 114.67      | 123.13   |
| 7   | AG    | 314 | ASP  | C-N-CA  | -5.60 | 114.67      | 123.13   |
| 7   | AM    | 126 | ILE  | N-CA-C  | 5.60  | 116.80      | 108.23   |
| 2   | CW    | 331 | ASN  | CA-C-O  | -5.60 | 112.49      | 119.38   |
| 5   | AE    | 765 | GLN  | CA-C-O  | -5.60 | 111.94      | 119.11   |
| 5   | G     | 574 | PHE  | N-CA-C  | -5.60 | 100.17      | 109.46   |
| 16  | Z     | 72  | LEU  | CB-CA-C | -5.60 | 101.33      | 110.85   |
| 5   | 9     | 690 | TYR  | N-CA-C  | 5.60  | 122.03      | 113.19   |
| 16  | CI    | 155 | ILE  | N-CA-C  | 5.60  | 116.01      | 108.17   |
| 16  | CT    | 185 | GLN  | CA-C-N  | -5.60 | 111.80      | 120.31   |
| 16  | CT    | 185 | GLN  | C-N-CA  | -5.60 | 111.80      | 120.31   |
| 2   | D     | 278 | GLY  | N-CA-C  | 5.59  | 119.30      | 111.19   |
| 16  | c     | 149 | ILE  | N-CA-C  | -5.59 | 104.90      | 111.00   |
| 5   | AO    | 165 | GLY  | N-CA-C  | -5.59 | 102.47      | 111.59   |
| 16  | Aq    | 147 | LYS  | N-CA-C  | -5.59 | 105.18      | 112.23   |
| 5   | AB    | 213 | ILE  | N-CA-C  | 5.59  | 116.00      | 108.17   |
| 7   | AG    | 506 | GLN  | CA-C-N  | 5.59  | 125.26      | 119.56   |
| 7   | AG    | 506 | GLN  | C-N-CA  | 5.59  | 125.26      | 119.56   |
| 5   | Bf    | 493 | LEU  | N-CA-C  | -5.59 | 104.81      | 111.69   |
| 3   | I     | 660 | ILE  | CA-C-O  | -5.59 | 114.62      | 120.76   |
| 3   | 1     | 110 | TYR  | N-CA-CB | -5.59 | 101.44      | 110.71   |
| 3   | 1     | 713 | GLU  | N-CA-C  | -5.59 | 105.19      | 111.28   |
| 3   | E     | 670 | LEU  | CA-C-N  | -5.58 | 111.03      | 120.58   |
| 3   | E     | 670 | LEU  | C-N-CA  | -5.58 | 111.03      | 120.58   |
| 5   | R     | 280 | LEU  | CA-C-N  | 5.58  | 125.78      | 120.31   |
| 5   | R     | 280 | LEU  | C-N-CA  | 5.58  | 125.78      | 120.31   |
| 16  | Aq    | 132 | GLN  | CA-C-O  | -5.58 | 112.52      | 120.51   |
| 2   | CW    | 158 | LYS  | N-CA-C  | -5.58 | 104.00      | 112.04   |
| 5   | M     | 162 | THR  | CA-C-N  | 5.58  | 125.20      | 119.56   |
| 5   | M     | 162 | THR  | C-N-CA  | 5.58  | 125.20      | 119.56   |
| 1   | i     | 250 | VAL  | N-CA-C  | 5.58  | 115.93      | 108.11   |
| 3   | BY    | 709 | ASP  | N-CA-C  | 5.58  | 122.69      | 110.80   |
| 2   | z     | 310 | LYS  | N-CA-C  | -5.58 | 105.82      | 113.30   |
| 5   | Bf    | 442 | ILE  | N-CA-C  | -5.58 | 106.76      | 111.56   |
| 5   | Bf    | 554 | ILE  | CA-C-N  | -5.58 | 112.80      | 120.28   |
| 5   | Bf    | 554 | ILE  | C-N-CA  | -5.58 | 112.80      | 120.28   |
| 16  | c     | 132 | GLN  | CA-C-O  | -5.58 | 112.53      | 120.51   |
| 7   | AG    | 510 | VAL  | N-CA-C  | -5.58 | 105.67      | 111.58   |
| 5   | AO    | 191 | SER  | O-C-N   | -5.58 | 116.89      | 123.25   |
| 16  | Ai    | 142 | ASN  | CB-CA-C | -5.58 | 99.50       | 110.10   |
| 2   | Ch    | 318 | ILE  | CA-C-N  | -5.58 | 112.28      | 121.92   |
| 2   | Ch    | 318 | ILE  | C-N-CA  | -5.58 | 112.28      | 121.92   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | q     | 267 | GLU  | N-CA-C  | -5.57 | 107.02      | 113.88   |
| 3   | n     | 441 | PHE  | N-CA-C  | -5.57 | 104.61      | 111.40   |
| 2   | y     | 310 | LYS  | N-CA-C  | -5.57 | 105.84      | 113.30   |
| 1   | A     | 203 | LYS  | N-CA-C  | 5.57  | 118.30      | 109.50   |
| 2   | CW    | 83  | GLU  | N-CA-C  | -5.57 | 104.84      | 111.69   |
| 3   | BY    | 43  | TRP  | N-CA-C  | 5.57  | 116.97      | 108.12   |
| 5   | Bt    | 278 | PHE  | N-CA-C  | 5.57  | 117.47      | 108.34   |
| 1   | CP    | 202 | TYR  | CA-C-N  | -5.57 | 113.94      | 122.62   |
| 1   | CP    | 202 | TYR  | C-N-CA  | -5.57 | 113.94      | 122.62   |
| 1   | CP    | 69  | ASN  | N-CA-C  | -5.56 | 105.36      | 111.82   |
| 7   | AG    | 126 | ILE  | CB-CA-C | -5.56 | 104.23      | 110.96   |
| 7   | AG    | 126 | ILE  | N-CA-C  | 5.56  | 116.74      | 108.23   |
| 3   | 1     | 133 | VAL  | N-CA-C  | 5.56  | 116.13      | 108.12   |
| 2   | D     | 82  | ARG  | CA-C-O  | -5.56 | 112.96      | 119.24   |
| 16  | CM    | 131 | VAL  | N-CA-C  | -5.56 | 102.35      | 109.30   |
| 16  | Z     | 33  | LEU  | CB-CA-C | -5.55 | 101.42      | 110.85   |
| 5   | M     | 281 | PRO  | N-CA-C  | 5.54  | 119.72      | 111.41   |
| 1   | i     | 258 | ILE  | N-CA-C  | -5.54 | 105.70      | 111.58   |
| 5   | v     | 611 | PRO  | N-CA-C  | 5.54  | 123.89      | 112.47   |
| 3   | 7     | 832 | PHE  | N-CA-C  | -5.54 | 105.32      | 111.36   |
| 5   | L     | 586 | GLY  | CA-C-N  | 5.54  | 132.12      | 121.54   |
| 5   | L     | 586 | GLY  | C-N-CA  | 5.54  | 132.12      | 121.54   |
| 5   | M     | 209 | SER  | N-CA-C  | -5.54 | 106.02      | 112.89   |
| 16  | Z     | 119 | ARG  | N-CA-C  | -5.54 | 106.36      | 114.39   |
| 3   | 7     | 894 | GLN  | N-CA-C  | -5.54 | 105.32      | 111.36   |
| 2   | Cd    | 326 | ALA  | N-CA-C  | -5.54 | 105.24      | 111.28   |
| 5   | R     | 316 | PHE  | N-CA-C  | -5.54 | 105.14      | 111.07   |
| 5   | AU    | 163 | PRO  | N-CA-C  | 5.54  | 123.88      | 112.47   |
| 5   | G     | 496 | PHE  | N-CA-C  | -5.54 | 105.16      | 111.14   |
| 1   | Ca    | 318 | GLN  | N-CA-C  | -5.54 | 100.93      | 109.52   |
| 3   | E     | 112 | ILE  | CB-CA-C | -5.54 | 105.42      | 110.63   |
| 5   | L     | 765 | GLN  | CA-C-O  | -5.54 | 112.02      | 119.11   |
| 7   | J     | 557 | LEU  | CA-C-O  | -5.54 | 114.91      | 121.66   |
| 5   | G     | 626 | LYS  | N-CA-C  | -5.53 | 105.66      | 112.90   |
| 1   | i     | 281 | SER  | N-CA-C  | 5.53  | 115.41      | 108.45   |
| 7   | 4     | 318 | THR  | N-CA-C  | -5.53 | 106.90      | 113.97   |
| 5   | AB    | 300 | ILE  | CA-C-N  | -5.53 | 115.83      | 122.90   |
| 5   | AB    | 300 | ILE  | C-N-CA  | -5.53 | 115.83      | 122.90   |
| 5   | AB    | 274 | ILE  | N-CA-C  | 5.52  | 116.32      | 107.98   |
| 1   | A     | 6   | ILE  | N-CA-C  | -5.52 | 99.78       | 108.23   |
| 5   | AE    | 442 | ILE  | N-CA-C  | -5.52 | 106.81      | 111.56   |
| 7   | AM    | 174 | ASN  | N-CA-C  | 5.52  | 121.89      | 113.61   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AE    | 546 | PRO  | N-CA-C  | 5.52  | 117.43      | 110.70   |
| 5   | M     | 252 | GLY  | N-CA-C  | -5.51 | 103.54      | 112.31   |
| 2   | f     | 322 | LYS  | CA-C-N  | 5.51  | 125.22      | 119.82   |
| 2   | f     | 322 | LYS  | C-N-CA  | 5.51  | 125.22      | 119.82   |
| 2   | z     | 56  | ASN  | N-CA-C  | -5.51 | 105.42      | 111.82   |
| 3   | E     | 31  | ASP  | CA-C-N  | -5.51 | 115.92      | 123.14   |
| 3   | E     | 31  | ASP  | C-N-CA  | -5.51 | 115.92      | 123.14   |
| 2   | y     | 56  | ASN  | N-CA-C  | -5.51 | 105.42      | 111.82   |
| 1   | i     | 95  | LEU  | N-CA-C  | -5.51 | 105.28      | 112.23   |
| 16  | Ai    | 113 | SER  | N-CA-C  | -5.51 | 102.37      | 110.52   |
| 3   | E     | 73  | LYS  | N-CA-C  | -5.51 | 105.69      | 112.90   |
| 7   | AG    | 550 | MET  | N-CA-C  | 5.51  | 117.36      | 111.36   |
| 2   | q     | 358 | ARG  | N-CA-C  | 5.50  | 120.68      | 113.30   |
| 3   | I     | 805 | GLN  | CA-C-N  | 5.50  | 128.00      | 120.46   |
| 3   | I     | 805 | GLN  | C-N-CA  | 5.50  | 128.00      | 120.46   |
| 3   | 1     | 43  | TRP  | N-CA-C  | 5.50  | 116.87      | 108.12   |
| 5   | AB    | 87  | VAL  | CB-CA-C | -5.50 | 102.96      | 110.77   |
| 2   | q     | 277 | VAL  | N-CA-C  | 5.50  | 116.56      | 111.45   |
| 5   | G     | 464 | LEU  | CA-C-N  | 5.50  | 131.60      | 121.70   |
| 5   | G     | 464 | LEU  | C-N-CA  | 5.50  | 131.60      | 121.70   |
| 1   | i     | 202 | TYR  | CA-C-N  | -5.50 | 114.04      | 122.62   |
| 1   | i     | 202 | TYR  | C-N-CA  | -5.50 | 114.04      | 122.62   |
| 5   | AU    | 16  | GLU  | N-CA-C  | 5.50  | 117.98      | 111.33   |
| 1   | Ca    | 90  | GLN  | N-CA-C  | 5.50  | 119.99      | 113.28   |
| 1   | i     | 203 | LYS  | N-CA-C  | 5.49  | 118.18      | 109.50   |
| 5   | AB    | 87  | VAL  | N-CA-C  | 5.49  | 115.77      | 107.75   |
| 1   | BD    | 214 | ILE  | N-CA-C  | -5.49 | 106.45      | 111.67   |
| 2   | Cd    | 329 | GLN  | CA-C-O  | -5.49 | 112.65      | 120.51   |
| 3   | E     | 110 | TYR  | N-CA-CB | -5.49 | 101.60      | 110.71   |
| 2   | BK    | 318 | ILE  | CA-C-O  | -5.49 | 114.43      | 120.96   |
| 1   | CP    | 342 | ASN  | CA-C-N  | -5.49 | 113.23      | 122.29   |
| 1   | CP    | 342 | ASN  | C-N-CA  | -5.49 | 113.23      | 122.29   |
| 7   | Bm    | 98  | SER  | N-CA-C  | -5.49 | 102.05      | 110.01   |
| 3   | I     | 507 | CYS  | CA-C-N  | 5.49  | 126.70      | 119.84   |
| 3   | I     | 507 | CYS  | C-N-CA  | 5.49  | 126.70      | 119.84   |
| 3   | I     | 847 | LEU  | CA-C-O  | -5.49 | 113.14      | 119.56   |
| 5   | L     | 464 | LEU  | CA-C-N  | 5.48  | 131.57      | 121.70   |
| 5   | L     | 464 | LEU  | C-N-CA  | 5.48  | 131.57      | 121.70   |
| 5   | R     | 59  | VAL  | CA-C-O  | -5.48 | 114.69      | 120.39   |
| 5   | 9     | 609 | ASP  | CA-C-N  | 5.48  | 131.86      | 123.96   |
| 5   | 9     | 609 | ASP  | C-N-CA  | 5.48  | 131.86      | 123.96   |
| 5   | AO    | 284 | LYS  | N-CA-C  | -5.48 | 104.84      | 112.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | Az    | 142 | ASN  | N-CA-CB | 5.48  | 119.82      | 110.50   |
| 1   | A     | 202 | TYR  | CA-C-N  | -5.48 | 114.07      | 122.62   |
| 1   | A     | 202 | TYR  | C-N-CA  | -5.48 | 114.07      | 122.62   |
| 5   | v     | 434 | TYR  | N-CA-C  | 5.48  | 114.61      | 108.25   |
| 1   | Ca    | 126 | GLN  | N-CA-C  | 5.48  | 118.11      | 109.39   |
| 3   | 7     | 588 | LEU  | N-CA-C  | -5.48 | 104.95      | 111.69   |
| 3   | 7     | 538 | ILE  | CA-C-N  | -5.48 | 112.94      | 120.28   |
| 3   | 7     | 538 | ILE  | C-N-CA  | -5.48 | 112.94      | 120.28   |
| 3   | E     | 609 | TRP  | CA-C-O  | -5.48 | 111.93      | 119.05   |
| 5   | R     | 293 | PRO  | N-CA-C  | 5.48  | 121.75      | 113.81   |
| 3   | n     | 762 | GLU  | CB-CA-C | -5.48 | 101.70      | 110.79   |
| 7   | 4     | 65  | CYS  | N-CA-C  | 5.48  | 117.40      | 109.07   |
| 1   | Ca    | 342 | ASN  | CA-C-N  | -5.48 | 113.25      | 122.29   |
| 1   | Ca    | 342 | ASN  | C-N-CA  | -5.48 | 113.25      | 122.29   |
| 2   | D     | 281 | ASN  | N-CA-C  | 5.47  | 126.33      | 111.00   |
| 5   | R     | 207 | ASP  | N-CA-C  | -5.47 | 96.68       | 107.69   |
| 16  | Z     | 41  | ASP  | N-CA-C  | 5.47  | 117.31      | 110.91   |
| 1   | CP    | 257 | ILE  | CA-C-O  | -5.47 | 114.61      | 120.85   |
| 2   | f     | 73  | LEU  | N-CA-C  | -5.47 | 104.96      | 111.69   |
| 3   | n     | 782 | GLU  | N-CA-C  | -5.47 | 105.70      | 112.38   |
| 5   | AO    | 78  | VAL  | N-CA-C  | 5.47  | 115.77      | 108.11   |
| 16  | CM    | 68  | THR  | N-CA-C  | 5.47  | 118.53      | 110.59   |
| 5   | AO    | 295 | ASN  | N-CA-C  | -5.47 | 105.25      | 113.89   |
| 2   | BK    | 158 | LYS  | N-CA-C  | -5.47 | 105.32      | 111.28   |
| 3   | E     | 155 | THR  | N-CA-C  | -5.47 | 107.61      | 114.56   |
| 5   | 9     | 506 | PHE  | N-CA-C  | -5.47 | 106.74      | 113.41   |
| 7   | AG    | 523 | VAL  | N-CA-C  | 5.47  | 118.91      | 112.35   |
| 1   | CP    | 42  | ARG  | N-CA-C  | -5.47 | 106.66      | 113.55   |
| 7   | J     | 110 | ASP  | N-CA-C  | 5.47  | 120.60      | 113.88   |
| 3   | 7     | 296 | PRO  | N-CA-C  | -5.47 | 101.92      | 110.50   |
| 1   | C     | 203 | LYS  | N-CA-C  | 5.46  | 118.14      | 109.50   |
| 7   | AM    | 259 | ILE  | N-CA-C  | 5.46  | 115.97      | 107.99   |
| 5   | M     | 106 | SER  | N-CA-C  | 5.46  | 117.40      | 108.55   |
| 3   | BY    | 31  | ASP  | CA-C-N  | -5.46 | 115.98      | 123.14   |
| 3   | BY    | 31  | ASP  | C-N-CA  | -5.46 | 115.98      | 123.14   |
| 5   | Bf    | 611 | PRO  | CA-C-N  | 5.46  | 131.53      | 121.70   |
| 5   | Bf    | 611 | PRO  | C-N-CA  | 5.46  | 131.53      | 121.70   |
| 3   | 1     | 602 | ASP  | N-CA-C  | -5.46 | 104.17      | 112.04   |
| 1   | Ca    | 434 | ILE  | CB-CA-C | -5.46 | 105.20      | 112.46   |
| 3   | 7     | 713 | GLU  | N-CA-C  | -5.46 | 105.33      | 111.28   |
| 1   | C     | 37  | GLN  | CA-C-N  | -5.46 | 113.25      | 121.05   |
| 1   | C     | 37  | GLN  | C-N-CA  | -5.46 | 113.25      | 121.05   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | f     | 147 | ILE  | CB-CA-C | -5.46 | 104.98      | 111.97   |
| 2   | s     | 37  | LYS  | CA-C-N  | -5.46 | 112.05      | 121.66   |
| 2   | s     | 37  | LYS  | C-N-CA  | -5.46 | 112.05      | 121.66   |
| 5   | 9     | 554 | ILE  | CA-C-N  | -5.46 | 112.42      | 120.28   |
| 5   | 9     | 554 | ILE  | C-N-CA  | -5.46 | 112.42      | 120.28   |
| 5   | AB    | 257 | ILE  | CB-CA-C | -5.46 | 102.36      | 110.33   |
| 3   | 7     | 733 | LYS  | N-CA-C  | -5.46 | 107.19      | 112.97   |
| 5   | AE    | 611 | PRO  | N-CA-C  | 5.46  | 123.71      | 112.47   |
| 7   | AM    | 513 | ASN  | N-CA-C  | 5.46  | 118.77      | 111.24   |
| 5   | AE    | 588 | PHE  | N-CA-C  | 5.46  | 119.68      | 113.19   |
| 5   | AE    | 641 | PHE  | CA-C-O  | -5.46 | 114.64      | 120.42   |
| 7   | Bm    | 192 | SER  | N-CA-C  | 5.46  | 115.44      | 108.24   |
| 3   | I     | 785 | VAL  | N-CA-C  | -5.45 | 107.06      | 111.91   |
| 7   | Bm    | 255 | LYS  | CA-C-N  | -5.45 | 116.00      | 123.14   |
| 7   | Bm    | 255 | LYS  | C-N-CA  | -5.45 | 116.00      | 123.14   |
| 7   | 4     | 314 | ASP  | CB-CA-C | -5.45 | 104.15      | 112.11   |
| 16  | Av    | 109 | ARG  | N-CA-C  | 5.45  | 117.70      | 109.41   |
| 7   | O     | 76  | PHE  | CA-C-O  | -5.45 | 113.59      | 120.84   |
| 7   | 4     | 345 | PHE  | N-CA-C  | -5.45 | 106.63      | 113.28   |
| 1   | BD    | 324 | VAL  | CA-C-N  | -5.45 | 115.20      | 122.72   |
| 1   | BD    | 324 | VAL  | C-N-CA  | -5.45 | 115.20      | 122.72   |
| 5   | Bf    | 741 | GLU  | N-CA-C  | -5.45 | 105.42      | 111.36   |
| 7   | Bm    | 506 | GLN  | CA-C-N  | 5.45  | 125.12      | 119.56   |
| 7   | Bm    | 506 | GLN  | C-N-CA  | 5.45  | 125.12      | 119.56   |
| 3   | 7     | 609 | TRP  | CA-C-O  | -5.45 | 111.97      | 119.05   |
| 5   | Bt    | 16  | GLU  | N-CA-C  | 5.45  | 117.22      | 111.28   |
| 5   | AB    | 59  | VAL  | CA-C-O  | -5.45 | 114.49      | 120.48   |
| 2   | Ch    | 280 | ILE  | CA-C-O  | -5.45 | 113.97      | 120.78   |
| 5   | AE    | 787 | THR  | N-CA-C  | -5.44 | 105.35      | 111.28   |
| 1   | C     | 202 | TYR  | CA-C-N  | -5.44 | 114.13      | 122.62   |
| 1   | C     | 202 | TYR  | C-N-CA  | -5.44 | 114.13      | 122.62   |
| 3   | 7     | 672 | TYR  | N-CA-C  | -5.44 | 105.77      | 112.90   |
| 7   | J     | 542 | GLN  | N-CA-C  | -5.44 | 106.31      | 113.17   |
| 16  | Az    | 38  | LYS  | N-CA-C  | -5.44 | 105.74      | 112.38   |
| 5   | M     | 175 | GLY  | N-CA-C  | -5.44 | 107.81      | 115.32   |
| 3   | I     | 598 | VAL  | N-CA-CB | -5.44 | 105.43      | 111.41   |
| 3   | n     | 31  | ASP  | CA-C-N  | -5.44 | 116.02      | 123.14   |
| 3   | n     | 31  | ASP  | C-N-CA  | -5.44 | 116.02      | 123.14   |
| 7   | AM    | 38  | ALA  | CA-C-N  | -5.44 | 113.15      | 120.82   |
| 7   | AM    | 38  | ALA  | C-N-CA  | -5.44 | 113.15      | 120.82   |
| 5   | AO    | 157 | ALA  | N-CA-C  | 5.44  | 120.28      | 113.43   |
| 5   | Bf    | 602 | ASP  | N-CA-C  | -5.44 | 105.00      | 111.69   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | k     | 280 | ILE  | O-C-N   | -5.43 | 115.78      | 122.57   |
| 3   | 1     | 112 | ILE  | CB-CA-C | -5.43 | 105.52      | 110.63   |
| 5   | Bt    | 10  | VAL  | N-CA-C  | 5.43  | 115.91      | 111.62   |
| 5   | AB    | 300 | ILE  | N-CA-C  | 5.43  | 116.55      | 108.46   |
| 16  | CM    | 171 | PHE  | CA-C-N  | 5.43  | 131.48      | 121.70   |
| 16  | CM    | 171 | PHE  | C-N-CA  | 5.43  | 131.48      | 121.70   |
| 5   | M     | 43  | ASN  | N-CA-C  | 5.43  | 119.07      | 111.74   |
| 1   | i     | 358 | ILE  | N-CA-C  | 5.43  | 115.67      | 107.80   |
| 2   | D     | 318 | ILE  | CA-C-O  | -5.43 | 114.50      | 120.96   |
| 2   | CW    | 93  | LEU  | CA-C-O  | -5.43 | 112.16      | 119.11   |
| 16  | An    | 38  | LYS  | N-CA-C  | -5.43 | 104.76      | 111.33   |
| 3   | E     | 662 | ILE  | CA-C-N  | -5.43 | 112.06      | 120.31   |
| 3   | E     | 662 | ILE  | C-N-CA  | -5.43 | 112.06      | 120.31   |
| 16  | An    | 142 | ASN  | N-CA-CB | 5.43  | 119.72      | 110.50   |
| 2   | f     | 136 | GLU  | CA-C-N  | -5.42 | 112.59      | 120.29   |
| 2   | f     | 136 | GLU  | C-N-CA  | -5.42 | 112.59      | 120.29   |
| 5   | 9     | 584 | LEU  | CA-C-N  | -5.42 | 112.54      | 121.92   |
| 5   | 9     | 584 | LEU  | C-N-CA  | -5.42 | 112.54      | 121.92   |
| 5   | AB    | 303 | GLY  | N-CA-C  | -5.42 | 108.71      | 114.67   |
| 2   | CW    | 22  | HIS  | N-CA-C  | 5.42  | 119.06      | 111.74   |
| 5   | AB    | 293 | PRO  | N-CA-C  | 5.42  | 123.63      | 112.47   |
| 7   | AM    | 38  | ALA  | N-CA-C  | 5.42  | 118.72      | 111.24   |
| 5   | R     | 295 | ASN  | N-CA-C  | -5.42 | 105.70      | 114.09   |
| 5   | v     | 756 | TYR  | CA-C-O  | -5.42 | 113.22      | 119.56   |
| 5   | Bf    | 585 | SER  | N-CA-C  | -5.42 | 106.84      | 113.50   |
| 2   | CW    | 108 | ARG  | CA-C-N  | -5.42 | 113.02      | 120.28   |
| 2   | CW    | 108 | ARG  | C-N-CA  | -5.42 | 113.02      | 120.28   |
| 3   | I     | 894 | GLN  | N-CA-C  | -5.41 | 105.46      | 111.36   |
| 7   | J     | 345 | PHE  | N-CA-C  | -5.41 | 106.68      | 113.28   |
| 3   | n     | 526 | LEU  | O-C-N   | -5.41 | 116.54      | 122.38   |
| 5   | Bf    | 816 | ASP  | N-CA-C  | -5.41 | 105.46      | 111.36   |
| 3   | E     | 132 | GLN  | CA-C-N  | -5.41 | 115.47      | 122.99   |
| 3   | E     | 132 | GLN  | C-N-CA  | -5.41 | 115.47      | 122.99   |
| 2   | BK    | 93  | LEU  | CA-C-N  | -5.41 | 112.41      | 122.09   |
| 2   | BK    | 93  | LEU  | C-N-CA  | -5.41 | 112.41      | 122.09   |
| 7   | O     | 534 | GLU  | CA-C-N  | -5.41 | 113.03      | 120.28   |
| 7   | O     | 534 | GLU  | C-N-CA  | -5.41 | 113.03      | 120.28   |
| 2   | q     | 328 | SER  | N-CA-C  | -5.41 | 107.33      | 114.31   |
| 3   | 1     | 31  | ASP  | CA-C-N  | -5.41 | 116.06      | 123.14   |
| 3   | 1     | 31  | ASP  | C-N-CA  | -5.41 | 116.06      | 123.14   |
| 5   | L     | 894 | GLN  | N-CA-C  | -5.41 | 105.47      | 111.36   |
| 7   | O     | 244 | CYS  | CA-C-N  | -5.41 | 112.42      | 121.39   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | O     | 244 | CYS  | C-N-CA  | -5.41 | 112.42      | 121.39   |
| 2   | Cd    | 89  | SER  | N-CA-C  | -5.40 | 105.47      | 111.36   |
| 3   | BY    | 682 | GLN  | CB-CA-C | -5.40 | 103.70      | 111.91   |
| 5   | Bf    | 803 | ASP  | N-CA-C  | 5.40  | 118.33      | 111.69   |
| 16  | CI    | 132 | GLN  | CA-C-O  | -5.40 | 112.79      | 120.51   |
| 2   | D     | 120 | LYS  | CA-C-N  | 5.40  | 127.78      | 120.44   |
| 2   | D     | 120 | LYS  | C-N-CA  | 5.40  | 127.78      | 120.44   |
| 2   | k     | 113 | GLN  | N-CA-C  | -5.40 | 105.48      | 111.36   |
| 5   | AE    | 597 | TRP  | CA-C-O  | -5.40 | 113.03      | 119.35   |
| 5   | AO    | 56  | THR  | CA-C-N  | -5.40 | 115.49      | 122.99   |
| 5   | AO    | 56  | THR  | C-N-CA  | -5.40 | 115.49      | 122.99   |
| 7   | J     | 88  | HIS  | CB-CA-C | -5.39 | 104.23      | 112.11   |
| 5   | L     | 664 | THR  | CA-C-N  | 5.39  | 125.33      | 119.78   |
| 5   | L     | 664 | THR  | C-N-CA  | 5.39  | 125.33      | 119.78   |
| 7   | AM    | 114 | ARG  | CA-C-N  | -5.39 | 115.16      | 123.14   |
| 7   | AM    | 114 | ARG  | C-N-CA  | -5.39 | 115.16      | 123.14   |
| 7   | AG    | 332 | GLY  | N-CA-C  | -5.39 | 106.25      | 112.29   |
| 7   | AM    | 545 | SER  | N-CA-C  | -5.39 | 105.40      | 111.28   |
| 5   | Bt    | 59  | VAL  | CA-C-O  | -5.39 | 114.79      | 120.39   |
| 2   | f     | 290 | ASN  | N-CA-C  | -5.39 | 99.33       | 110.80   |
| 3   | 7     | 493 | TYR  | N-CA-C  | -5.39 | 105.57      | 111.82   |
| 7   | AG    | 88  | HIS  | CB-CA-C | -5.39 | 104.25      | 112.11   |
| 7   | Bm    | 110 | ASP  | N-CA-C  | 5.39  | 119.98      | 113.41   |
| 1   | A     | 213 | LEU  | N-CA-C  | 5.38  | 118.03      | 110.23   |
| 5   | AE    | 506 | PHE  | N-CA-C  | -5.38 | 106.84      | 113.41   |
| 16  | Av    | 153 | ALA  | CA-C-N  | 5.38  | 130.24      | 121.74   |
| 16  | Av    | 153 | ALA  | C-N-CA  | 5.38  | 130.24      | 121.74   |
| 7   | 4     | 109 | GLN  | CA-C-N  | 5.38  | 129.82      | 120.68   |
| 7   | 4     | 109 | GLN  | C-N-CA  | 5.38  | 129.82      | 120.68   |
| 16  | CT    | 27  | THR  | N-CA-C  | 5.38  | 116.45      | 108.86   |
| 2   | Cd    | 30  | GLU  | N-CA-C  | -5.38 | 106.39      | 113.17   |
| 7   | J     | 331 | THR  | N-CA-C  | 5.38  | 116.82      | 109.18   |
| 5   | 9     | 584 | LEU  | CA-C-O  | -5.38 | 115.24      | 120.89   |
| 5   | AB    | 222 | TYR  | N-CA-C  | 5.38  | 117.67      | 108.90   |
| 7   | Bm    | 38  | ALA  | N-CA-C  | 5.38  | 118.66      | 111.24   |
| 7   | AM    | 151 | ASP  | N-CA-C  | 5.38  | 122.25      | 110.80   |
| 16  | CI    | 37  | ILE  | N-CA-C  | -5.38 | 106.56      | 111.67   |
| 5   | L     | 584 | LEU  | CA-C-O  | -5.37 | 112.83      | 120.51   |
| 5   | AB    | 194 | GLU  | CA-C-N  | -5.37 | 115.05      | 122.30   |
| 5   | AB    | 194 | GLU  | C-N-CA  | -5.37 | 115.05      | 122.30   |
| 3   | n     | 752 | LYS  | N-CA-C  | 5.37  | 116.68      | 108.30   |
| 16  | CI    | 40  | GLN  | N-CA-C  | 5.37  | 116.82      | 110.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 7     | 144 | SER  | N-CA-C  | -5.37 | 102.25      | 110.14   |
| 5   | AE    | 926 | GLN  | N-CA-C  | -5.37 | 105.99      | 112.54   |
| 7   | O     | 200 | TRP  | CA-C-N  | 5.37  | 129.50      | 121.72   |
| 7   | O     | 200 | TRP  | C-N-CA  | 5.37  | 129.50      | 121.72   |
| 2   | k     | 48  | GLY  | N-CA-C  | -5.37 | 106.29      | 112.73   |
| 5   | AE    | 503 | SER  | O-C-N   | -5.37 | 116.40      | 123.16   |
| 16  | A7    | 185 | GLN  | CA-C-N  | -5.37 | 112.15      | 120.31   |
| 16  | A7    | 185 | GLN  | C-N-CA  | -5.37 | 112.15      | 120.31   |
| 16  | c     | 31  | LYS  | N-CA-C  | -5.36 | 107.28      | 113.88   |
| 2   | Cd    | 53  | LYS  | N-CA-C  | -5.36 | 105.43      | 111.28   |
| 7   | 4     | 76  | PHE  | CA-C-O  | -5.36 | 112.84      | 120.51   |
| 3   | 7     | 866 | ILE  | N-CA-C  | -5.36 | 105.16      | 111.00   |
| 2   | BR    | 104 | LEU  | N-CA-C  | -5.36 | 105.88      | 112.90   |
| 3   | BY    | 516 | MET  | CA-C-N  | 5.36  | 125.03      | 119.56   |
| 3   | BY    | 516 | MET  | C-N-CA  | 5.36  | 125.03      | 119.56   |
| 16  | CT    | 109 | ARG  | N-CA-C  | 5.36  | 117.54      | 109.23   |
| 7   | O     | 533 | THR  | CA-C-O  | -5.36 | 115.27      | 120.89   |
| 5   | 9     | 597 | TRP  | N-CA-C  | -5.36 | 106.25      | 112.89   |
| 7   | Bm    | 147 | LEU  | N-CA-C  | 5.35  | 117.99      | 110.23   |
| 5   | Bt    | 188 | THR  | N-CA-C  | -5.35 | 107.12      | 113.97   |
| 7   | J     | 506 | GLN  | CA-C-N  | 5.35  | 125.02      | 119.56   |
| 7   | J     | 506 | GLN  | C-N-CA  | 5.35  | 125.02      | 119.56   |
| 5   | Bt    | 261 | ASN  | CA-C-N  | 5.35  | 129.74      | 122.19   |
| 5   | Bt    | 261 | ASN  | C-N-CA  | 5.35  | 129.74      | 122.19   |
| 5   | L     | 539 | TYR  | N-CA-C  | 5.35  | 118.97      | 112.23   |
| 3   | BY    | 599 | VAL  | N-CA-CB | -5.35 | 102.41      | 111.50   |
| 3   | I     | 153 | ILE  | CB-CA-C | -5.35 | 104.92      | 112.14   |
| 5   | AO    | 312 | LEU  | N-CA-C  | -5.35 | 105.49      | 112.23   |
| 1   | A     | 434 | ILE  | CB-CA-C | -5.34 | 105.35      | 112.46   |
| 16  | CB    | 139 | LYS  | CA-C-O  | -5.34 | 112.87      | 120.51   |
| 1   | Ca    | 398 | LEU  | N-CA-C  | -5.34 | 103.44      | 110.39   |
| 7   | 4     | 521 | ASN  | CA-C-N  | 5.34  | 127.39      | 120.44   |
| 7   | 4     | 521 | ASN  | C-N-CA  | 5.34  | 127.39      | 120.44   |
| 5   | AE    | 465 | TYR  | CA-C-N  | 5.34  | 126.52      | 119.84   |
| 5   | AE    | 465 | TYR  | C-N-CA  | 5.34  | 126.52      | 119.84   |
| 7   | AG    | 542 | GLN  | N-CA-C  | -5.34 | 106.44      | 113.17   |
| 5   | AU    | 319 | GLU  | CA-C-N  | 5.34  | 131.74      | 121.54   |
| 5   | AU    | 319 | GLU  | C-N-CA  | 5.34  | 131.74      | 121.54   |
| 16  | Aq    | 144 | ILE  | CB-CA-C | -5.34 | 107.17      | 111.71   |
| 2   | f     | 91  | ILE  | N-CA-CB | 5.34  | 118.59      | 110.58   |
| 3   | 7     | 459 | LEU  | CA-C-N  | 5.34  | 125.03      | 119.64   |
| 3   | 7     | 459 | LEU  | C-N-CA  | 5.34  | 125.03      | 119.64   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AB    | 261 | ASN  | N-CA-C  | -5.34 | 106.35      | 112.92   |
| 1   | C     | 364 | VAL  | N-CA-C  | 5.34  | 119.51      | 112.04   |
| 5   | M     | 1   | MET  | CA-C-N  | 5.34  | 131.31      | 121.70   |
| 5   | M     | 1   | MET  | C-N-CA  | 5.34  | 131.31      | 121.70   |
| 5   | L     | 638 | LEU  | N-CA-C  | -5.34 | 105.13      | 111.69   |
| 5   | AO    | 305 | GLY  | N-CA-C  | -5.34 | 108.34      | 114.69   |
| 16  | Av    | 39  | HIS  | N-CA-C  | -5.34 | 98.68       | 108.02   |
| 5   | Bf    | 765 | GLN  | CA-C-O  | -5.33 | 112.28      | 119.11   |
| 5   | G     | 646 | ASN  | CA-C-N  | 5.33  | 124.95      | 119.56   |
| 5   | G     | 646 | ASN  | C-N-CA  | 5.33  | 124.95      | 119.56   |
| 3   | n     | 451 | VAL  | CB-CA-C | -5.33 | 105.06      | 112.04   |
| 3   | n     | 670 | LEU  | CA-C-O  | -5.33 | 112.70      | 119.31   |
| 5   | G     | 624 | TYR  | N-CA-C  | -5.33 | 105.55      | 111.36   |
| 3   | l     | 660 | ILE  | CA-C-O  | -5.33 | 114.90      | 120.76   |
| 16  | c     | 108 | LEU  | CB-CA-C | -5.33 | 103.81      | 111.91   |
| 1   | CP    | 208 | HIS  | N-CA-C  | -5.33 | 103.32      | 109.93   |
| 1   | CP    | 214 | ILE  | N-CA-C  | -5.33 | 107.23      | 111.81   |
| 16  | Az    | 169 | PRO  | N-CA-C  | -5.33 | 102.83      | 111.14   |
| 5   | G     | 442 | ILE  | N-CA-C  | -5.33 | 106.98      | 111.56   |
| 5   | v     | 573 | ASN  | N-CA-C  | 5.33  | 118.93      | 111.74   |
| 5   | AO    | 209 | SER  | N-CA-C  | -5.33 | 106.63      | 113.23   |
| 2   | s     | 27  | LEU  | N-CA-C  | 5.32  | 118.26      | 109.85   |
| 3   | E     | 471 | ARG  | CA-C-O  | -5.32 | 113.12      | 120.52   |
| 3   | I     | 837 | MET  | CA-C-O  | -5.32 | 114.89      | 121.06   |
| 5   | AU    | 102 | GLY  | N-CA-C  | -5.32 | 105.65      | 114.48   |
| 16  | CB    | 35  | TYR  | N-CA-C  | 5.32  | 113.86      | 108.75   |
| 1   | CP    | 126 | GLN  | N-CA-C  | 5.32  | 117.77      | 108.52   |
| 5   | R     | 194 | GLU  | CA-C-N  | -5.32 | 115.35      | 122.42   |
| 5   | R     | 194 | GLU  | C-N-CA  | -5.32 | 115.35      | 122.42   |
| 2   | Ch    | 357 | ARG  | CA-C-O  | -5.32 | 113.34      | 119.56   |
| 16  | Z     | 147 | LYS  | CA-C-N  | -5.32 | 111.64      | 120.68   |
| 16  | Z     | 147 | LYS  | C-N-CA  | -5.32 | 111.64      | 120.68   |
| 7   | AG    | 152 | ASP  | CB-CA-C | -5.32 | 104.64      | 111.50   |
| 7   | AG    | 239 | HIS  | CA-C-N  | 5.32  | 125.64      | 119.47   |
| 7   | AG    | 239 | HIS  | C-N-CA  | 5.32  | 125.64      | 119.47   |
| 7   | J     | 166 | MET  | N-CA-CB | -5.31 | 102.61      | 110.53   |
| 3   | l     | 128 | ILE  | N-CA-C  | -5.31 | 101.88      | 108.89   |
| 1   | A     | 179 | MET  | N-CA-C  | -5.31 | 104.39      | 112.04   |
| 2   | BR    | 321 | SER  | N-CA-C  | 5.31  | 119.86      | 112.90   |
| 3   | I     | 831 | LYS  | N-CA-C  | -5.31 | 105.57      | 111.36   |
| 5   | L     | 930 | ILE  | N-CA-C  | -5.31 | 105.36      | 110.72   |
| 2   | y     | 14  | LEU  | CA-C-N  | 5.31  | 127.39      | 120.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | y     | 14  | LEU  | C-N-CA  | 5.31  | 127.39      | 120.28   |
| 7   | J     | 246 | ILE  | N-CA-CB | -5.31 | 104.74      | 111.64   |
| 2   | s     | 91  | ILE  | N-CA-C  | -5.31 | 105.36      | 110.72   |
| 16  | CM    | 173 | ILE  | CA-C-N  | 5.31  | 131.25      | 121.70   |
| 16  | CM    | 173 | ILE  | C-N-CA  | 5.31  | 131.25      | 121.70   |
| 2   | Cd    | 48  | GLY  | N-CA-C  | -5.31 | 106.29      | 113.24   |
| 1   | C     | 388 | TRP  | N-CA-CB | 5.30  | 117.00      | 110.53   |
| 5   | R     | 256 | GLY  | N-CA-C  | -5.30 | 104.94      | 112.37   |
| 2   | f     | 265 | ASP  | CA-C-N  | -5.30 | 113.66      | 120.34   |
| 2   | f     | 265 | ASP  | C-N-CA  | -5.30 | 113.66      | 120.34   |
| 2   | k     | 280 | ILE  | CA-C-O  | -5.30 | 114.15      | 120.78   |
| 7   | AG    | 345 | PHE  | N-CA-C  | -5.30 | 106.81      | 113.28   |
| 3   | BY    | 755 | ALA  | CA-C-O  | -5.30 | 114.80      | 120.42   |
| 16  | CI    | 185 | GLN  | CA-C-N  | -5.30 | 112.25      | 120.31   |
| 16  | CI    | 185 | GLN  | C-N-CA  | -5.30 | 112.25      | 120.31   |
| 7   | 4     | 233 | VAL  | N-CA-C  | -5.30 | 102.21      | 109.37   |
| 3   | n     | 558 | VAL  | N-CA-C  | 5.30  | 120.36      | 109.34   |
| 2   | q     | 9   | ARG  | N-CA-C  | -5.30 | 105.50      | 111.28   |
| 2   | D     | 108 | ARG  | CA-C-N  | -5.30 | 112.77      | 120.29   |
| 2   | D     | 108 | ARG  | C-N-CA  | -5.30 | 112.77      | 120.29   |
| 3   | 1     | 32  | VAL  | N-CA-C  | 5.30  | 115.53      | 108.11   |
| 3   | 1     | 516 | MET  | CA-C-N  | 5.30  | 124.96      | 119.56   |
| 3   | 1     | 516 | MET  | C-N-CA  | 5.30  | 124.96      | 119.56   |
| 7   | Bm    | 186 | ARG  | CB-CA-C | -5.30 | 102.20      | 110.94   |
| 16  | Aq    | 109 | ARG  | N-CA-C  | 5.30  | 117.44      | 109.23   |
| 7   | Bm    | 165 | PHE  | N-CA-C  | -5.30 | 101.02      | 109.07   |
| 1   | Ca    | 200 | ILE  | N-CA-C  | 5.30  | 116.02      | 110.62   |
| 1   | i     | 174 | PHE  | N-CA-C  | 5.29  | 118.06      | 108.69   |
| 5   | Bt    | 38  | VAL  | CA-C-N  | -5.29 | 113.19      | 121.87   |
| 5   | Bt    | 38  | VAL  | C-N-CA  | -5.29 | 113.19      | 121.87   |
| 2   | s     | 265 | ASP  | O-C-N   | -5.29 | 116.51      | 122.12   |
| 5   | AO    | 291 | ILE  | N-CA-C  | 5.29  | 115.58      | 108.17   |
| 2   | z     | 14  | LEU  | CA-C-N  | 5.29  | 127.37      | 120.28   |
| 2   | z     | 14  | LEU  | C-N-CA  | 5.29  | 127.37      | 120.28   |
| 5   | AU    | 141 | GLN  | CA-C-N  | 5.29  | 129.65      | 122.19   |
| 5   | AU    | 141 | GLN  | C-N-CA  | 5.29  | 129.65      | 122.19   |
| 2   | Ch    | 278 | GLY  | N-CA-C  | 5.29  | 118.86      | 111.19   |
| 7   | J     | 158 | TRP  | N-CA-C  | 5.29  | 122.06      | 110.80   |
| 3   | 1     | 339 | GLN  | N-CA-C  | 5.29  | 117.05      | 111.28   |
| 5   | AB    | 242 | THR  | N-CA-C  | -5.29 | 107.48      | 114.04   |
| 7   | AM    | 285 | TYR  | CA-C-N  | -5.29 | 114.60      | 122.74   |
| 7   | AM    | 285 | TYR  | C-N-CA  | -5.29 | 114.60      | 122.74   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | Ca    | 414 | LYS  | N-CA-C  | -5.29 | 105.60      | 111.36   |
| 2   | s     | 14  | LEU  | CA-C-N  | 5.29  | 127.36      | 120.28   |
| 2   | s     | 14  | LEU  | C-N-CA  | 5.29  | 127.36      | 120.28   |
| 5   | v     | 762 | LEU  | N-CA-C  | -5.29 | 106.33      | 112.89   |
| 2   | y     | 86  | ASN  | N-CA-C  | -5.29 | 105.19      | 111.69   |
| 5   | AE    | 622 | ILE  | CA-C-O  | -5.29 | 115.89      | 121.44   |
| 5   | Bf    | 764 | ARG  | N-CA-C  | -5.29 | 105.60      | 111.36   |
| 7   | Bm    | 202 | LEU  | CA-C-O  | -5.29 | 112.89      | 119.28   |
| 16  | Z     | 172 | ASP  | N-CA-CB | 5.28  | 119.48      | 110.50   |
| 3   | 1     | 144 | SER  | N-CA-C  | -5.28 | 102.37      | 110.14   |
| 3   | 7     | 816 | ASP  | N-CA-C  | -5.28 | 105.60      | 111.36   |
| 16  | CB    | 35  | TYR  | CB-CA-C | -5.28 | 108.76      | 116.53   |
| 3   | n     | 752 | LYS  | CA-C-N  | 5.28  | 129.05      | 120.60   |
| 3   | n     | 752 | LYS  | C-N-CA  | 5.28  | 129.05      | 120.60   |
| 5   | AO    | 249 | PHE  | N-CA-C  | 5.28  | 118.30      | 110.48   |
| 1   | i     | 131 | ASN  | CA-C-N  | 5.28  | 125.20      | 119.76   |
| 1   | i     | 131 | ASN  | C-N-CA  | 5.28  | 125.20      | 119.76   |
| 3   | BY    | 660 | ILE  | CA-C-O  | -5.28 | 114.95      | 120.76   |
| 16  | CT    | 186 | LEU  | N-CA-C  | -5.28 | 105.69      | 111.82   |
| 16  | c     | 60  | GLU  | N-CA-C  | 5.28  | 118.29      | 110.48   |
| 16  | Ai    | 132 | GLN  | CA-C-N  | -5.28 | 113.87      | 121.42   |
| 16  | Ai    | 132 | GLN  | C-N-CA  | -5.28 | 113.87      | 121.42   |
| 3   | BY    | 736 | ASN  | N-CA-C  | -5.28 | 105.61      | 111.36   |
| 7   | J     | 524 | PRO  | N-CA-C  | -5.28 | 103.16      | 111.34   |
| 2   | z     | 308 | LEU  | CA-C-N  | 5.28  | 131.20      | 121.70   |
| 2   | z     | 308 | LEU  | C-N-CA  | 5.28  | 131.20      | 121.70   |
| 3   | n     | 331 | ILE  | CB-CA-C | -5.28 | 105.22      | 111.97   |
| 5   | 9     | 618 | THR  | N-CA-C  | -5.28 | 105.42      | 111.07   |
| 5   | AU    | 289 | PHE  | N-CA-C  | 5.28  | 117.09      | 109.07   |
| 3   | BY    | 331 | ILE  | CB-CA-C | -5.28 | 105.22      | 111.97   |
| 5   | v     | 765 | GLN  | CA-C-O  | -5.27 | 112.36      | 119.11   |
| 2   | z     | 86  | ASN  | N-CA-C  | -5.27 | 105.20      | 111.69   |
| 7   | J     | 314 | ASP  | CB-CA-C | -5.27 | 104.80      | 111.86   |
| 1   | CP    | 281 | SER  | N-CA-C  | 5.27  | 115.09      | 108.45   |
| 3   | 1     | 331 | ILE  | N-CA-CB | 5.27  | 116.71      | 110.55   |
| 2   | BR    | 48  | GLY  | N-CA-C  | -5.27 | 106.27      | 113.27   |
| 5   | Bt    | 209 | SER  | N-CA-C  | -5.27 | 106.36      | 112.89   |
| 5   | M     | 237 | LEU  | CA-C-N  | 5.26  | 125.26      | 119.89   |
| 5   | M     | 237 | LEU  | C-N-CA  | 5.26  | 125.26      | 119.89   |
| 3   | n     | 493 | TYR  | N-CA-C  | -5.26 | 105.71      | 111.82   |
| 16  | Ai    | 71  | SER  | N-CA-C  | -5.26 | 105.54      | 111.28   |
| 16  | CM    | 141 | LYS  | O-C-N   | -5.26 | 115.59      | 122.59   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 59  | ASP  | CA-C-N  | 5.26  | 129.61      | 122.19   |
| 1   | A     | 59  | ASP  | C-N-CA  | 5.26  | 129.61      | 122.19   |
| 3   | 1     | 294 | GLU  | N-CA-C  | 5.26  | 119.25      | 112.41   |
| 16  | Z     | 68  | THR  | N-CA-C  | 5.26  | 117.32      | 110.53   |
| 2   | y     | 308 | LEU  | CA-C-N  | 5.26  | 131.17      | 121.70   |
| 2   | y     | 308 | LEU  | C-N-CA  | 5.26  | 131.17      | 121.70   |
| 16  | Ai    | 118 | HIS  | N-CA-C  | 5.26  | 122.00      | 110.80   |
| 5   | AO    | 242 | THR  | N-CA-C  | -5.26 | 107.41      | 113.88   |
| 1   | Ca    | 196 | TRP  | CB-CA-C | -5.26 | 101.44      | 110.22   |
| 3   | E     | 32  | VAL  | N-CA-C  | 5.25  | 115.47      | 108.11   |
| 5   | AE    | 756 | TYR  | CA-C-O  | -5.25 | 113.41      | 119.56   |
| 5   | Bt    | 349 | LEU  | N-CA-CB | 5.25  | 119.21      | 111.43   |
| 1   | i     | 90  | GLN  | N-CA-C  | 5.25  | 119.69      | 113.28   |
| 7   | Bm    | 513 | ASN  | N-CA-C  | 5.25  | 118.49      | 111.24   |
| 3   | 1     | 493 | TYR  | N-CA-C  | -5.25 | 105.73      | 111.82   |
| 3   | 1     | 125 | THR  | N-CA-C  | -5.25 | 101.39      | 109.52   |
| 3   | 1     | 666 | LEU  | CA-C-N  | -5.25 | 111.86      | 121.52   |
| 3   | 1     | 666 | LEU  | C-N-CA  | -5.25 | 111.86      | 121.52   |
| 5   | AU    | 59  | VAL  | O-C-N   | -5.25 | 116.96      | 123.10   |
| 7   | AM    | 126 | ILE  | CB-CA-C | -5.25 | 104.61      | 110.96   |
| 3   | I     | 51  | ASP  | N-CA-C  | 5.24  | 117.63      | 110.55   |
| 5   | v     | 474 | LYS  | N-CA-C  | -5.24 | 106.57      | 113.12   |
| 5   | L     | 474 | LYS  | N-CA-C  | -5.24 | 106.95      | 113.55   |
| 7   | O     | 46  | HIS  | CA-C-N  | 5.24  | 128.99      | 120.60   |
| 7   | O     | 46  | HIS  | C-N-CA  | 5.24  | 128.99      | 120.60   |
| 1   | A     | 131 | ASN  | CA-C-N  | 5.24  | 125.16      | 119.76   |
| 1   | A     | 131 | ASN  | C-N-CA  | 5.24  | 125.16      | 119.76   |
| 5   | AE    | 435 | PRO  | N-CA-C  | -5.24 | 102.97      | 111.19   |
| 5   | AU    | 290 | ASP  | CB-CA-C | -5.24 | 102.71      | 110.62   |
| 2   | BK    | 20  | GLU  | N-CA-C  | -5.24 | 106.39      | 112.89   |
| 5   | Bt    | 322 | GLN  | N-CA-C  | -5.24 | 105.47      | 111.07   |
| 3   | I     | 128 | ILE  | N-CA-C  | -5.24 | 101.98      | 108.89   |
| 2   | BR    | 274 | ARG  | CA-C-N  | 5.24  | 131.13      | 121.70   |
| 2   | BR    | 274 | ARG  | C-N-CA  | 5.24  | 131.13      | 121.70   |
| 7   | J     | 76  | PHE  | CA-C-O  | -5.24 | 113.02      | 120.51   |
| 7   | O     | 51  | THR  | CB-CA-C | -5.24 | 100.55      | 109.03   |
| 5   | 9     | 611 | PRO  | CA-C-O  | -5.24 | 117.35      | 121.38   |
| 3   | E     | 740 | GLN  | CB-CA-C | -5.23 | 102.56      | 110.83   |
| 3   | n     | 445 | PRO  | N-CA-C  | 5.23  | 118.55      | 111.22   |
| 1   | BD    | 202 | TYR  | CA-C-N  | -5.23 | 113.66      | 122.29   |
| 1   | BD    | 202 | TYR  | C-N-CA  | -5.23 | 113.66      | 122.29   |
| 16  | CI    | 132 | GLN  | N-CA-C  | -5.23 | 99.66       | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | BY    | 301 | ILE  | N-CA-C  | 5.23  | 115.84      | 108.36   |
| 7   | Bm    | 169 | PHE  | N-CA-C  | 5.23  | 116.36      | 108.46   |
| 2   | Cd    | 308 | LEU  | CA-C-N  | 5.23  | 131.11      | 121.70   |
| 2   | Cd    | 308 | LEU  | C-N-CA  | 5.23  | 131.11      | 121.70   |
| 5   | 9     | 612 | GLU  | CA-C-N  | -5.23 | 111.99      | 120.72   |
| 5   | 9     | 612 | GLU  | C-N-CA  | -5.23 | 111.99      | 120.72   |
| 5   | AE    | 584 | LEU  | CA-C-O  | -5.23 | 113.65      | 119.40   |
| 2   | BK    | 360 | GLN  | N-CA-C  | 5.23  | 121.94      | 110.80   |
| 3   | n     | 735 | LEU  | N-CA-C  | -5.22 | 105.67      | 111.36   |
| 3   | 7     | 211 | LYS  | N-CA-C  | -5.22 | 105.19      | 112.45   |
| 7   | AM    | 187 | LEU  | N-CA-C  | 5.22  | 118.46      | 110.20   |
| 3   | I     | 837 | MET  | O-C-N   | -5.22 | 117.21      | 123.27   |
| 5   | AE    | 729 | ILE  | N-CA-C  | -5.22 | 105.62      | 110.53   |
| 7   | Bm    | 98  | SER  | CB-CA-C | 5.22  | 118.90      | 109.61   |
| 1   | C     | 417 | LYS  | N-CA-C  | -5.22 | 107.58      | 114.31   |
| 5   | M     | 207 | ASP  | N-CA-C  | -5.22 | 97.20       | 107.69   |
| 3   | 1     | 114 | SER  | N-CA-C  | -5.22 | 106.15      | 112.88   |
| 16  | An    | 97  | ILE  | N-CA-C  | -5.22 | 105.76      | 110.82   |
| 2   | Cd    | 272 | LYS  | CA-C-N  | 5.22  | 129.43      | 120.72   |
| 2   | Cd    | 272 | LYS  | C-N-CA  | 5.22  | 129.43      | 120.72   |
| 3   | 7     | 677 | PRO  | N-CA-C  | -5.21 | 105.46      | 110.47   |
| 7   | AM    | 180 | VAL  | N-CA-C  | 5.21  | 115.36      | 107.75   |
| 3   | n     | 660 | ILE  | CA-C-O  | -5.21 | 115.03      | 120.76   |
| 1   | A     | 76  | LYS  | N-CA-C  | 5.21  | 116.89      | 108.34   |
| 5   | AO    | 124 | THR  | N-CA-C  | -5.21 | 106.83      | 114.39   |
| 7   | 4     | 541 | GLN  | O-C-N   | -5.21 | 116.12      | 122.22   |
| 16  | Z     | 29  | LEU  | CA-C-N  | 5.21  | 125.72      | 119.94   |
| 16  | Z     | 29  | LEU  | C-N-CA  | 5.21  | 125.72      | 119.94   |
| 2   | Ch    | 280 | ILE  | O-C-N   | -5.21 | 116.06      | 122.57   |
| 7   | AM    | 345 | PHE  | CA-C-O  | -5.21 | 112.99      | 119.18   |
| 1   | C     | 398 | LEU  | CA-C-N  | 5.20  | 126.55      | 120.98   |
| 1   | C     | 398 | LEU  | C-N-CA  | 5.20  | 126.55      | 120.98   |
| 3   | E     | 526 | LEU  | O-C-N   | -5.20 | 116.76      | 122.38   |
| 7   | 4     | 88  | HIS  | CB-CA-C | -5.20 | 104.08      | 112.09   |
| 3   | BY    | 833 | ILE  | CA-C-N  | 5.20  | 127.25      | 120.28   |
| 3   | BY    | 833 | ILE  | C-N-CA  | 5.20  | 127.25      | 120.28   |
| 1   | C     | 217 | ILE  | N-CA-C  | -5.20 | 100.27      | 108.23   |
| 7   | AG    | 328 | TYR  | N-CA-CB | -5.20 | 103.00      | 111.22   |
| 5   | Bt    | 235 | PHE  | N-CA-C  | 5.20  | 116.43      | 108.42   |
| 2   | CW    | 325 | ILE  | N-CA-CB | -5.20 | 107.38      | 111.64   |
| 2   | Cd    | 310 | LYS  | N-CA-C  | -5.20 | 106.33      | 113.30   |
| 7   | AG    | 200 | TRP  | CA-C-N  | 5.20  | 129.33      | 122.42   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AG    | 200 | TRP  | C-N-CA  | 5.20  | 129.33      | 122.42   |
| 2   | Ch    | 93  | LEU  | CA-C-O  | -5.20 | 112.46      | 119.11   |
| 3   | I     | 110 | TYR  | N-CA-CB | -5.20 | 102.09      | 110.71   |
| 7   | J     | 76  | PHE  | CA-C-N  | -5.20 | 109.12      | 121.80   |
| 7   | J     | 76  | PHE  | C-N-CA  | -5.20 | 109.12      | 121.80   |
| 7   | AM    | 325 | SER  | CA-C-N  | -5.20 | 113.79      | 122.62   |
| 7   | AM    | 325 | SER  | C-N-CA  | -5.20 | 113.79      | 122.62   |
| 1   | A     | 69  | ASN  | N-CA-C  | -5.19 | 106.90      | 113.18   |
| 5   | G     | 506 | PHE  | N-CA-C  | -5.19 | 107.08      | 113.41   |
| 5   | L     | 588 | PHE  | N-CA-C  | 5.19  | 119.48      | 113.20   |
| 5   | R     | 237 | LEU  | CA-C-N  | 5.19  | 125.18      | 119.89   |
| 5   | R     | 237 | LEU  | C-N-CA  | 5.19  | 125.18      | 119.89   |
| 1   | BD    | 60  | ASN  | N-CA-CB | -5.19 | 104.29      | 112.13   |
| 3   | BY    | 538 | ILE  | CA-C-N  | -5.19 | 113.32      | 120.28   |
| 3   | BY    | 538 | ILE  | C-N-CA  | -5.19 | 113.32      | 120.28   |
| 3   | 7     | 128 | ILE  | N-CA-C  | -5.19 | 102.04      | 108.89   |
| 2   | BR    | 313 | THR  | CA-C-O  | -5.19 | 114.00      | 119.97   |
| 5   | G     | 622 | ILE  | CA-C-O  | -5.19 | 116.22      | 121.67   |
| 7   | AM    | 239 | HIS  | N-CA-C  | -5.19 | 102.63      | 109.84   |
| 5   | Bf    | 583 | PHE  | N-CA-C  | -5.19 | 107.02      | 113.55   |
| 3   | E     | 147 | ASN  | N-CA-C  | 5.18  | 117.05      | 108.13   |
| 7   | 4     | 38  | ALA  | CA-C-N  | -5.18 | 113.51      | 120.82   |
| 7   | 4     | 38  | ALA  | C-N-CA  | -5.18 | 113.51      | 120.82   |
| 5   | AO    | 181 | ASN  | N-CA-C  | -5.18 | 100.64      | 108.67   |
| 16  | A7    | 129 | LEU  | N-CA-C  | 5.18  | 117.01      | 111.36   |
| 3   | BY    | 90  | PHE  | CA-C-N  | 5.18  | 129.79      | 123.10   |
| 3   | BY    | 90  | PHE  | C-N-CA  | 5.18  | 129.79      | 123.10   |
| 1   | Ca    | 388 | TRP  | N-CA-CB | 5.18  | 117.57      | 110.57   |
| 1   | i     | 164 | TYR  | N-CA-C  | -5.18 | 100.72      | 108.96   |
| 5   | v     | 577 | VAL  | CA-C-N  | 5.18  | 127.53      | 120.54   |
| 5   | v     | 577 | VAL  | C-N-CA  | 5.18  | 127.53      | 120.54   |
| 5   | AB    | 138 | TRP  | N-CA-C  | 5.18  | 116.94      | 109.07   |
| 3   | E     | 599 | VAL  | CA-C-N  | -5.18 | 114.39      | 122.05   |
| 3   | E     | 599 | VAL  | C-N-CA  | -5.18 | 114.39      | 122.05   |
| 3   | I     | 670 | LEU  | CA-C-O  | -5.18 | 112.89      | 119.31   |
| 5   | AB    | 267 | ILE  | N-CA-C  | 5.18  | 115.36      | 108.11   |
| 3   | BY    | 493 | TYR  | N-CA-C  | -5.18 | 105.76      | 111.71   |
| 7   | Bm    | 306 | GLN  | N-CA-C  | -5.18 | 102.62      | 110.28   |
| 3   | n     | 765 | GLU  | N-CA-C  | 5.17  | 119.65      | 113.23   |
| 2   | CW    | 29  | ILE  | CA-C-N  | -5.17 | 113.36      | 120.71   |
| 2   | CW    | 29  | ILE  | C-N-CA  | -5.17 | 113.36      | 120.71   |
| 3   | E     | 97  | TYR  | N-CA-C  | -5.17 | 104.56      | 111.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 756 | TYR  | CA-C-O  | -5.17 | 113.51      | 119.56   |
| 7   | 4     | 76  | PHE  | CA-C-N  | -5.17 | 109.19      | 121.80   |
| 7   | 4     | 76  | PHE  | C-N-CA  | -5.17 | 109.19      | 121.80   |
| 3   | E     | 331 | ILE  | CB-CA-C | -5.17 | 105.36      | 111.97   |
| 5   | L     | 645 | GLN  | CA-C-N  | 5.17  | 127.67      | 120.65   |
| 5   | L     | 645 | GLN  | C-N-CA  | 5.17  | 127.67      | 120.65   |
| 2   | s     | 332 | VAL  | N-CA-C  | -5.17 | 105.37      | 111.00   |
| 1   | CP    | 414 | LYS  | N-CA-C  | -5.17 | 105.73      | 111.36   |
| 3   | BY    | 803 | ALA  | N-CA-C  | -5.17 | 106.66      | 113.17   |
| 7   | AM    | 521 | ASN  | CA-C-N  | 5.16  | 127.15      | 120.44   |
| 7   | AM    | 521 | ASN  | C-N-CA  | 5.16  | 127.15      | 120.44   |
| 1   | C     | 334 | ALA  | N-CA-C  | -5.16 | 102.05      | 110.20   |
| 3   | 7     | 797 | GLU  | N-CA-C  | -5.16 | 105.66      | 111.28   |
| 7   | Bm    | 305 | ARG  | N-CA-C  | 5.16  | 116.92      | 109.07   |
| 5   | AO    | 186 | GLU  | CA-C-N  | -5.16 | 116.30      | 122.90   |
| 5   | AO    | 186 | GLU  | C-N-CA  | -5.16 | 116.30      | 122.90   |
| 2   | s     | 136 | GLU  | CA-C-N  | -5.16 | 111.76      | 120.58   |
| 2   | s     | 136 | GLU  | C-N-CA  | -5.16 | 111.76      | 120.58   |
| 5   | R     | 208 | SER  | N-CA-C  | 5.16  | 118.69      | 110.70   |
| 5   | AO    | 59  | VAL  | CA-C-O  | -5.16 | 114.81      | 120.48   |
| 5   | AO    | 235 | PHE  | N-CA-C  | 5.15  | 116.68      | 108.79   |
| 1   | BD    | 90  | GLN  | N-CA-C  | 5.15  | 119.57      | 113.28   |
| 3   | E     | 491 | LYS  | N-CA-C  | -5.15 | 107.54      | 113.88   |
| 3   | 7     | 676 | THR  | CA-C-N  | 5.15  | 123.42      | 119.66   |
| 3   | 7     | 676 | THR  | C-N-CA  | 5.15  | 123.42      | 119.66   |
| 16  | CI    | 40  | GLN  | CA-C-N  | -5.15 | 115.04      | 122.36   |
| 16  | CI    | 40  | GLN  | C-N-CA  | -5.15 | 115.04      | 122.36   |
| 3   | 1     | 147 | ASN  | N-CA-C  | 5.15  | 116.99      | 108.13   |
| 7   | 4     | 332 | GLY  | CA-C-O  | -5.15 | 118.87      | 122.22   |
| 5   | AO    | 43  | ASN  | N-CA-C  | 5.15  | 121.77      | 110.80   |
| 2   | BK    | 279 | GLY  | CA-C-N  | 5.15  | 131.24      | 121.97   |
| 2   | BK    | 279 | GLY  | C-N-CA  | 5.15  | 131.24      | 121.97   |
| 2   | z     | 265 | ASP  | O-C-N   | -5.15 | 115.93      | 122.27   |
| 16  | A7    | 146 | GLN  | CA-C-N  | -5.15 | 112.98      | 120.29   |
| 16  | A7    | 146 | GLN  | C-N-CA  | -5.15 | 112.98      | 120.29   |
| 3   | 7     | 479 | LEU  | N-CA-C  | 5.15  | 119.64      | 112.90   |
| 5   | R     | 270 | SER  | CA-C-O  | -5.15 | 113.05      | 119.38   |
| 3   | 7     | 324 | VAL  | N-CA-CB | -5.14 | 104.98      | 111.41   |
| 16  | Av    | 132 | GLN  | N-CA-C  | -5.14 | 99.84       | 110.80   |
| 16  | CB    | 142 | ASN  | N-CA-CB | 5.14  | 119.25      | 110.50   |
| 1   | Ca    | 287 | GLN  | CA-C-N  | 5.14  | 128.60      | 123.04   |
| 1   | Ca    | 287 | GLN  | C-N-CA  | 5.14  | 128.60      | 123.04   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 805 | LEU  | N-CA-CB | -5.14 | 102.52      | 110.13   |
| 3   | 1     | 559 | SER  | O-C-N   | -5.14 | 116.17      | 122.34   |
| 5   | AE    | 504 | ASP  | N-CA-C  | -5.14 | 106.16      | 112.90   |
| 1   | BD    | 258 | ILE  | CB-CA-C | -5.14 | 107.46      | 113.22   |
| 5   | R     | 291 | ILE  | N-CA-C  | 5.14  | 115.37      | 108.17   |
| 2   | k     | 350 | GLU  | N-CA-C  | 5.14  | 118.01      | 107.37   |
| 5   | L     | 486 | MET  | N-CA-C  | -5.14 | 106.27      | 112.54   |
| 2   | y     | 265 | ASP  | O-C-N   | -5.14 | 115.95      | 122.27   |
| 3   | 1     | 538 | ILE  | CA-C-N  | -5.14 | 113.39      | 120.28   |
| 3   | 1     | 538 | ILE  | C-N-CA  | -5.14 | 113.39      | 120.28   |
| 5   | Bf    | 521 | GLU  | N-CA-C  | 5.14  | 116.57      | 111.07   |
| 16  | Z     | 98  | LEU  | CA-C-O  | -5.14 | 112.39      | 119.12   |
| 7   | 4     | 513 | ASN  | N-CA-C  | 5.14  | 118.33      | 111.24   |
| 1   | C     | 10  | ALA  | CA-C-N  | 5.14  | 127.16      | 120.28   |
| 1   | C     | 10  | ALA  | C-N-CA  | 5.14  | 127.16      | 120.28   |
| 1   | C     | 117 | THR  | CA-C-N  | -5.14 | 115.95      | 122.37   |
| 1   | C     | 117 | THR  | C-N-CA  | -5.14 | 115.95      | 122.37   |
| 2   | D     | 158 | LYS  | N-CA-C  | -5.14 | 105.59      | 111.14   |
| 2   | y     | 307 | TYR  | N-CA-C  | 5.14  | 119.26      | 112.89   |
| 3   | 7     | 625 | LEU  | CA-C-N  | -5.14 | 112.38      | 120.60   |
| 3   | 7     | 625 | LEU  | C-N-CA  | -5.14 | 112.38      | 120.60   |
| 5   | Bf    | 468 | PHE  | N-CA-C  | 5.14  | 117.56      | 109.39   |
| 2   | z     | 307 | TYR  | N-CA-C  | 5.14  | 119.26      | 112.89   |
| 5   | AU    | 56  | THR  | CA-C-N  | -5.13 | 115.95      | 122.37   |
| 5   | AU    | 56  | THR  | C-N-CA  | -5.13 | 115.95      | 122.37   |
| 2   | Cd    | 235 | GLU  | CA-C-N  | 5.13  | 127.42      | 120.38   |
| 2   | Cd    | 235 | GLU  | C-N-CA  | 5.13  | 127.42      | 120.38   |
| 5   | G     | 503 | SER  | O-C-N   | -5.13 | 116.95      | 123.01   |
| 3   | 7     | 153 | ILE  | CB-CA-C | -5.13 | 105.21      | 112.14   |
| 5   | 9     | 504 | ASP  | N-CA-C  | -5.13 | 105.38      | 111.69   |
| 7   | J     | 114 | ARG  | CA-C-N  | -5.13 | 115.55      | 123.14   |
| 7   | J     | 114 | ARG  | C-N-CA  | -5.13 | 115.55      | 123.14   |
| 1   | CP    | 117 | THR  | CA-C-N  | -5.13 | 115.96      | 122.37   |
| 1   | CP    | 117 | THR  | C-N-CA  | -5.13 | 115.96      | 122.37   |
| 1   | CP    | 222 | TYR  | CA-C-O  | -5.13 | 113.32      | 121.94   |
| 3   | 1     | 211 | LYS  | N-CA-C  | -5.13 | 105.32      | 112.45   |
| 7   | 4     | 324 | GLN  | CA-C-N  | 5.13  | 131.34      | 121.54   |
| 7   | 4     | 324 | GLN  | C-N-CA  | 5.13  | 131.34      | 121.54   |
| 5   | Bt    | 252 | GLY  | CA-C-N  | -5.13 | 114.39      | 122.08   |
| 5   | Bt    | 252 | GLY  | C-N-CA  | -5.13 | 114.39      | 122.08   |
| 1   | CP    | 213 | LEU  | N-CA-C  | 5.13  | 117.67      | 110.23   |
| 2   | s     | 25  | GLN  | CA-C-N  | 5.12  | 125.04      | 119.76   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | s     | 25  | GLN  | C-N-CA  | 5.12  | 125.04      | 119.76   |
| 7   | AG    | 541 | GLN  | O-C-N   | -5.12 | 115.44      | 122.46   |
| 7   | AG    | 544 | TYR  | N-CA-C  | -5.12 | 107.20      | 113.50   |
| 7   | Bm    | 252 | HIS  | N-CA-CB | -5.12 | 102.40      | 110.49   |
| 3   | I     | 173 | CYS  | N-CA-C  | 5.12  | 116.08      | 108.60   |
| 7   | 4     | 346 | ASP  | CA-C-N  | 5.12  | 130.92      | 121.70   |
| 7   | 4     | 346 | ASP  | C-N-CA  | 5.12  | 130.92      | 121.70   |
| 2   | BK    | 93  | LEU  | CA-C-O  | -5.12 | 112.56      | 119.11   |
| 2   | BK    | 265 | ASP  | N-CA-C  | -5.12 | 105.88      | 111.82   |
| 16  | CB    | 38  | LYS  | N-CA-C  | -5.12 | 105.82      | 111.71   |
| 1   | Ca    | 425 | ARG  | CB-CA-C | -5.12 | 104.13      | 111.91   |
| 7   | J     | 126 | ILE  | CB-CA-C | -5.12 | 104.77      | 110.96   |
| 16  | CM    | 123 | PHE  | N-CA-C  | -5.12 | 105.78      | 111.36   |
| 3   | E     | 662 | ILE  | N-CA-C  | -5.12 | 105.86      | 110.82   |
| 5   | R     | 233 | SER  | N-CA-C  | 5.12  | 116.85      | 109.07   |
| 3   | BY    | 32  | VAL  | N-CA-C  | 5.12  | 115.28      | 108.11   |
| 1   | C     | 434 | ILE  | CB-CA-C | -5.12 | 105.65      | 112.46   |
| 5   | 9     | 602 | ASP  | N-CA-C  | -5.12 | 105.78      | 112.23   |
| 3   | n     | 133 | VAL  | N-CA-C  | 5.12  | 115.27      | 108.11   |
| 7   | AM    | 506 | GLN  | CA-C-N  | 5.12  | 124.78      | 119.56   |
| 7   | AM    | 506 | GLN  | C-N-CA  | 5.12  | 124.78      | 119.56   |
| 7   | AM    | 534 | GLU  | CA-C-N  | -5.12 | 113.43      | 120.28   |
| 7   | AM    | 534 | GLU  | C-N-CA  | -5.12 | 113.43      | 120.28   |
| 7   | Bm    | 38  | ALA  | CA-C-N  | -5.12 | 113.61      | 120.82   |
| 7   | Bm    | 38  | ALA  | C-N-CA  | -5.12 | 113.61      | 120.82   |
| 5   | R     | 43  | ASN  | N-CA-C  | 5.11  | 121.69      | 110.80   |
| 2   | k     | 158 | LYS  | N-CA-C  | -5.11 | 105.78      | 111.36   |
| 5   | 9     | 489 | ILE  | CB-CA-C | -5.11 | 105.16      | 112.22   |
| 5   | AU    | 63  | ASN  | CA-C-N  | 5.11  | 131.41      | 122.82   |
| 5   | AU    | 63  | ASN  | C-N-CA  | 5.11  | 131.41      | 122.82   |
| 5   | Bt    | 300 | ILE  | CA-C-N  | -5.11 | 116.36      | 122.90   |
| 5   | Bt    | 300 | ILE  | C-N-CA  | -5.11 | 116.36      | 122.90   |
| 5   | 9     | 435 | PRO  | N-CA-C  | -5.11 | 103.16      | 111.19   |
| 3   | E     | 43  | TRP  | N-CA-C  | 5.11  | 116.25      | 108.12   |
| 3   | E     | 670 | LEU  | CA-C-O  | -5.11 | 112.97      | 119.31   |
| 5   | L     | 581 | TRP  | N-CA-C  | 5.11  | 121.11      | 109.81   |
| 7   | 4     | 154 | THR  | N-CA-C  | 5.11  | 116.44      | 109.18   |
| 5   | AB    | 329 | ARG  | N-CA-C  | -5.11 | 107.17      | 113.41   |
| 7   | Bm    | 146 | LEU  | CB-CA-C | -5.11 | 104.14      | 111.70   |
| 1   | C     | 126 | GLN  | N-CA-C  | 5.11  | 117.41      | 108.52   |
| 3   | 7     | 775 | TYR  | N-CA-C  | -5.11 | 105.71      | 111.28   |
| 1   | A     | 208 | HIS  | N-CA-C  | -5.11 | 103.60      | 109.93   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | AG    | 76  | PHE  | N-CA-C  | -5.11 | 102.02      | 109.63   |
| 7   | AG    | 113 | ILE  | N-CA-C  | -5.11 | 100.53      | 108.86   |
| 5   | Bf    | 496 | PHE  | N-CA-C  | -5.11 | 105.17      | 111.40   |
| 1   | CP    | 388 | TRP  | N-CA-CB | 5.11  | 117.46      | 110.57   |
| 7   | O     | 81  | ARG  | CA-C-N  | 5.11  | 125.01      | 119.85   |
| 7   | O     | 81  | ARG  | C-N-CA  | 5.11  | 125.01      | 119.85   |
| 5   | R     | 309 | LYS  | N-CA-CB | 5.11  | 119.18      | 110.50   |
| 7   | 4     | 56  | ASP  | CA-C-N  | 5.11  | 126.22      | 119.84   |
| 7   | 4     | 56  | ASP  | C-N-CA  | 5.11  | 126.22      | 119.84   |
| 5   | Bt    | 194 | GLU  | CA-C-N  | -5.11 | 115.41      | 122.30   |
| 5   | Bt    | 194 | GLU  | C-N-CA  | -5.11 | 115.41      | 122.30   |
| 5   | G     | 625 | PHE  | CA-C-N  | -5.10 | 112.13      | 121.52   |
| 5   | G     | 625 | PHE  | C-N-CA  | -5.10 | 112.13      | 121.52   |
| 5   | R     | 337 | TYR  | CA-C-O  | -5.10 | 113.11      | 119.18   |
| 16  | c     | 129 | LEU  | N-CA-C  | 5.10  | 116.92      | 111.36   |
| 1   | i     | 71  | ASN  | CA-C-N  | -5.10 | 114.88      | 122.74   |
| 1   | i     | 71  | ASN  | C-N-CA  | -5.10 | 114.88      | 122.74   |
| 16  | A7    | 132 | GLN  | N-CA-C  | -5.10 | 99.93       | 110.80   |
| 5   | Bt    | 1   | MET  | CA-C-N  | 5.10  | 130.88      | 121.70   |
| 5   | Bt    | 1   | MET  | C-N-CA  | 5.10  | 130.88      | 121.70   |
| 2   | Ch    | 22  | HIS  | N-CA-C  | 5.10  | 118.63      | 111.74   |
| 5   | AB    | 332 | GLU  | N-CA-C  | 5.10  | 117.61      | 109.96   |
| 5   | G     | 512 | PRO  | CA-C-N  | -5.10 | 113.45      | 120.28   |
| 5   | G     | 512 | PRO  | C-N-CA  | -5.10 | 113.45      | 120.28   |
| 5   | L     | 741 | GLU  | N-CA-C  | -5.10 | 105.80      | 111.36   |
| 5   | M     | 155 | TYR  | CA-C-N  | 5.10  | 128.11      | 120.87   |
| 5   | M     | 155 | TYR  | C-N-CA  | 5.10  | 128.11      | 120.87   |
| 3   | n     | 144 | SER  | N-CA-C  | -5.10 | 102.64      | 110.14   |
| 3   | n     | 326 | ASP  | CA-C-O  | -5.10 | 114.95      | 120.81   |
| 5   | AB    | 125 | LYS  | CA-C-N  | -5.10 | 114.89      | 122.74   |
| 5   | AB    | 125 | LYS  | C-N-CA  | -5.10 | 114.89      | 122.74   |
| 1   | BD    | 358 | ILE  | N-CA-C  | 5.10  | 115.25      | 108.11   |
| 16  | CM    | 29  | LEU  | CA-C-N  | 5.10  | 125.60      | 119.94   |
| 16  | CM    | 29  | LEU  | C-N-CA  | 5.10  | 125.60      | 119.94   |
| 2   | z     | 82  | ARG  | N-CA-C  | -5.10 | 105.81      | 112.23   |
| 7   | J     | 534 | GLU  | N-CA-C  | -5.10 | 107.61      | 113.88   |
| 2   | f     | 32  | ALA  | O-C-N   | -5.10 | 116.72      | 122.12   |
| 2   | k     | 93  | LEU  | CA-C-N  | -5.10 | 114.49      | 122.49   |
| 2   | k     | 93  | LEU  | C-N-CA  | -5.10 | 114.49      | 122.49   |
| 3   | 7     | 110 | TYR  | N-CA-CB | -5.10 | 102.25      | 110.71   |
| 3   | 7     | 143 | VAL  | N-CA-C  | 5.10  | 115.19      | 107.80   |
| 5   | AU    | 21  | ARG  | CA-C-N  | -5.10 | 116.01      | 122.43   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AU    | 21  | ARG  | C-N-CA  | -5.10 | 116.01      | 122.43   |
| 1   | Ca    | 282 | THR  | N-CA-C  | -5.10 | 102.01      | 109.81   |
| 3   | E     | 807 | ALA  | N-CA-C  | -5.10 | 105.91      | 111.82   |
| 1   | i     | 161 | GLY  | N-CA-C  | -5.09 | 103.64      | 111.64   |
| 5   | v     | 626 | LYS  | CA-C-N  | -5.09 | 113.82      | 120.44   |
| 5   | v     | 626 | LYS  | C-N-CA  | -5.09 | 113.82      | 120.44   |
| 7   | 4     | 333 | GLY  | CA-C-N  | 5.09  | 129.23      | 120.72   |
| 7   | 4     | 333 | GLY  | C-N-CA  | 5.09  | 129.23      | 120.72   |
| 7   | AM    | 252 | HIS  | N-CA-CB | -5.09 | 102.44      | 110.49   |
| 1   | BD    | 237 | PHE  | CA-C-N  | -5.09 | 116.87      | 123.19   |
| 1   | BD    | 237 | PHE  | C-N-CA  | -5.09 | 116.87      | 123.19   |
| 1   | A     | 287 | GLN  | CA-C-N  | 5.09  | 128.54      | 123.04   |
| 1   | A     | 287 | GLN  | C-N-CA  | 5.09  | 128.54      | 123.04   |
| 5   | v     | 576 | PHE  | CB-CA-C | -5.09 | 99.11       | 109.65   |
| 5   | AB    | 130 | ILE  | CB-CA-C | -5.09 | 104.18      | 111.31   |
| 16  | CI    | 40  | GLN  | O-C-N   | -5.09 | 116.73      | 122.03   |
| 1   | CP    | 282 | THR  | N-CA-C  | -5.09 | 102.02      | 109.81   |
| 2   | Cd    | 86  | ASN  | CA-C-N  | -5.09 | 112.02      | 120.68   |
| 2   | Cd    | 86  | ASN  | C-N-CA  | -5.09 | 112.02      | 120.68   |
| 5   | Bf    | 464 | LEU  | CA-C-N  | 5.09  | 130.86      | 121.70   |
| 5   | Bf    | 464 | LEU  | C-N-CA  | 5.09  | 130.86      | 121.70   |
| 2   | CW    | 326 | ALA  | N-CA-C  | 5.09  | 116.83      | 111.28   |
| 3   | I     | 544 | GLN  | N-CA-CB | 5.08  | 117.35      | 110.59   |
| 7   | J     | 239 | HIS  | N-CA-C  | -5.08 | 103.18      | 109.64   |
| 3   | n     | 278 | ILE  | CB-CA-C | -5.08 | 103.92      | 110.84   |
| 3   | E     | 211 | LYS  | N-CA-C  | -5.08 | 105.38      | 112.45   |
| 2   | k     | 93  | LEU  | CA-C-O  | -5.08 | 112.60      | 119.11   |
| 5   | AB    | 44  | HIS  | N-CA-C  | 5.08  | 117.72      | 111.82   |
| 16  | Ai    | 29  | LEU  | CA-C-N  | 5.08  | 125.58      | 119.94   |
| 16  | Ai    | 29  | LEU  | C-N-CA  | 5.08  | 125.58      | 119.94   |
| 1   | CP    | 343 | ALA  | N-CA-C  | 5.08  | 117.11      | 109.23   |
| 7   | J     | 202 | LEU  | CA-C-N  | -5.08 | 112.04      | 120.68   |
| 7   | J     | 202 | LEU  | C-N-CA  | -5.08 | 112.04      | 120.68   |
| 2   | f     | 328 | SER  | N-CA-C  | -5.08 | 103.82      | 110.53   |
| 2   | y     | 82  | ARG  | N-CA-C  | -5.08 | 105.83      | 112.23   |
| 16  | Av    | 49  | VAL  | N-CA-C  | -5.08 | 105.59      | 110.72   |
| 5   | M     | 63  | ASN  | CA-C-N  | 5.08  | 130.49      | 122.36   |
| 5   | M     | 63  | ASN  | C-N-CA  | 5.08  | 130.49      | 122.36   |
| 5   | AU    | 181 | ASN  | N-CA-C  | -5.08 | 99.05       | 107.99   |
| 1   | CP    | 95  | LEU  | N-CA-C  | -5.08 | 105.83      | 112.23   |
| 3   | E     | 799 | GLU  | CA-C-N  | -5.08 | 112.97      | 120.28   |
| 3   | E     | 799 | GLU  | C-N-CA  | -5.08 | 112.97      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | L     | 621 | PHE  | CA-C-N | 5.08  | 130.73      | 123.27   |
| 5   | L     | 621 | PHE  | C-N-CA | 5.08  | 130.73      | 123.27   |
| 2   | Ch    | 34  | LEU  | N-CA-C | -5.08 | 105.66      | 111.14   |
| 1   | C     | 5   | ASN  | CA-C-N | -5.07 | 114.66      | 121.66   |
| 1   | C     | 5   | ASN  | C-N-CA | -5.07 | 114.66      | 121.66   |
| 5   | L     | 468 | PHE  | CA-C-N | 5.07  | 127.59      | 120.28   |
| 5   | L     | 468 | PHE  | C-N-CA | 5.07  | 127.59      | 120.28   |
| 3   | n     | 274 | SER  | CA-C-N | 5.07  | 129.19      | 120.72   |
| 3   | n     | 274 | SER  | C-N-CA | 5.07  | 129.19      | 120.72   |
| 5   | v     | 585 | SER  | N-CA-C | -5.07 | 107.14      | 113.38   |
| 5   | AB    | 267 | ILE  | CA-C-N | 5.07  | 129.55      | 121.99   |
| 5   | AB    | 267 | ILE  | C-N-CA | 5.07  | 129.55      | 121.99   |
| 16  | A7    | 133 | ASN  | CA-C-N | 5.07  | 127.97      | 120.82   |
| 16  | A7    | 133 | ASN  | C-N-CA | 5.07  | 127.97      | 120.82   |
| 1   | BD    | 131 | ASN  | CA-C-N | 5.07  | 125.00      | 119.78   |
| 1   | BD    | 131 | ASN  | C-N-CA | 5.07  | 125.00      | 119.78   |
| 1   | i     | 288 | HIS  | CA-C-O | 5.07  | 121.53      | 118.33   |
| 5   | 9     | 633 | LYS  | N-CA-C | -5.07 | 107.75      | 114.04   |
| 5   | AE    | 611 | PRO  | CA-C-N | 5.07  | 130.83      | 121.70   |
| 5   | AE    | 611 | PRO  | C-N-CA | 5.07  | 130.83      | 121.70   |
| 1   | C     | 250 | VAL  | N-CA-C | 5.07  | 115.21      | 108.11   |
| 3   | n     | 529 | THR  | N-CA-C | -5.07 | 105.20      | 111.33   |
| 16  | Ai    | 98  | LEU  | CA-C-O | -5.07 | 112.48      | 119.12   |
| 5   | R     | 279 | ARG  | N-CA-C | 5.07  | 117.08      | 109.23   |
| 2   | f     | 87  | LEU  | N-CA-C | -5.07 | 105.84      | 112.23   |
| 2   | q     | 93  | LEU  | CA-C-O | -5.07 | 112.46      | 119.05   |
| 5   | AB    | 290 | ASP  | CA-C-N | -5.07 | 116.53      | 123.12   |
| 5   | AB    | 290 | ASP  | C-N-CA | -5.07 | 116.53      | 123.12   |
| 3   | BY    | 313 | LEU  | CA-C-N | -5.07 | 116.50      | 123.14   |
| 3   | BY    | 313 | LEU  | C-N-CA | -5.07 | 116.50      | 123.14   |
| 1   | CP    | 386 | TYR  | CA-C-N | -5.07 | 114.71      | 122.62   |
| 1   | CP    | 386 | TYR  | C-N-CA | -5.07 | 114.71      | 122.62   |
| 3   | E     | 481 | LEU  | N-CA-C | 5.07  | 117.53      | 111.71   |
| 16  | CI    | 178 | SER  | N-CA-C | -5.07 | 105.22      | 111.40   |
| 1   | Ca    | 281 | SER  | N-CA-C | 5.07  | 114.83      | 108.45   |
| 5   | G     | 621 | PHE  | CA-C-N | 5.06  | 130.68      | 122.68   |
| 5   | G     | 621 | PHE  | C-N-CA | 5.06  | 130.68      | 122.68   |
| 7   | O     | 38  | ALA  | CA-C-N | -5.06 | 113.68      | 120.82   |
| 7   | O     | 38  | ALA  | C-N-CA | -5.06 | 113.68      | 120.82   |
| 3   | 1     | 155 | THR  | N-CA-C | -5.06 | 108.13      | 114.56   |
| 16  | An    | 136 | GLU  | N-CA-C | -5.06 | 105.84      | 111.36   |
| 16  | CM    | 169 | PRO  | CA-C-N | -5.06 | 113.70      | 122.10   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | CM    | 169 | PRO  | C-N-CA  | -5.06 | 113.70      | 122.10   |
| 2   | Cd    | 291 | TYR  | CA-C-O  | -5.06 | 112.19      | 120.80   |
| 7   | J     | 267 | HIS  | CA-C-N  | -5.06 | 115.97      | 123.05   |
| 7   | J     | 267 | HIS  | C-N-CA  | -5.06 | 115.97      | 123.05   |
| 5   | v     | 650 | VAL  | N-CA-C  | 5.06  | 119.87      | 109.34   |
| 7   | AM    | 125 | SER  | CA-C-N  | 5.06  | 128.70      | 122.37   |
| 7   | AM    | 125 | SER  | C-N-CA  | 5.06  | 128.70      | 122.37   |
| 1   | CP    | 26  | ASN  | N-CA-C  | -5.06 | 102.30      | 110.14   |
| 3   | n     | 602 | ASP  | N-CA-C  | -5.06 | 106.79      | 113.17   |
| 3   | l     | 598 | VAL  | N-CA-CB | -5.06 | 105.84      | 111.41   |
| 2   | k     | 25  | GLN  | N-CA-C  | 5.06  | 117.84      | 108.94   |
| 2   | s     | 29  | ILE  | O-C-N   | -5.06 | 112.58      | 121.84   |
| 5   | R     | 93  | HIS  | CA-C-N  | -5.06 | 116.55      | 123.12   |
| 5   | R     | 93  | HIS  | C-N-CA  | -5.06 | 116.55      | 123.12   |
| 3   | n     | 51  | ASP  | N-CA-C  | 5.06  | 117.38      | 110.55   |
| 5   | AE    | 608 | ASN  | O-C-N   | -5.06 | 115.23      | 122.41   |
| 2   | Cd    | 321 | SER  | N-CA-C  | 5.06  | 119.32      | 112.04   |
| 5   | v     | 583 | PHE  | CA-C-N  | -5.05 | 114.68      | 121.71   |
| 5   | v     | 583 | PHE  | C-N-CA  | -5.05 | 114.68      | 121.71   |
| 7   | AG    | 125 | SER  | CA-C-N  | 5.05  | 128.69      | 122.37   |
| 7   | AG    | 125 | SER  | C-N-CA  | 5.05  | 128.69      | 122.37   |
| 7   | AM    | 294 | SER  | CA-C-O  | -5.05 | 113.31      | 119.32   |
| 16  | Ai    | 139 | LYS  | CA-C-O  | -5.05 | 113.34      | 119.61   |
| 5   | Bf    | 504 | ASP  | N-CA-C  | -5.05 | 106.28      | 112.90   |
| 7   | Bm    | 166 | MET  | CB-CA-C | 5.05  | 118.09      | 109.24   |
| 1   | C     | 196 | TRP  | N-CA-CB | -5.05 | 102.03      | 110.37   |
| 5   | AB    | 135 | CYS  | CA-C-N  | -5.05 | 116.03      | 123.00   |
| 5   | AB    | 135 | CYS  | C-N-CA  | -5.05 | 116.03      | 123.00   |
| 1   | A     | 388 | TRP  | N-CA-CB | 5.05  | 117.39      | 110.57   |
| 5   | Bf    | 567 | GLN  | N-CA-C  | -5.05 | 105.77      | 111.28   |
| 16  | CB    | 136 | GLU  | N-CA-C  | -5.05 | 105.85      | 111.36   |
| 16  | CM    | 40  | GLN  | N-CA-C  | 5.05  | 115.00      | 107.88   |
| 1   | Ca    | 250 | VAL  | N-CA-C  | 5.05  | 115.18      | 108.11   |
| 1   | Ca    | 334 | ALA  | N-CA-C  | -5.05 | 102.22      | 110.20   |
| 1   | A     | 10  | ALA  | CA-C-N  | 5.05  | 127.05      | 120.28   |
| 1   | A     | 10  | ALA  | C-N-CA  | 5.05  | 127.05      | 120.28   |
| 5   | 9     | 581 | TRP  | N-CA-C  | 5.05  | 120.47      | 113.45   |
| 7   | AG    | 38  | ALA  | CA-C-N  | -5.05 | 113.70      | 120.82   |
| 7   | AG    | 38  | ALA  | C-N-CA  | -5.05 | 113.70      | 120.82   |
| 5   | M     | 98  | LEU  | N-CA-C  | -5.05 | 102.17      | 109.59   |
| 7   | 4     | 345 | PHE  | CA-C-O  | -5.05 | 113.17      | 119.18   |
| 7   | AG    | 205 | GLN  | CB-CA-C | -5.05 | 104.56      | 111.73   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | AG    | 534 | GLU  | CA-C-N | -5.05 | 113.52      | 120.28   |
| 7   | AG    | 534 | GLU  | C-N-CA | -5.05 | 113.52      | 120.28   |
| 5   | AU    | 295 | ASN  | N-CA-C | -5.05 | 106.27      | 114.09   |
| 5   | Bf    | 584 | LEU  | CA-C-N | -5.05 | 113.19      | 121.92   |
| 5   | Bf    | 584 | LEU  | C-N-CA | -5.05 | 113.19      | 121.92   |
| 1   | CP    | 270 | TYR  | N-CA-C | -5.05 | 101.08      | 109.46   |
| 7   | Bm    | 324 | GLN  | CA-C-N | 5.04  | 131.17      | 121.54   |
| 7   | Bm    | 324 | GLN  | C-N-CA | 5.04  | 131.17      | 121.54   |
| 5   | G     | 756 | TYR  | CA-C-O | -5.04 | 113.66      | 119.56   |
| 5   | AO    | 121 | ASN  | CA-C-N | 5.04  | 124.70      | 119.56   |
| 5   | AO    | 121 | ASN  | C-N-CA | 5.04  | 124.70      | 119.56   |
| 16  | Aq    | 89  | ILE  | CA-C-N | 5.04  | 131.17      | 121.54   |
| 16  | Aq    | 89  | ILE  | C-N-CA | 5.04  | 131.17      | 121.54   |
| 3   | BY    | 97  | TYR  | N-CA-C | -5.04 | 104.28      | 111.24   |
| 5   | Bf    | 519 | GLN  | N-CA-C | 5.04  | 119.52      | 113.17   |
| 1   | C     | 213 | LEU  | N-CA-C | 5.04  | 117.54      | 110.23   |
| 3   | E     | 313 | LEU  | CA-C-N | -5.04 | 116.54      | 123.14   |
| 3   | E     | 313 | LEU  | C-N-CA | -5.04 | 116.54      | 123.14   |
| 3   | n     | 36  | LYS  | O-C-N  | -5.04 | 116.78      | 122.12   |
| 5   | R     | 4   | ILE  | N-CA-C | 5.04  | 115.83      | 108.58   |
| 5   | R     | 162 | THR  | CA-C-N | 5.04  | 124.70      | 119.56   |
| 5   | R     | 162 | THR  | C-N-CA | 5.04  | 124.70      | 119.56   |
| 16  | Ai    | 172 | ASP  | CA-C-N | 5.04  | 131.03      | 121.97   |
| 16  | Ai    | 172 | ASP  | C-N-CA | 5.04  | 131.03      | 121.97   |
| 3   | BY    | 36  | LYS  | O-C-N  | -5.04 | 116.78      | 122.12   |
| 1   | A     | 386 | TYR  | CA-C-N | -5.03 | 114.77      | 122.62   |
| 1   | A     | 386 | TYR  | C-N-CA | -5.03 | 114.77      | 122.62   |
| 1   | C     | 258 | ILE  | N-CA-C | -5.03 | 106.25      | 111.58   |
| 3   | E     | 232 | TYR  | N-CA-C | 5.03  | 117.45      | 109.50   |
| 5   | AB    | 252 | GLY  | CA-C-N | -5.03 | 114.53      | 122.08   |
| 5   | AB    | 252 | GLY  | C-N-CA | -5.03 | 114.53      | 122.08   |
| 5   | AO    | 122 | PRO  | CA-C-N | -5.03 | 115.13      | 122.28   |
| 5   | AO    | 122 | PRO  | C-N-CA | -5.03 | 115.13      | 122.28   |
| 2   | z     | 249 | THR  | N-CA-C | -5.03 | 105.87      | 111.36   |
| 2   | D     | 280 | ILE  | O-C-N  | -5.03 | 116.28      | 122.57   |
| 5   | R     | 282 | LYS  | CA-C-O | -5.03 | 114.65      | 120.49   |
| 2   | D     | 113 | GLN  | N-CA-C | -5.03 | 105.88      | 111.36   |
| 5   | G     | 581 | TRP  | N-CA-C | 5.03  | 120.44      | 113.45   |
| 1   | i     | 222 | TYR  | CA-C-O | -5.03 | 113.49      | 121.94   |
| 5   | v     | 715 | SER  | N-CA-C | -5.03 | 105.80      | 111.28   |
| 16  | A7    | 139 | LYS  | N-CA-C | -5.03 | 106.92      | 113.16   |
| 3   | BY    | 551 | GLU  | N-CA-C | 5.03  | 117.49      | 111.71   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | Av    | 57  | ARG  | CA-C-N | -5.03 | 115.16      | 122.65   |
| 16  | Av    | 57  | ARG  | C-N-CA | -5.03 | 115.16      | 122.65   |
| 7   | Bm    | 332 | GLY  | CA-C-O | -5.03 | 118.76      | 122.23   |
| 3   | I     | 255 | ILE  | N-CA-C | -5.03 | 103.09      | 109.58   |
| 2   | k     | 31  | SER  | N-CA-C | 5.03  | 121.51      | 110.80   |
| 1   | BD    | 414 | LYS  | N-CA-C | -5.03 | 105.88      | 111.36   |
| 5   | Bf    | 756 | TYR  | CA-C-O | -5.03 | 113.68      | 119.56   |
| 3   | 1     | 520 | VAL  | N-CA-C | -5.03 | 105.50      | 110.62   |
| 7   | AG    | 113 | ILE  | CA-C-N | -5.03 | 115.78      | 122.72   |
| 7   | AG    | 113 | ILE  | C-N-CA | -5.03 | 115.78      | 122.72   |
| 2   | y     | 249 | THR  | N-CA-C | -5.02 | 105.88      | 111.36   |
| 5   | AU    | 337 | TYR  | CA-C-O | -5.02 | 113.39      | 119.27   |
| 16  | CB    | 98  | LEU  | CA-C-O | -5.02 | 112.54      | 119.12   |
| 3   | n     | 312 | TYR  | N-CA-C | 5.02  | 117.16      | 109.07   |
| 5   | 9     | 423 | LYS  | N-CA-C | -5.02 | 105.89      | 111.36   |
| 1   | C     | 414 | LYS  | N-CA-C | -5.02 | 105.89      | 111.36   |
| 7   | O     | 243 | THR  | N-CA-C | -5.02 | 103.31      | 110.59   |
| 16  | Az    | 97  | ILE  | N-CA-C | -5.02 | 105.53      | 111.00   |
| 16  | CM    | 56  | GLU  | N-CA-C | 5.02  | 119.25      | 113.18   |
| 5   | AB    | 316 | PHE  | N-CA-C | -5.02 | 105.89      | 111.36   |
| 2   | BR    | 83  | GLU  | N-CA-C | -5.02 | 105.81      | 111.28   |
| 2   | CW    | 34  | LEU  | N-CA-C | -5.02 | 105.52      | 111.69   |
| 5   | M     | 251 | HIS  | N-CA-C | 5.02  | 116.56      | 111.14   |
| 7   | O     | 56  | ASP  | CA-C-N | 5.02  | 126.11      | 119.84   |
| 7   | O     | 56  | ASP  | C-N-CA | 5.02  | 126.11      | 119.84   |
| 5   | Bf    | 430 | LYS  | N-CA-C | 5.02  | 120.05      | 113.88   |
| 5   | M     | 13  | TYR  | N-CA-C | -5.01 | 105.26      | 112.13   |
| 3   | 1     | 526 | LEU  | O-C-N  | -5.01 | 116.96      | 122.38   |
| 5   | AE    | 741 | GLU  | N-CA-C | -5.01 | 105.89      | 111.36   |
| 5   | AU    | 153 | ALA  | CA-C-N | -5.01 | 113.75      | 120.82   |
| 5   | AU    | 153 | ALA  | C-N-CA | -5.01 | 113.75      | 120.82   |
| 3   | 1     | 309 | ASP  | N-CA-C | -5.01 | 99.61       | 108.23   |
| 3   | 7     | 326 | ASP  | CA-C-O | -5.01 | 115.05      | 120.81   |
| 5   | AU    | 328 | GLU  | N-CA-C | -5.01 | 107.11      | 113.18   |
| 3   | E     | 837 | MET  | CA-C-O | -5.01 | 115.65      | 121.26   |
| 3   | 1     | 235 | ILE  | N-CA-C | 5.01  | 115.19      | 108.17   |
| 16  | Aq    | 146 | GLN  | O-C-N  | -5.01 | 116.44      | 122.15   |
| 16  | Az    | 98  | LEU  | CA-C-O | -5.01 | 112.69      | 119.11   |
| 7   | Bm    | 318 | THR  | N-CA-C | -5.01 | 107.55      | 113.97   |
| 7   | J     | 202 | LEU  | O-C-N  | -5.01 | 116.11      | 122.27   |
| 2   | BK    | 21  | LEU  | N-CA-C | -5.01 | 106.42      | 112.88   |
| 3   | n     | 784 | GLN  | CA-C-O | -5.01 | 113.35      | 120.51   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | Bm    | 154 | THR  | CA-C-N | -5.01 | 114.81      | 122.87   |
| 7   | Bm    | 154 | THR  | C-N-CA | -5.01 | 114.81      | 122.87   |
| 5   | G     | 608 | ASN  | O-C-N  | -5.00 | 115.30      | 122.41   |
| 7   | AG    | 230 | MET  | N-CA-C | 5.00  | 117.51      | 111.40   |
| 7   | AM    | 324 | GLN  | CA-C-N | 5.00  | 131.10      | 121.54   |
| 7   | AM    | 324 | GLN  | C-N-CA | 5.00  | 131.10      | 121.54   |
| 7   | Bm    | 48  | ASP  | CA-C-O | -5.00 | 113.36      | 120.51   |
| 1   | A     | 26  | ASN  | N-CA-C | -5.00 | 102.00      | 109.95   |
| 2   | D     | 93  | LEU  | CA-C-O | -5.00 | 112.71      | 119.11   |
| 2   | BK    | 357 | ARG  | CA-C-O | -5.00 | 114.50      | 120.55   |
| 5   | Bt    | 279 | ARG  | N-CA-C | 5.00  | 117.88      | 110.48   |

There are no chirality outliers.

All (579) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 11  | 0     | 46  | UNK  | Mainchain         |
| 3   | 1     | 326 | ASP  | Mainchain         |
| 3   | 1     | 36  | LYS  | Mainchain         |
| 3   | 1     | 445 | PRO  | Mainchain         |
| 3   | 1     | 471 | ARG  | Mainchain         |
| 3   | 1     | 526 | LEU  | Mainchain         |
| 3   | 1     | 609 | TRP  | Mainchain         |
| 3   | 1     | 631 | VAL  | Mainchain         |
| 3   | 1     | 666 | LEU  | Mainchain         |
| 3   | 1     | 733 | LYS  | Peptide,Mainchain |
| 7   | 4     | 202 | LEU  | Mainchain         |
| 7   | 4     | 325 | SER  | Peptide,Mainchain |
| 7   | 4     | 345 | PHE  | Mainchain         |
| 7   | 4     | 48  | ASP  | Peptide,Mainchain |
| 7   | 4     | 522 | PHE  | Mainchain         |
| 7   | 4     | 533 | THR  | Mainchain         |
| 7   | 4     | 541 | GLN  | Mainchain         |
| 7   | 4     | 557 | LEU  | Peptide,Mainchain |
| 7   | 4     | 76  | PHE  | Peptide,Mainchain |
| 3   | 7     | 326 | ASP  | Mainchain         |
| 3   | 7     | 36  | LYS  | Mainchain         |
| 3   | 7     | 445 | PRO  | Mainchain         |
| 3   | 7     | 453 | TRP  | Mainchain         |
| 3   | 7     | 471 | ARG  | Mainchain         |
| 3   | 7     | 526 | LEU  | Mainchain         |
| 3   | 7     | 609 | TRP  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 3   | 7     | 733 | LYS  | Mainchain         |
| 3   | 7     | 784 | GLN  | Peptide,Mainchain |
| 3   | 7     | 792 | GLN  | Mainchain         |
| 3   | 7     | 803 | ALA  | Mainchain         |
| 3   | 7     | 808 | GLU  | Mainchain         |
| 3   | 7     | 837 | MET  | Peptide,Mainchain |
| 3   | 7     | 847 | LEU  | Mainchain         |
| 3   | 7     | 863 | ASP  | Mainchain         |
| 3   | 7     | 880 | LEU  | Mainchain         |
| 5   | 9     | 483 | TYR  | Mainchain         |
| 5   | 9     | 492 | CYS  | Mainchain         |
| 5   | 9     | 503 | SER  | Mainchain         |
| 5   | 9     | 584 | LEU  | Peptide,Mainchain |
| 5   | 9     | 597 | TRP  | Mainchain         |
| 5   | 9     | 608 | ASN  | Mainchain         |
| 5   | 9     | 649 | SER  | Peptide,Mainchain |
| 1   | A     | 155 | ASP  | Mainchain         |
| 1   | A     | 222 | TYR  | Peptide,Mainchain |
| 1   | A     | 301 | GLU  | Mainchain         |
| 1   | A     | 349 | VAL  | Peptide,Mainchain |
| 1   | A     | 94  | LEU  | Mainchain         |
| 16  | A7    | 132 | GLN  | Peptide,Mainchain |
| 16  | A7    | 154 | THR  | Peptide,Mainchain |
| 16  | A7    | 40  | GLN  | Mainchain         |
| 5   | AB    | 124 | THR  | Mainchain         |
| 5   | AB    | 236 | ALA  | Mainchain         |
| 5   | AB    | 253 | ASN  | Mainchain         |
| 5   | AB    | 270 | SER  | Mainchain         |
| 5   | AB    | 31  | ASN  | Peptide,Mainchain |
| 5   | AB    | 337 | TYR  | Mainchain         |
| 5   | AB    | 59  | VAL  | Peptide,Mainchain |
| 5   | AE    | 475 | TYR  | Mainchain         |
| 5   | AE    | 483 | TYR  | Mainchain         |
| 5   | AE    | 492 | CYS  | Mainchain         |
| 5   | AE    | 503 | SER  | Mainchain         |
| 5   | AE    | 584 | LEU  | Mainchain         |
| 5   | AE    | 597 | TRP  | Mainchain         |
| 5   | AE    | 608 | ASN  | Mainchain         |
| 5   | AE    | 649 | SER  | Peptide,Mainchain |
| 5   | AE    | 728 | GLN  | Mainchain         |
| 5   | AE    | 756 | TYR  | Mainchain         |
| 5   | AE    | 765 | GLN  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 5   | AE    | 782 | LYS  | Mainchain         |
| 5   | AE    | 857 | ARG  | Mainchain         |
| 5   | AE    | 876 | GLN  | Mainchain         |
| 5   | AE    | 893 | LYS  | Mainchain         |
| 5   | AE    | 919 | THR  | Mainchain         |
| 5   | AE    | 927 | MET  | Mainchain         |
| 7   | AG    | 202 | LEU  | Mainchain         |
| 7   | AG    | 325 | SER  | Mainchain         |
| 7   | AG    | 345 | PHE  | Mainchain         |
| 7   | AG    | 48  | ASP  | Mainchain         |
| 7   | AG    | 522 | PHE  | Mainchain         |
| 7   | AG    | 533 | THR  | Mainchain         |
| 7   | AG    | 541 | GLN  | Mainchain         |
| 7   | AG    | 557 | LEU  | Mainchain         |
| 7   | AG    | 76  | PHE  | Peptide,Mainchain |
| 7   | AM    | 294 | SER  | Mainchain         |
| 7   | AM    | 304 | GLY  | Mainchain         |
| 7   | AM    | 325 | SER  | Peptide,Mainchain |
| 7   | AM    | 345 | PHE  | Mainchain         |
| 7   | AM    | 48  | ASP  | Peptide,Mainchain |
| 7   | AM    | 522 | PHE  | Mainchain         |
| 7   | AM    | 533 | THR  | Mainchain         |
| 7   | AM    | 541 | GLN  | Mainchain         |
| 7   | AM    | 557 | LEU  | Mainchain         |
| 7   | AM    | 76  | PHE  | Peptide,Mainchain |
| 5   | AO    | 191 | SER  | Peptide,Mainchain |
| 5   | AO    | 236 | ALA  | Mainchain         |
| 5   | AO    | 253 | ASN  | Mainchain         |
| 5   | AO    | 270 | SER  | Mainchain         |
| 5   | AO    | 31  | ASN  | Peptide,Mainchain |
| 5   | AO    | 337 | TYR  | Mainchain         |
| 5   | AO    | 59  | VAL  | Mainchain         |
| 15  | AP    | 30  | UNK  | Mainchain         |
| 15  | AP    | 44  | UNK  | Mainchain         |
| 13  | AS    | 75  | UNK  | Mainchain         |
| 5   | AU    | 124 | THR  | Mainchain         |
| 5   | AU    | 236 | ALA  | Mainchain         |
| 5   | AU    | 253 | ASN  | Mainchain         |
| 5   | AU    | 283 | ASN  | Peptide,Mainchain |
| 5   | AU    | 31  | ASN  | Peptide,Mainchain |
| 5   | AU    | 337 | TYR  | Mainchain         |
| 5   | AU    | 59  | VAL  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 14  | AZ    | 11  | UNK  | Mainchain         |
| 14  | AZ    | 62  | UNK  | Mainchain         |
| 14  | AZ    | 84  | UNK  | Mainchain         |
| 15  | Aa    | 30  | UNK  | Mainchain         |
| 15  | Aa    | 44  | UNK  | Mainchain         |
| 16  | Ai    | 125 | ALA  | Mainchain         |
| 16  | Ai    | 132 | GLN  | Mainchain         |
| 16  | Ai    | 139 | LYS  | Mainchain         |
| 16  | Ai    | 146 | GLN  | Mainchain         |
| 16  | Ai    | 98  | LEU  | Mainchain         |
| 14  | Am    | 11  | UNK  | Mainchain         |
| 14  | Am    | 64  | UNK  | Mainchain         |
| 14  | Am    | 84  | UNK  | Mainchain         |
| 16  | An    | 125 | ALA  | Mainchain         |
| 16  | An    | 132 | GLN  | Mainchain         |
| 16  | An    | 139 | LYS  | Mainchain         |
| 16  | An    | 35  | TYR  | Peptide,Mainchain |
| 16  | Aq    | 132 | GLN  | Peptide,Mainchain |
| 16  | Aq    | 146 | GLN  | Mainchain         |
| 16  | Aq    | 154 | THR  | Peptide,Mainchain |
| 16  | Aq    | 40  | GLN  | Mainchain         |
| 14  | As    | 11  | UNK  | Mainchain         |
| 14  | As    | 62  | UNK  | Mainchain         |
| 14  | As    | 84  | UNK  | Mainchain         |
| 16  | Av    | 127 | LYS  | Mainchain         |
| 16  | Av    | 132 | GLN  | Peptide,Mainchain |
| 16  | Av    | 154 | THR  | Peptide,Mainchain |
| 16  | Av    | 37  | ILE  | Mainchain         |
| 16  | Az    | 132 | GLN  | Mainchain         |
| 16  | Az    | 139 | LYS  | Mainchain         |
| 16  | Az    | 98  | LEU  | Mainchain         |
| 11  | B2    | 46  | UNK  | Mainchain         |
| 6   | B4    | 105 | UNK  | Mainchain         |
| 6   | B4    | 78  | UNK  | Peptide,Mainchain |
| 15  | B5    | 30  | UNK  | Mainchain         |
| 15  | B5    | 44  | UNK  | Mainchain         |
| 1   | BD    | 155 | ASP  | Mainchain         |
| 1   | BD    | 222 | TYR  | Peptide,Mainchain |
| 1   | BD    | 301 | GLU  | Mainchain         |
| 1   | BD    | 349 | VAL  | Peptide,Mainchain |
| 1   | BD    | 94  | LEU  | Mainchain         |
| 2   | BK    | 12  | LEU  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | BK    | 233 | ILE  | Peptide,Mainchain |
| 2   | BK    | 318 | ILE  | Mainchain         |
| 2   | BK    | 331 | ASN  | Mainchain         |
| 2   | BK    | 357 | ARG  | Peptide,Mainchain |
| 2   | BK    | 82  | ARG  | Mainchain         |
| 2   | BK    | 93  | LEU  | Mainchain         |
| 4   | BO    | 68  | UNK  | Mainchain         |
| 2   | BR    | 117 | GLN  | Mainchain         |
| 2   | BR    | 136 | GLU  | Mainchain         |
| 2   | BR    | 239 | GLN  | Mainchain         |
| 2   | BR    | 240 | LEU  | Mainchain         |
| 2   | BR    | 265 | ASP  | Mainchain         |
| 2   | BR    | 29  | ILE  | Peptide,Mainchain |
| 2   | BR    | 313 | THR  | Mainchain         |
| 2   | BR    | 37  | LYS  | Mainchain         |
| 2   | BR    | 53  | LYS  | Mainchain         |
| 6   | BV    | 105 | UNK  | Mainchain         |
| 6   | BV    | 78  | UNK  | Peptide,Mainchain |
| 3   | BY    | 326 | ASP  | Mainchain         |
| 3   | BY    | 36  | LYS  | Mainchain         |
| 3   | BY    | 445 | PRO  | Mainchain         |
| 3   | BY    | 471 | ARG  | Mainchain         |
| 3   | BY    | 526 | LEU  | Mainchain         |
| 3   | BY    | 533 | PHE  | Mainchain         |
| 3   | BY    | 556 | PRO  | Peptide           |
| 3   | BY    | 609 | TRP  | Mainchain         |
| 3   | BY    | 631 | VAL  | Mainchain         |
| 3   | BY    | 670 | LEU  | Mainchain         |
| 3   | BY    | 733 | LYS  | Mainchain         |
| 3   | BY    | 755 | ALA  | Mainchain         |
| 3   | BY    | 785 | VAL  | Mainchain         |
| 3   | BY    | 792 | GLN  | Mainchain         |
| 3   | BY    | 803 | ALA  | Mainchain         |
| 3   | BY    | 837 | MET  | Mainchain         |
| 3   | BY    | 847 | LEU  | Mainchain         |
| 3   | BY    | 880 | LEU  | Mainchain         |
| 4   | BZ    | 68  | UNK  | Mainchain         |
| 5   | Bf    | 483 | TYR  | Mainchain         |
| 5   | Bf    | 492 | CYS  | Mainchain         |
| 5   | Bf    | 503 | SER  | Mainchain         |
| 5   | Bf    | 584 | LEU  | Mainchain         |
| 5   | Bf    | 597 | TRP  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 5   | Bf    | 608 | ASN  | Mainchain         |
| 5   | Bf    | 649 | SER  | Mainchain         |
| 5   | Bf    | 749 | ILE  | Mainchain         |
| 5   | Bf    | 756 | TYR  | Mainchain         |
| 5   | Bf    | 765 | GLN  | Mainchain         |
| 5   | Bf    | 858 | MET  | Mainchain         |
| 6   | Bg    | 105 | UNK  | Mainchain         |
| 6   | Bg    | 78  | UNK  | Peptide,Mainchain |
| 7   | Bm    | 202 | LEU  | Mainchain         |
| 7   | Bm    | 294 | SER  | Mainchain         |
| 7   | Bm    | 325 | SER  | Peptide,Mainchain |
| 7   | Bm    | 345 | PHE  | Mainchain         |
| 7   | Bm    | 48  | ASP  | Peptide,Mainchain |
| 7   | Bm    | 522 | PHE  | Mainchain         |
| 7   | Bm    | 533 | THR  | Mainchain         |
| 7   | Bm    | 541 | GLN  | Mainchain         |
| 7   | Bm    | 557 | LEU  | Mainchain         |
| 7   | Bm    | 76  | PHE  | Peptide,Mainchain |
| 11  | Bq    | 46  | UNK  | Mainchain         |
| 5   | Bt    | 124 | THR  | Mainchain         |
| 5   | Bt    | 236 | ALA  | Mainchain         |
| 5   | Bt    | 253 | ASN  | Mainchain         |
| 5   | Bt    | 270 | SER  | Mainchain         |
| 5   | Bt    | 31  | ASN  | Peptide,Mainchain |
| 5   | Bt    | 337 | TYR  | Mainchain         |
| 5   | Bt    | 59  | VAL  | Mainchain         |
| 4   | Bw    | 68  | UNK  | Mainchain         |
| 1   | C     | 222 | TYR  | Mainchain         |
| 1   | C     | 301 | GLU  | Mainchain         |
| 1   | C     | 349 | VAL  | Peptide,Mainchain |
| 1   | C     | 94  | LEU  | Mainchain         |
| 16  | CB    | 125 | ALA  | Mainchain         |
| 16  | CB    | 132 | GLN  | Mainchain         |
| 16  | CB    | 139 | LYS  | Mainchain         |
| 16  | CB    | 175 | GLY  | Mainchain         |
| 16  | CB    | 98  | LEU  | Mainchain         |
| 14  | CE    | 11  | UNK  | Mainchain         |
| 14  | CE    | 62  | UNK  | Mainchain         |
| 14  | CE    | 84  | UNK  | Mainchain         |
| 15  | CF    | 30  | UNK  | Mainchain         |
| 15  | CF    | 44  | UNK  | Mainchain         |
| 16  | CI    | 132 | GLN  | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 16  | CI    | 154 | THR  | Peptide,Mainchain |
| 16  | CI    | 40  | GLN  | Mainchain         |
| 16  | CM    | 125 | ALA  | Mainchain         |
| 16  | CM    | 132 | GLN  | Mainchain         |
| 16  | CM    | 139 | LYS  | Mainchain         |
| 16  | CM    | 98  | LEU  | Mainchain         |
| 11  | CO    | 46  | UNK  | Mainchain         |
| 1   | CP    | 155 | ASP  | Mainchain         |
| 1   | CP    | 222 | TYR  | Peptide,Mainchain |
| 1   | CP    | 301 | GLU  | Mainchain         |
| 1   | CP    | 349 | VAL  | Peptide,Mainchain |
| 1   | CP    | 94  | LEU  | Mainchain         |
| 16  | CT    | 132 | GLN  | Peptide,Mainchain |
| 16  | CT    | 154 | THR  | Peptide,Mainchain |
| 16  | CT    | 40  | GLN  | Mainchain         |
| 2   | CW    | 101 | LYS  | Mainchain         |
| 2   | CW    | 12  | LEU  | Mainchain         |
| 2   | CW    | 123 | LEU  | Mainchain         |
| 2   | CW    | 233 | ILE  | Peptide,Mainchain |
| 2   | CW    | 318 | ILE  | Mainchain         |
| 2   | CW    | 331 | ASN  | Mainchain         |
| 2   | CW    | 357 | ARG  | Peptide,Mainchain |
| 2   | CW    | 82  | ARG  | Mainchain         |
| 2   | CW    | 93  | LEU  | Mainchain         |
| 1   | Ca    | 132 | PRO  | Mainchain         |
| 1   | Ca    | 155 | ASP  | Mainchain         |
| 1   | Ca    | 222 | TYR  | Peptide,Mainchain |
| 1   | Ca    | 301 | GLU  | Mainchain         |
| 1   | Ca    | 349 | VAL  | Peptide,Mainchain |
| 1   | Ca    | 94  | LEU  | Mainchain         |
| 15  | Cc    | 30  | UNK  | Mainchain         |
| 15  | Cc    | 44  | UNK  | Mainchain         |
| 2   | Cd    | 136 | GLU  | Mainchain         |
| 2   | Cd    | 265 | ASP  | Mainchain         |
| 2   | Cd    | 29  | ILE  | Mainchain         |
| 2   | Cd    | 291 | TYR  | Mainchain         |
| 2   | Cd    | 32  | ALA  | Mainchain         |
| 2   | Cd    | 329 | GLN  | Peptide,Mainchain |
| 2   | Cd    | 347 | LYS  | Mainchain         |
| 2   | Cd    | 354 | GLU  | Peptide,Mainchain |
| 2   | Cd    | 37  | LYS  | Mainchain         |
| 2   | Cd    | 44  | LYS  | Peptide,Mainchain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | Cd    | 53  | LYS  | Mainchain         |
| 2   | Cd    | 86  | ASN  | Mainchain         |
| 2   | Ch    | 12  | LEU  | Mainchain         |
| 2   | Ch    | 233 | ILE  | Peptide,Mainchain |
| 2   | Ch    | 237 | GLN  | Mainchain         |
| 2   | Ch    | 318 | ILE  | Peptide,Mainchain |
| 2   | Ch    | 331 | ASN  | Mainchain         |
| 2   | Ch    | 342 | LEU  | Mainchain         |
| 2   | Ch    | 357 | ARG  | Mainchain         |
| 2   | Ch    | 82  | ARG  | Mainchain         |
| 2   | Ch    | 93  | LEU  | Mainchain         |
| 2   | D     | 12  | LEU  | Mainchain         |
| 2   | D     | 233 | ILE  | Peptide,Mainchain |
| 2   | D     | 318 | ILE  | Mainchain         |
| 2   | D     | 331 | ASN  | Mainchain         |
| 2   | D     | 357 | ARG  | Mainchain         |
| 2   | D     | 82  | ARG  | Mainchain         |
| 2   | D     | 93  | LEU  | Mainchain         |
| 3   | E     | 326 | ASP  | Mainchain         |
| 3   | E     | 36  | LYS  | Mainchain         |
| 3   | E     | 445 | PRO  | Mainchain         |
| 3   | E     | 471 | ARG  | Mainchain         |
| 3   | E     | 526 | LEU  | Mainchain         |
| 3   | E     | 609 | TRP  | Mainchain         |
| 3   | E     | 631 | VAL  | Mainchain         |
| 3   | E     | 662 | ILE  | Mainchain         |
| 3   | E     | 670 | LEU  | Mainchain         |
| 3   | E     | 733 | LYS  | Mainchain         |
| 3   | E     | 784 | GLN  | Peptide,Mainchain |
| 3   | E     | 785 | VAL  | Mainchain         |
| 3   | E     | 791 | GLN  | Mainchain         |
| 3   | E     | 803 | ALA  | Mainchain         |
| 3   | E     | 837 | MET  | Peptide,Mainchain |
| 4   | F     | 68  | UNK  | Mainchain         |
| 5   | G     | 483 | TYR  | Mainchain         |
| 5   | G     | 492 | CYS  | Mainchain         |
| 5   | G     | 503 | SER  | Mainchain         |
| 5   | G     | 584 | LEU  | Mainchain         |
| 5   | G     | 597 | TRP  | Mainchain         |
| 5   | G     | 608 | ASN  | Mainchain         |
| 5   | G     | 625 | PHE  | Mainchain         |
| 5   | G     | 649 | SER  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 5   | G     | 733 | GLU  | Mainchain         |
| 5   | G     | 749 | ILE  | Mainchain         |
| 5   | G     | 756 | TYR  | Mainchain         |
| 5   | G     | 765 | GLN  | Mainchain         |
| 6   | H     | 105 | UNK  | Mainchain         |
| 6   | H     | 78  | UNK  | Peptide,Mainchain |
| 3   | I     | 326 | ASP  | Mainchain         |
| 3   | I     | 36  | LYS  | Mainchain         |
| 3   | I     | 445 | PRO  | Mainchain         |
| 3   | I     | 471 | ARG  | Mainchain         |
| 3   | I     | 526 | LEU  | Mainchain         |
| 3   | I     | 609 | TRP  | Mainchain         |
| 3   | I     | 631 | VAL  | Mainchain         |
| 3   | I     | 662 | ILE  | Mainchain         |
| 3   | I     | 670 | LEU  | Mainchain         |
| 3   | I     | 784 | GLN  | Peptide,Mainchain |
| 3   | I     | 785 | VAL  | Mainchain         |
| 3   | I     | 826 | ARG  | Mainchain         |
| 3   | I     | 833 | ILE  | Mainchain         |
| 3   | I     | 837 | MET  | Peptide,Mainchain |
| 3   | I     | 847 | LEU  | Mainchain         |
| 3   | I     | 921 | LYS  | Mainchain         |
| 7   | J     | 202 | LEU  | Mainchain         |
| 7   | J     | 294 | SER  | Mainchain         |
| 7   | J     | 325 | SER  | Mainchain         |
| 7   | J     | 345 | PHE  | Mainchain         |
| 7   | J     | 48  | ASP  | Mainchain         |
| 7   | J     | 522 | PHE  | Mainchain         |
| 7   | J     | 533 | THR  | Mainchain         |
| 7   | J     | 541 | GLN  | Mainchain         |
| 7   | J     | 76  | PHE  | Peptide,Mainchain |
| 5   | L     | 483 | TYR  | Mainchain         |
| 5   | L     | 492 | CYS  | Mainchain         |
| 5   | L     | 503 | SER  | Mainchain         |
| 5   | L     | 584 | LEU  | Mainchain         |
| 5   | L     | 597 | TRP  | Mainchain         |
| 5   | L     | 608 | ASN  | Mainchain         |
| 5   | L     | 649 | SER  | Peptide,Mainchain |
| 5   | L     | 749 | ILE  | Mainchain         |
| 5   | L     | 756 | TYR  | Mainchain         |
| 5   | L     | 765 | GLN  | Mainchain         |
| 5   | L     | 858 | MET  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 5   | L     | 875 | ILE  | Mainchain         |
| 5   | L     | 893 | LYS  | Mainchain         |
| 5   | L     | 908 | GLU  | Mainchain         |
| 5   | L     | 919 | THR  | Mainchain         |
| 5   | L     | 927 | MET  | Mainchain         |
| 5   | M     | 236 | ALA  | Mainchain         |
| 5   | M     | 253 | ASN  | Mainchain         |
| 5   | M     | 270 | SER  | Mainchain         |
| 5   | M     | 31  | ASN  | Peptide,Mainchain |
| 5   | M     | 320 | MET  | Mainchain         |
| 5   | M     | 337 | TYR  | Mainchain         |
| 5   | M     | 341 | LYS  | Peptide           |
| 5   | M     | 59  | VAL  | Mainchain         |
| 7   | O     | 202 | LEU  | Mainchain         |
| 7   | O     | 294 | SER  | Mainchain         |
| 7   | O     | 325 | SER  | Peptide,Mainchain |
| 7   | O     | 345 | PHE  | Mainchain         |
| 7   | O     | 48  | ASP  | Mainchain         |
| 7   | O     | 522 | PHE  | Mainchain         |
| 7   | O     | 533 | THR  | Mainchain         |
| 7   | O     | 541 | GLN  | Mainchain         |
| 7   | O     | 557 | LEU  | Mainchain         |
| 7   | O     | 76  | PHE  | Peptide,Mainchain |
| 5   | R     | 124 | THR  | Mainchain         |
| 5   | R     | 236 | ALA  | Mainchain         |
| 5   | R     | 253 | ASN  | Mainchain         |
| 5   | R     | 270 | SER  | Mainchain         |
| 5   | R     | 282 | LYS  | Peptide,Mainchain |
| 5   | R     | 283 | ASN  | Mainchain         |
| 5   | R     | 31  | ASN  | Peptide,Mainchain |
| 5   | R     | 337 | TYR  | Mainchain         |
| 5   | R     | 59  | VAL  | Mainchain         |
| 14  | V     | 11  | UNK  | Mainchain         |
| 14  | V     | 64  | UNK  | Mainchain         |
| 14  | V     | 84  | UNK  | Mainchain         |
| 15  | W     | 30  | UNK  | Mainchain         |
| 15  | W     | 44  | UNK  | Mainchain         |
| 16  | Z     | 125 | ALA  | Mainchain         |
| 16  | Z     | 132 | GLN  | Mainchain         |
| 16  | Z     | 139 | LYS  | Mainchain         |
| 16  | Z     | 147 | LYS  | Mainchain         |
| 16  | Z     | 98  | LEU  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 14  | a     | 11  | UNK  | Mainchain         |
| 14  | a     | 64  | UNK  | Mainchain         |
| 14  | a     | 84  | UNK  | Mainchain         |
| 16  | c     | 132 | GLN  | Peptide,Mainchain |
| 16  | c     | 154 | THR  | Peptide,Mainchain |
| 16  | c     | 40  | GLN  | Mainchain         |
| 4   | d     | 68  | UNK  | Mainchain         |
| 2   | f     | 136 | GLU  | Mainchain         |
| 2   | f     | 265 | ASP  | Mainchain         |
| 2   | f     | 29  | ILE  | Mainchain         |
| 2   | f     | 32  | ALA  | Mainchain         |
| 2   | f     | 347 | LYS  | Mainchain         |
| 2   | f     | 354 | GLU  | Peptide,Mainchain |
| 2   | f     | 37  | LYS  | Mainchain         |
| 2   | f     | 44  | LYS  | Mainchain         |
| 2   | f     | 53  | LYS  | Mainchain         |
| 2   | f     | 86  | ASN  | Mainchain         |
| 1   | i     | 155 | ASP  | Mainchain         |
| 1   | i     | 222 | TYR  | Mainchain         |
| 1   | i     | 301 | GLU  | Mainchain         |
| 1   | i     | 349 | VAL  | Peptide,Mainchain |
| 1   | i     | 94  | LEU  | Mainchain         |
| 2   | k     | 12  | LEU  | Mainchain         |
| 2   | k     | 233 | ILE  | Peptide,Mainchain |
| 2   | k     | 318 | ILE  | Mainchain         |
| 2   | k     | 331 | ASN  | Mainchain         |
| 2   | k     | 350 | GLU  | Peptide,Mainchain |
| 2   | k     | 355 | TYR  | Mainchain         |
| 2   | k     | 357 | ARG  | Mainchain         |
| 2   | k     | 82  | ARG  | Mainchain         |
| 2   | k     | 93  | LEU  | Mainchain         |
| 6   | l     | 105 | UNK  | Mainchain         |
| 6   | l     | 78  | UNK  | Peptide,Mainchain |
| 3   | n     | 326 | ASP  | Mainchain         |
| 3   | n     | 36  | LYS  | Mainchain         |
| 3   | n     | 445 | PRO  | Mainchain         |
| 3   | n     | 471 | ARG  | Mainchain         |
| 3   | n     | 526 | LEU  | Mainchain         |
| 3   | n     | 609 | TRP  | Mainchain         |
| 3   | n     | 631 | VAL  | Mainchain         |
| 3   | n     | 662 | ILE  | Mainchain         |
| 3   | n     | 670 | LEU  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 3   | n     | 733 | LYS  | Mainchain         |
| 3   | n     | 784 | GLN  | Peptide,Mainchain |
| 4   | o     | 68  | UNK  | Mainchain         |
| 2   | q     | 12  | LEU  | Mainchain         |
| 2   | q     | 233 | ILE  | Peptide,Mainchain |
| 2   | q     | 318 | ILE  | Mainchain         |
| 2   | q     | 357 | ARG  | Mainchain         |
| 2   | q     | 82  | ARG  | Mainchain         |
| 2   | q     | 93  | LEU  | Mainchain         |
| 2   | s     | 136 | GLU  | Mainchain         |
| 2   | s     | 239 | GLN  | Mainchain         |
| 2   | s     | 265 | ASP  | Mainchain         |
| 2   | s     | 29  | ILE  | Peptide,Mainchain |
| 2   | s     | 314 | GLU  | Mainchain         |
| 2   | s     | 32  | ALA  | Mainchain         |
| 2   | s     | 354 | GLU  | Peptide,Mainchain |
| 2   | s     | 37  | LYS  | Mainchain         |
| 5   | v     | 483 | TYR  | Mainchain         |
| 5   | v     | 492 | CYS  | Mainchain         |
| 5   | v     | 503 | SER  | Mainchain         |
| 5   | v     | 584 | LEU  | Mainchain         |
| 5   | v     | 597 | TRP  | Mainchain         |
| 5   | v     | 608 | ASN  | Mainchain         |
| 5   | v     | 649 | SER  | Mainchain         |
| 5   | v     | 749 | ILE  | Mainchain         |
| 5   | v     | 756 | TYR  | Mainchain         |
| 5   | v     | 765 | GLN  | Mainchain         |
| 6   | w     | 105 | UNK  | Mainchain         |
| 6   | w     | 78  | UNK  | Peptide,Mainchain |
| 2   | y     | 239 | GLN  | Mainchain         |
| 2   | y     | 265 | ASP  | Mainchain         |
| 2   | y     | 32  | ALA  | Mainchain         |
| 2   | y     | 329 | GLN  | Mainchain         |
| 2   | y     | 347 | LYS  | Mainchain         |
| 2   | y     | 354 | GLU  | Mainchain         |
| 2   | y     | 37  | LYS  | Mainchain         |
| 2   | y     | 44  | LYS  | Peptide,Mainchain |
| 2   | y     | 53  | LYS  | Mainchain         |
| 2   | y     | 86  | ASN  | Mainchain         |
| 2   | z     | 239 | GLN  | Mainchain         |
| 2   | z     | 265 | ASP  | Mainchain         |
| 2   | z     | 32  | ALA  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | z     | 329 | GLN  | Mainchain         |
| 2   | z     | 347 | LYS  | Mainchain         |
| 2   | z     | 354 | GLU  | Mainchain         |
| 2   | z     | 37  | LYS  | Mainchain         |
| 2   | z     | 44  | LYS  | Peptide,Mainchain |
| 2   | z     | 53  | LYS  | Mainchain         |
| 2   | z     | 86  | ASN  | Mainchain         |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2129  | 0        | 926      | 2       | 0            |
| 1   | BD    | 2129  | 0        | 926      | 2       | 0            |
| 1   | C     | 2129  | 0        | 926      | 7       | 0            |
| 1   | CP    | 2129  | 0        | 926      | 4       | 0            |
| 1   | Ca    | 2129  | 0        | 926      | 5       | 0            |
| 1   | i     | 2129  | 0        | 926      | 1       | 0            |
| 2   | BK    | 1415  | 0        | 597      | 4       | 0            |
| 2   | BR    | 1288  | 0        | 542      | 5       | 0            |
| 2   | CW    | 1415  | 0        | 596      | 6       | 0            |
| 2   | Cd    | 1288  | 0        | 542      | 10      | 0            |
| 2   | Ch    | 1415  | 0        | 597      | 8       | 0            |
| 2   | D     | 1415  | 0        | 597      | 4       | 0            |
| 2   | f     | 1288  | 0        | 542      | 9       | 0            |
| 2   | k     | 1415  | 0        | 597      | 9       | 0            |
| 2   | q     | 1415  | 0        | 597      | 4       | 0            |
| 2   | s     | 1288  | 0        | 542      | 10      | 0            |
| 2   | y     | 1288  | 0        | 542      | 5       | 0            |
| 2   | z     | 1288  | 0        | 542      | 5       | 0            |
| 3   | 1     | 3082  | 0        | 1317     | 8       | 0            |
| 3   | 7     | 4040  | 0        | 1741     | 15      | 0            |
| 3   | BY    | 3841  | 0        | 1655     | 18      | 0            |
| 3   | E     | 3597  | 0        | 1547     | 14      | 0            |
| 3   | I     | 4040  | 0        | 1741     | 10      | 0            |
| 3   | n     | 3302  | 0        | 1411     | 12      | 0            |
| 4   | BO    | 755   | 0        | 158      | 7       | 0            |
| 4   | BZ    | 755   | 0        | 158      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | Bw    | 755   | 0        | 158      | 5       | 0            |
| 4   | F     | 755   | 0        | 157      | 5       | 0            |
| 4   | d     | 755   | 0        | 159      | 6       | 0            |
| 4   | o     | 755   | 0        | 157      | 3       | 0            |
| 5   | 9     | 1510  | 0        | 629      | 6       | 0            |
| 5   | AB    | 1752  | 0        | 772      | 1       | 0            |
| 5   | AE    | 2584  | 0        | 1093     | 11      | 0            |
| 5   | AO    | 1752  | 0        | 772      | 3       | 0            |
| 5   | AU    | 1752  | 0        | 772      | 7       | 0            |
| 5   | Bf    | 2334  | 0        | 990      | 8       | 0            |
| 5   | Bt    | 1752  | 0        | 772      | 5       | 0            |
| 5   | G     | 2064  | 0        | 867      | 9       | 0            |
| 5   | L     | 2584  | 0        | 1093     | 10      | 0            |
| 5   | M     | 1752  | 0        | 772      | 6       | 0            |
| 5   | R     | 1752  | 0        | 772      | 4       | 0            |
| 5   | v     | 1790  | 0        | 744      | 5       | 0            |
| 6   | B4    | 820   | 0        | 167      | 0       | 0            |
| 6   | BV    | 820   | 0        | 167      | 0       | 0            |
| 6   | Bg    | 820   | 0        | 167      | 0       | 0            |
| 6   | H     | 820   | 0        | 167      | 0       | 0            |
| 6   | l     | 820   | 0        | 167      | 0       | 0            |
| 6   | w     | 820   | 0        | 166      | 0       | 0            |
| 7   | 4     | 1806  | 0        | 792      | 15      | 0            |
| 7   | AG    | 1806  | 0        | 792      | 17      | 0            |
| 7   | AM    | 1806  | 0        | 792      | 17      | 0            |
| 7   | Bm    | 1806  | 0        | 792      | 17      | 0            |
| 7   | J     | 1806  | 0        | 792      | 10      | 0            |
| 7   | O     | 1806  | 0        | 792      | 10      | 0            |
| 8   | 5     | 835   | 0        | 169      | 0       | 0            |
| 8   | Bc    | 835   | 0        | 169      | 0       | 0            |
| 8   | Bn    | 835   | 0        | 169      | 0       | 0            |
| 8   | CA    | 835   | 0        | 169      | 0       | 0            |
| 8   | K     | 835   | 0        | 169      | 0       | 0            |
| 8   | t     | 835   | 0        | 169      | 0       | 0            |
| 9   | 2     | 805   | 0        | 165      | 2       | 0            |
| 9   | AC    | 805   | 0        | 165      | 1       | 0            |
| 9   | Bj    | 805   | 0        | 165      | 0       | 0            |
| 9   | Bu    | 805   | 0        | 165      | 0       | 0            |
| 9   | CH    | 805   | 0        | 165      | 0       | 0            |
| 9   | N     | 805   | 0        | 165      | 0       | 0            |
| 10  | AJ    | 160   | 0        | 34       | 0       | 0            |
| 10  | AW    | 160   | 0        | 34       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | Ac    | 160   | 0        | 35       | 0       | 0            |
| 10  | B1    | 160   | 0        | 34       | 0       | 0            |
| 10  | P     | 160   | 0        | 34       | 0       | 0            |
| 10  | U     | 160   | 0        | 34       | 0       | 0            |
| 11  | 0     | 525   | 0        | 107      | 0       | 0            |
| 11  | AK    | 525   | 0        | 107      | 1       | 0            |
| 11  | B2    | 525   | 0        | 107      | 0       | 0            |
| 11  | Bq    | 525   | 0        | 107      | 0       | 0            |
| 11  | CO    | 525   | 0        | 107      | 0       | 0            |
| 11  | Q     | 525   | 0        | 107      | 1       | 0            |
| 12  | AR    | 165   | 0        | 35       | 0       | 0            |
| 12  | Ae    | 165   | 0        | 35       | 0       | 0            |
| 12  | Ak    | 165   | 0        | 35       | 0       | 0            |
| 12  | B8    | 165   | 0        | 35       | 0       | 0            |
| 12  | S     | 165   | 0        | 35       | 0       | 0            |
| 12  | X     | 165   | 0        | 35       | 0       | 0            |
| 13  | AH    | 635   | 0        | 129      | 1       | 0            |
| 13  | AS    | 635   | 0        | 130      | 0       | 0            |
| 13  | B9    | 635   | 0        | 129      | 1       | 0            |
| 13  | Bx    | 635   | 0        | 129      | 1       | 0            |
| 13  | CV    | 635   | 0        | 129      | 1       | 0            |
| 13  | T     | 635   | 0        | 129      | 1       | 0            |
| 14  | AZ    | 765   | 0        | 158      | 3       | 0            |
| 14  | Am    | 765   | 0        | 157      | 7       | 0            |
| 14  | As    | 765   | 0        | 158      | 3       | 0            |
| 14  | CE    | 765   | 0        | 157      | 4       | 0            |
| 14  | V     | 765   | 0        | 157      | 2       | 0            |
| 14  | a     | 765   | 0        | 158      | 3       | 0            |
| 15  | AP    | 510   | 0        | 105      | 3       | 0            |
| 15  | Aa    | 510   | 0        | 104      | 0       | 0            |
| 15  | B5    | 510   | 0        | 104      | 2       | 0            |
| 15  | CF    | 510   | 0        | 104      | 2       | 0            |
| 15  | Cc    | 510   | 0        | 104      | 1       | 0            |
| 15  | W     | 510   | 0        | 104      | 1       | 0            |
| 16  | A7    | 783   | 0        | 350      | 3       | 0            |
| 16  | Ai    | 748   | 0        | 330      | 1       | 0            |
| 16  | An    | 748   | 0        | 330      | 2       | 0            |
| 16  | Aq    | 783   | 0        | 350      | 4       | 0            |
| 16  | Av    | 783   | 0        | 350      | 3       | 0            |
| 16  | Az    | 748   | 0        | 330      | 1       | 0            |
| 16  | CB    | 748   | 0        | 330      | 1       | 0            |
| 16  | CI    | 783   | 0        | 350      | 5       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 16  | CM    | 748    | 0        | 330      | 3       | 0            |
| 16  | CT    | 783    | 0        | 350      | 4       | 0            |
| 16  | Z     | 748    | 0        | 330      | 2       | 0            |
| 16  | c     | 783    | 0        | 350      | 4       | 0            |
| All | All   | 130144 | 0        | 48035    | 442     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:Cd:330:ALA:H | 2:Cd:332:VAL:H | 1.41                     | 0.69              |
| 1:BD:234:THR:O | 1:BD:235:PRO:C | 2.43                     | 0.62              |
| 1:CP:234:THR:O | 1:CP:235:PRO:C | 2.43                     | 0.62              |
| 1:A:234:THR:O  | 1:A:235:PRO:C  | 2.43                     | 0.61              |
| 14:CE:72:UNK:O | 14:CE:73:UNK:C | 2.48                     | 0.61              |
| 14:AZ:72:UNK:O | 14:AZ:73:UNK:C | 2.49                     | 0.60              |
| 2:q:152:TYR:O  | 2:q:153:LEU:C  | 2.41                     | 0.60              |
| 2:BK:152:TYR:O | 2:BK:153:LEU:C | 2.44                     | 0.60              |
| 2:Ch:152:TYR:O | 2:Ch:153:LEU:C | 2.44                     | 0.60              |
| 14:a:72:UNK:O  | 14:a:73:UNK:C  | 2.50                     | 0.59              |
| 3:E:799:GLU:O  | 3:E:803:ALA:N  | 2.36                     | 0.59              |
| 14:V:72:UNK:O  | 14:V:73:UNK:C  | 2.48                     | 0.59              |
| 14:Am:72:UNK:O | 14:Am:73:UNK:C | 2.49                     | 0.59              |
| 14:a:5:UNK:HA  | 14:a:6:UNK:C   | 2.33                     | 0.58              |
| 3:I:682:GLN:O  | 3:I:683:ALA:C  | 2.44                     | 0.58              |
| 2:k:152:TYR:O  | 2:k:153:LEU:C  | 2.46                     | 0.58              |
| 14:As:72:UNK:O | 14:As:73:UNK:C | 2.49                     | 0.58              |
| 14:CE:5:UNK:HA | 14:CE:6:UNK:C  | 2.34                     | 0.58              |
| 7:AG:142:ASP:O | 7:AG:144:GLY:N | 2.38                     | 0.56              |
| 3:BY:555:ASN:C | 3:BY:556:PRO:O | 2.42                     | 0.56              |
| 5:Bt:230:LEU:N | 5:Bt:351:PHE:O | 2.39                     | 0.56              |
| 7:AG:146:LEU:N | 7:AG:157:LEU:O | 2.39                     | 0.56              |
| 7:Bm:231:ASP:O | 7:Bm:232:THR:C | 2.48                     | 0.56              |
| 14:As:5:UNK:HA | 14:As:6:UNK:C  | 2.36                     | 0.56              |
| 1:Ca:234:THR:O | 1:Ca:235:PRO:C | 2.48                     | 0.56              |
| 5:AU:230:LEU:N | 5:AU:351:PHE:O | 2.40                     | 0.55              |
| 5:Bt:317:ILE:O | 5:Bt:321:ASN:N | 2.39                     | 0.55              |
| 7:AM:553:TYR:O | 7:AM:557:LEU:N | 2.40                     | 0.55              |
| 3:BY:799:GLU:O | 3:BY:803:ALA:N | 2.38                     | 0.55              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 5:R:230:LEU:N   | 5:R:351:PHE:O  | 2.40                     | 0.55              |
| 2:s:44:LYS:O    | 2:s:45:THR:C   | 2.48                     | 0.55              |
| 5:M:230:LEU:N   | 5:M:351:PHE:O  | 2.39                     | 0.55              |
| 5:AO:230:LEU:N  | 5:AO:351:PHE:O | 2.40                     | 0.55              |
| 3:n:754:ASP:O   | 3:n:755:ALA:C  | 2.50                     | 0.54              |
| 2:y:84:ASN:O    | 2:y:88:GLN:N   | 2.38                     | 0.54              |
| 2:z:84:ASN:O    | 2:z:88:GLN:N   | 2.38                     | 0.54              |
| 5:AU:153:ALA:O  | 5:AU:154:SER:C | 2.46                     | 0.54              |
| 3:E:746:GLU:O   | 3:E:747:LYS:CB | 2.56                     | 0.54              |
| 3:1:287:MET:O   | 3:1:288:GLU:C  | 2.50                     | 0.54              |
| 5:AB:230:LEU:N  | 5:AB:351:PHE:O | 2.41                     | 0.54              |
| 7:AM:544:TYR:O  | 7:AM:545:SER:C | 2.51                     | 0.54              |
| 3:1:682:GLN:O   | 3:1:683:ALA:C  | 2.50                     | 0.54              |
| 5:v:626:LYS:O   | 5:v:627:HIS:C  | 2.49                     | 0.53              |
| 2:BR:90:GLU:O   | 2:BR:92:ILE:N  | 2.42                     | 0.53              |
| 5:M:320:MET:O   | 5:M:323:GLN:N  | 2.41                     | 0.53              |
| 3:7:682:GLN:O   | 3:7:683:ALA:C  | 2.51                     | 0.53              |
| 5:Bt:323:GLN:O  | 5:Bt:327:LEU:N | 2.42                     | 0.53              |
| 5:L:597:TRP:O   | 5:L:600:LEU:N  | 2.41                     | 0.52              |
| 7:J:544:TYR:O   | 7:J:545:SER:C  | 2.52                     | 0.52              |
| 1:C:38:GLU:O    | 1:C:39:LEU:C   | 2.52                     | 0.52              |
| 2:D:152:TYR:O   | 2:D:153:LEU:C  | 2.51                     | 0.52              |
| 1:C:37:GLN:O    | 1:C:38:GLU:C   | 2.47                     | 0.52              |
| 7:O:201:ASP:O   | 7:O:205:GLN:N  | 2.43                     | 0.52              |
| 3:BY:682:GLN:O  | 3:BY:684:VAL:N | 2.43                     | 0.51              |
| 3:I:287:MET:O   | 3:I:288:GLU:C  | 2.54                     | 0.51              |
| 7:Bm:178:SER:CB | 7:Bm:236:VAL:H | 2.22                     | 0.51              |
| 3:7:287:MET:O   | 3:7:288:GLU:C  | 2.53                     | 0.51              |
| 5:AE:466:PRO:O  | 5:AE:705:GLU:N | 2.44                     | 0.51              |
| 16:CI:53:ALA:O  | 16:CI:54:PRO:C | 2.53                     | 0.51              |
| 5:L:706:THR:O   | 5:L:707:GLU:C  | 2.53                     | 0.51              |
| 16:Aq:93:ILE:C  | 16:Aq:94:PRO:O | 2.48                     | 0.50              |
| 2:Ch:296:ASP:C  | 2:Ch:297:LYS:O | 2.46                     | 0.50              |
| 1:C:234:THR:O   | 1:C:235:PRO:C  | 2.54                     | 0.50              |
| 2:f:83:GLU:O    | 2:f:87:LEU:N   | 2.44                     | 0.50              |
| 5:9:597:TRP:O   | 5:9:600:LEU:N  | 2.45                     | 0.50              |
| 5:v:556:GLU:C   | 5:v:557:ILE:O  | 2.51                     | 0.50              |
| 7:AM:553:TYR:O  | 7:AM:554:MET:C | 2.53                     | 0.50              |
| 7:AG:163:LYS:O  | 7:AG:164:LYS:C | 2.55                     | 0.50              |
| 2:BR:41:ASP:O   | 2:BR:45:THR:N  | 2.45                     | 0.50              |
| 3:BY:559:SER:HA | 3:BY:562:LYS:H | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:682:GLN:O    | 3:E:683:ALA:C    | 2.54                     | 0.50              |
| 7:O:38:ALA:O     | 7:O:39:LEU:C     | 2.54                     | 0.50              |
| 3:E:287:MET:O    | 3:E:288:GLU:C    | 2.55                     | 0.49              |
| 5:L:575:LYS:C    | 5:L:576:PHE:O    | 2.51                     | 0.49              |
| 3:7:792:GLN:O    | 3:7:795:LYS:N    | 2.44                     | 0.49              |
| 7:J:524:PRO:O    | 7:J:525:LYS:CB   | 2.61                     | 0.49              |
| 5:M:323:GLN:O    | 5:M:327:LEU:N    | 2.46                     | 0.49              |
| 7:O:524:PRO:O    | 7:O:525:LYS:CB   | 2.61                     | 0.49              |
| 5:L:927:MET:O    | 5:L:930:ILE:N    | 2.46                     | 0.49              |
| 2:y:328:SER:C    | 2:y:330:ALA:H    | 2.19                     | 0.49              |
| 5:AU:285:GLY:HA3 | 7:Bm:143:GLY:HA3 | 1.94                     | 0.49              |
| 7:J:138:SER:O    | 7:J:147:LEU:N    | 2.44                     | 0.49              |
| 7:AG:231:ASP:O   | 7:AG:232:THR:C   | 2.55                     | 0.49              |
| 7:AM:524:PRO:O   | 7:AM:525:LYS:CB  | 2.61                     | 0.49              |
| 2:z:328:SER:C    | 2:z:330:ALA:H    | 2.19                     | 0.49              |
| 5:v:706:THR:O    | 5:v:707:GLU:C    | 2.55                     | 0.49              |
| 5:AU:282:LYS:HA  | 7:Bm:140:SER:O   | 2.13                     | 0.49              |
| 2:y:304:GLN:O    | 2:y:308:LEU:N    | 2.41                     | 0.48              |
| 7:Bm:159:ARG:H   | 7:Bm:166:MET:CB  | 2.26                     | 0.48              |
| 2:Cd:28:GLN:C    | 2:Cd:30:GLU:H    | 2.21                     | 0.48              |
| 3:7:799:GLU:O    | 3:7:803:ALA:N    | 2.47                     | 0.48              |
| 5:AE:927:MET:O   | 5:AE:930:ILE:N   | 2.46                     | 0.48              |
| 7:AG:144:GLY:O   | 7:AG:160:LEU:N   | 2.44                     | 0.48              |
| 7:AG:524:PRO:O   | 7:AG:525:LYS:CB  | 2.62                     | 0.48              |
| 4:BO:15:UNK:O    | 4:BO:19:UNK:N    | 2.46                     | 0.48              |
| 15:B5:44:UNK:O   | 15:B5:45:UNK:C   | 2.61                     | 0.48              |
| 2:z:304:GLN:O    | 2:z:308:LEU:N    | 2.41                     | 0.48              |
| 7:J:144:GLY:O    | 7:J:160:LEU:N    | 2.44                     | 0.48              |
| 2:y:328:SER:C    | 2:y:330:ALA:N    | 2.71                     | 0.48              |
| 2:z:328:SER:C    | 2:z:330:ALA:N    | 2.71                     | 0.48              |
| 3:n:682:GLN:O    | 3:n:684:VAL:N    | 2.47                     | 0.48              |
| 7:4:159:ARG:H    | 7:4:166:MET:CB   | 2.27                     | 0.48              |
| 14:Am:-16:UNK:O  | 14:Am:-12:UNK:N  | 2.46                     | 0.48              |
| 7:Bm:524:PRO:O   | 7:Bm:525:LYS:CB  | 2.62                     | 0.48              |
| 16:CT:42:TYR:O   | 16:CT:43:LYS:C   | 2.55                     | 0.48              |
| 7:4:524:PRO:O    | 7:4:525:LYS:CB   | 2.62                     | 0.48              |
| 15:AP:44:UNK:O   | 15:AP:45:UNK:C   | 2.61                     | 0.48              |
| 5:AE:575:LYS:C   | 5:AE:576:PHE:O   | 2.53                     | 0.48              |
| 7:AM:517:THR:O   | 7:AM:518:TYR:C   | 2.56                     | 0.47              |
| 2:BK:108:ARG:O   | 2:BK:112:LEU:N   | 2.42                     | 0.47              |
| 5:Bf:575:LYS:C   | 5:Bf:576:PHE:O   | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:Bm:163:LYS:O   | 7:Bm:164:LYS:C   | 2.57                     | 0.47              |
| 3:BY:792:GLN:O   | 3:BY:795:LYS:N   | 2.47                     | 0.47              |
| 5:Bf:483:TYR:O   | 5:Bf:486:MET:N   | 2.46                     | 0.47              |
| 2:f:136:GLU:O    | 2:f:139:ALA:N    | 2.47                     | 0.47              |
| 16:CM:173:ILE:CB | 16:CM:174:GLU:HA | 2.44                     | 0.47              |
| 3:E:799:GLU:O    | 3:E:800:SER:C    | 2.54                     | 0.47              |
| 5:G:575:LYS:C    | 5:G:576:PHE:O    | 2.51                     | 0.47              |
| 5:9:626:LYS:O    | 5:9:627:HIS:C    | 2.56                     | 0.47              |
| 5:L:803:ASP:O    | 5:L:804:LEU:C    | 2.55                     | 0.47              |
| 5:R:53:GLY:O     | 5:R:54:ASN:C     | 2.58                     | 0.47              |
| 3:n:631:VAL:O    | 3:n:634:PHE:N    | 2.48                     | 0.47              |
| 3:BY:631:VAL:O   | 3:BY:634:PHE:N   | 2.46                     | 0.47              |
| 3:n:765:GLU:C    | 3:n:767:ILE:H    | 2.23                     | 0.47              |
| 4:Bw:15:UNK:O    | 4:Bw:19:UNK:N    | 2.47                     | 0.47              |
| 16:c:53:ALA:O    | 16:c:54:PRO:C    | 2.57                     | 0.47              |
| 3:1:429:LEU:O    | 3:1:430:ASP:CB   | 2.63                     | 0.47              |
| 7:O:544:TYR:O    | 7:O:545:SER:C    | 2.55                     | 0.47              |
| 11:Q:55:UNK:O    | 11:Q:59:UNK:N    | 2.48                     | 0.47              |
| 7:4:201:ASP:O    | 7:4:205:GLN:N    | 2.48                     | 0.47              |
| 2:Ch:342:LEU:O   | 2:Ch:345:LEU:N   | 2.48                     | 0.47              |
| 3:E:92:GLU:O     | 3:E:93:LYS:C     | 2.58                     | 0.46              |
| 4:F:15:UNK:O     | 4:F:19:UNK:N     | 2.48                     | 0.46              |
| 3:n:287:MET:O    | 3:n:288:GLU:C    | 2.58                     | 0.46              |
| 14:a:11:UNK:O    | 14:a:14:UNK:N    | 2.48                     | 0.46              |
| 3:7:595:SER:O    | 3:7:599:VAL:HA   | 2.15                     | 0.46              |
| 7:AG:142:ASP:C   | 7:AG:144:GLY:H   | 2.23                     | 0.46              |
| 7:AM:280:ILE:O   | 7:AM:281:HIS:C   | 2.56                     | 0.46              |
| 14:Am:-28:UNK:O  | 14:Am:-24:UNK:N  | 2.48                     | 0.46              |
| 15:Cc:44:UNK:O   | 15:Cc:45:UNK:C   | 2.62                     | 0.46              |
| 4:d:15:UNK:O     | 4:d:19:UNK:N     | 2.48                     | 0.46              |
| 7:4:108:GLY:C    | 7:4:110:ASP:H    | 2.22                     | 0.46              |
| 7:AM:342:LYS:O   | 7:AM:343:THR:C   | 2.57                     | 0.46              |
| 16:CT:73:LEU:O   | 16:CT:74:VAL:C   | 2.54                     | 0.46              |
| 5:M:317:ILE:O    | 5:M:321:ASN:N    | 2.49                     | 0.46              |
| 2:k:331:ASN:O    | 2:k:332:VAL:C    | 2.59                     | 0.46              |
| 2:q:246:GLN:HA   | 2:q:248:HIS:N    | 2.30                     | 0.46              |
| 7:O:163:LYS:O    | 7:O:164:LYS:C    | 2.58                     | 0.46              |
| 4:d:33:UNK:CB    | 4:d:34:UNK:HA    | 2.46                     | 0.46              |
| 2:k:270:ARG:O    | 2:k:271:LEU:C    | 2.58                     | 0.46              |
| 2:CW:152:TYR:O   | 2:CW:153:LEU:C   | 2.57                     | 0.46              |
| 7:J:38:ALA:O     | 7:J:39:LEU:C     | 2.58                     | 0.46              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 5:R:285:GLY:O   | 5:R:303:GLY:N   | 2.48                     | 0.46              |
| 15:W:44:UNK:O   | 15:W:45:UNK:C   | 2.63                     | 0.46              |
| 5:9:424:LEU:O   | 5:9:425:ARG:C   | 2.57                     | 0.46              |
| 16:CI:42:TYR:O  | 16:CI:43:LYS:C  | 2.56                     | 0.46              |
| 2:Cd:327:LEU:O  | 2:Cd:329:GLN:N  | 2.49                     | 0.46              |
| 2:s:291:TYR:O   | 2:s:292:MET:C   | 2.58                     | 0.46              |
| 7:4:87:GLY:O    | 7:4:88:HIS:C    | 2.59                     | 0.46              |
| 2:BR:117:GLN:O  | 2:BR:120:LYS:N  | 2.48                     | 0.46              |
| 2:Cd:240:LEU:O  | 2:Cd:241:ARG:C  | 2.57                     | 0.46              |
| 5:L:893:LYS:O   | 5:L:896:LYS:N   | 2.48                     | 0.46              |
| 4:o:16:UNK:O    | 4:o:17:UNK:C    | 2.63                     | 0.46              |
| 2:s:41:ASP:O    | 2:s:45:THR:N    | 2.47                     | 0.46              |
| 2:s:44:LYS:O    | 2:s:47:GLU:N    | 2.49                     | 0.46              |
| 5:9:523:LEU:O   | 5:9:524:ALA:C   | 2.55                     | 0.46              |
| 7:AG:559:ASN:O  | 7:AG:560:ARG:C  | 2.57                     | 0.46              |
| 16:CI:178:SER:C | 16:CI:179:TYR:O | 2.53                     | 0.46              |
| 16:CT:93:ILE:C  | 16:CT:94:PRO:O  | 2.46                     | 0.46              |
| 7:AM:231:ASP:O  | 7:AM:232:THR:C  | 2.59                     | 0.46              |
| 16:Av:53:ALA:O  | 16:Av:54:PRO:C  | 2.55                     | 0.46              |
| 4:d:32:UNK:O    | 4:d:33:UNK:C    | 2.64                     | 0.45              |
| 7:4:534:GLU:C   | 7:4:535:ALA:O   | 2.47                     | 0.45              |
| 7:AG:517:THR:O  | 7:AG:518:TYR:C  | 2.58                     | 0.45              |
| 3:BY:558:VAL:O  | 3:BY:562:LYS:N  | 2.49                     | 0.45              |
| 16:c:42:TYR:O   | 16:c:43:LYS:C   | 2.57                     | 0.45              |
| 5:v:575:LYS:C   | 5:v:576:PHE:O   | 2.54                     | 0.45              |
| 7:Bm:280:ILE:O  | 7:Bm:281:HIS:C  | 2.54                     | 0.45              |
| 3:n:96:GLY:O    | 3:n:97:TYR:C    | 2.59                     | 0.45              |
| 16:An:30:GLY:O  | 16:An:31:LYS:C  | 2.57                     | 0.45              |
| 16:Aq:42:TYR:O  | 16:Aq:43:LYS:C  | 2.56                     | 0.45              |
| 16:A7:42:TYR:O  | 16:A7:43:LYS:C  | 2.58                     | 0.45              |
| 3:BY:745:LEU:C  | 3:BY:746:GLU:O  | 2.53                     | 0.45              |
| 5:AU:285:GLY:O  | 5:AU:303:GLY:N  | 2.48                     | 0.45              |
| 4:F:16:UNK:O    | 4:F:20:UNK:N    | 2.50                     | 0.45              |
| 5:G:598:LEU:O   | 5:G:599:GLN:C   | 2.56                     | 0.45              |
| 4:o:-2:UNK:O    | 4:o:-1:UNK:C    | 2.64                     | 0.45              |
| 7:4:342:LYS:O   | 7:4:343:THR:C   | 2.58                     | 0.45              |
| 5:M:266:ALA:O   | 5:M:275:ALA:N   | 2.49                     | 0.45              |
| 2:s:136:GLU:O   | 2:s:139:ALA:N   | 2.49                     | 0.45              |
| 3:1:92:GLU:O    | 3:1:93:LYS:C    | 2.59                     | 0.45              |
| 7:4:144:GLY:O   | 7:4:160:LEU:N   | 2.49                     | 0.45              |
| 1:BD:375:ASN:O  | 1:BD:376:LEU:C  | 2.56                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 14:V:11:UNK:O   | 14:V:14:UNK:N   | 2.49                     | 0.45              |
| 2:f:78:GLN:O    | 2:f:82:ARG:N    | 2.47                     | 0.45              |
| 2:s:32:ALA:O    | 2:s:34:LEU:N    | 2.50                     | 0.45              |
| 5:G:610:THR:C   | 5:G:612:GLU:HA  | 2.42                     | 0.45              |
| 5:Bf:858:MET:O  | 5:Bf:861:ASP:N  | 2.48                     | 0.45              |
| 2:Ch:108:ARG:O  | 2:Ch:109:LEU:C  | 2.56                     | 0.45              |
| 7:AG:342:LYS:O  | 7:AG:343:THR:C  | 2.59                     | 0.45              |
| 5:Bf:881:GLU:O  | 5:Bf:882:ASP:C  | 2.57                     | 0.45              |
| 3:n:732:LEU:C   | 3:n:734:GLU:H   | 2.24                     | 0.45              |
| 7:4:517:THR:O   | 7:4:518:TYR:C   | 2.59                     | 0.45              |
| 3:7:795:LYS:O   | 3:7:799:GLU:N   | 2.50                     | 0.45              |
| 16:Aq:146:GLN:O | 16:Aq:147:LYS:C | 2.56                     | 0.45              |
| 3:BY:287:MET:O  | 3:BY:288:GLU:C  | 2.58                     | 0.45              |
| 1:CP:374:ASN:O  | 1:CP:375:ASN:C  | 2.60                     | 0.45              |
| 7:O:69:SER:HA   | 7:O:88:HIS:O    | 2.17                     | 0.44              |
| 2:f:265:ASP:O   | 2:f:268:ILE:N   | 2.50                     | 0.44              |
| 7:Bm:245:LEU:N  | 7:Bm:257:THR:O  | 2.49                     | 0.44              |
| 3:BY:555:ASN:O  | 3:BY:556:PRO:C  | 2.58                     | 0.44              |
| 3:I:826:ARG:O   | 3:I:829:ASP:N   | 2.50                     | 0.44              |
| 16:c:95:ASP:O   | 16:c:96:ARG:C   | 2.61                     | 0.44              |
| 2:k:111:GLN:O   | 2:k:115:GLU:N   | 2.51                     | 0.44              |
| 3:7:828:ASN:O   | 3:7:832:PHE:N   | 2.44                     | 0.44              |
| 7:J:243:THR:O   | 7:J:244:CYS:C   | 2.60                     | 0.44              |
| 2:s:312:ASN:O   | 2:s:313:THR:C   | 2.59                     | 0.44              |
| 9:2:25:UNK:O    | 9:2:29:UNK:N    | 2.51                     | 0.44              |
| 5:AU:320:MET:C  | 5:AU:321:ASN:O  | 2.56                     | 0.44              |
| 7:Bm:320:VAL:O  | 7:Bm:321:GLN:C  | 2.57                     | 0.44              |
| 2:Cd:286:VAL:O  | 2:Cd:287:GLN:C  | 2.60                     | 0.44              |
| 7:Bm:342:LYS:O  | 7:Bm:343:THR:C  | 2.58                     | 0.44              |
| 7:AM:45:GLY:O   | 7:AM:46:HIS:C   | 2.57                     | 0.44              |
| 7:AM:320:VAL:O  | 7:AM:321:GLN:C  | 2.59                     | 0.44              |
| 16:CM:172:ASP:O | 16:CM:173:ILE:C | 2.60                     | 0.44              |
| 3:E:795:LYS:O   | 3:E:799:GLU:N   | 2.51                     | 0.44              |
| 5:G:794:GLN:O   | 5:G:795:GLU:C   | 2.58                     | 0.44              |
| 2:f:308:LEU:N   | 2:f:309:ASN:HA  | 2.32                     | 0.44              |
| 14:AZ:5:UNK:HA  | 14:AZ:6:UNK:C   | 2.47                     | 0.44              |
| 4:BO:33:UNK:CB  | 4:BO:34:UNK:HA  | 2.47                     | 0.44              |
| 5:G:575:LYS:O   | 5:G:576:PHE:C   | 2.61                     | 0.44              |
| 2:s:108:ARG:O   | 2:s:109:LEU:C   | 2.59                     | 0.44              |
| 5:v:597:TRP:O   | 5:v:600:LEU:N   | 2.51                     | 0.44              |
| 7:4:243:THR:O   | 7:4:244:CYS:C   | 2.61                     | 0.44              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 3:BY:92:GLU:O  | 3:BY:93:LYS:C   | 2.60                     | 0.44              |
| 4:BZ:15:UNK:O  | 4:BZ:19:UNK:N   | 2.50                     | 0.44              |
| 4:Bw:20:UNK:O  | 4:Bw:21:UNK:C   | 2.65                     | 0.44              |
| 15:CF:44:UNK:O | 15:CF:45:UNK:C  | 2.64                     | 0.44              |
| 4:F:32:UNK:O   | 4:F:33:UNK:C    | 2.65                     | 0.44              |
| 4:Bw:34:UNK:O  | 4:Bw:35:UNK:C   | 2.61                     | 0.44              |
| 13:B9:-7:UNK:O | 13:B9:-6:UNK:C  | 2.66                     | 0.44              |
| 16:Av:42:TYR:O | 16:Av:43:LYS:C  | 2.59                     | 0.43              |
| 4:Bw:33:UNK:CB | 4:Bw:34:UNK:HA  | 2.48                     | 0.43              |
| 1:C:362:ASN:O  | 1:C:363:PRO:C   | 2.61                     | 0.43              |
| 3:E:732:LEU:C  | 3:E:734:GLU:H   | 2.25                     | 0.43              |
| 5:L:858:MET:O  | 5:L:861:ASP:N   | 2.51                     | 0.43              |
| 16:Z:119:ARG:O | 16:Z:120:CYS:C  | 2.59                     | 0.43              |
| 7:4:69:SER:HA  | 7:4:88:HIS:O    | 2.18                     | 0.43              |
| 7:O:320:VAL:O  | 7:O:321:GLN:C   | 2.60                     | 0.43              |
| 16:Z:62:GLU:O  | 16:Z:63:LYS:C   | 2.61                     | 0.43              |
| 7:AG:45:GLY:O  | 7:AG:46:HIS:C   | 2.60                     | 0.43              |
| 16:CT:53:ALA:O | 16:CT:54:PRO:C  | 2.60                     | 0.43              |
| 3:I:884:TYR:O  | 3:I:885:LYS:C   | 2.61                     | 0.43              |
| 3:1:152:ASN:O  | 3:1:156:TYR:N   | 2.51                     | 0.43              |
| 14:CE:11:UNK:O | 14:CE:14:UNK:N  | 2.51                     | 0.43              |
| 13:CV:-7:UNK:O | 13:CV:-6:UNK:C  | 2.65                     | 0.43              |
| 5:L:431:HIS:O  | 5:L:432:LYS:C   | 2.62                     | 0.43              |
| 5:R:308:PHE:HA | 5:R:309:LYS:CB  | 2.49                     | 0.43              |
| 5:AE:523:LEU:O | 5:AE:524:ALA:C  | 2.58                     | 0.43              |
| 5:AE:773:LYS:O | 5:AE:774:GLN:C  | 2.60                     | 0.43              |
| 13:AH:-7:UNK:O | 13:AH:-6:UNK:C  | 2.66                     | 0.43              |
| 4:BO:32:UNK:O  | 4:BO:33:UNK:C   | 2.67                     | 0.43              |
| 1:CP:432:PRO:O | 1:CP:434:ILE:N  | 2.52                     | 0.43              |
| 2:CW:12:LEU:O  | 2:CW:15:ARG:N   | 2.51                     | 0.43              |
| 2:k:351:ILE:O  | 2:k:352:LEU:C   | 2.59                     | 0.43              |
| 3:1:631:VAL:O  | 3:1:634:PHE:N   | 2.47                     | 0.43              |
| 5:AE:728:GLN:O | 5:AE:731:SER:N  | 2.52                     | 0.43              |
| 15:AP:50:UNK:O | 15:AP:54:UNK:N  | 2.52                     | 0.43              |
| 15:CF:50:UNK:O | 15:CF:54:UNK:N  | 2.52                     | 0.43              |
| 3:n:756:LEU:O  | 3:n:757:MET:C   | 2.61                     | 0.43              |
| 4:F:33:UNK:CB  | 4:F:34:UNK:HA   | 2.49                     | 0.43              |
| 16:c:116:PHE:O | 16:c:117:GLU:C  | 2.59                     | 0.43              |
| 2:k:310:LYS:O  | 2:k:311:GLU:C   | 2.61                     | 0.43              |
| 3:n:307:ASN:O  | 3:n:308:ILE:C   | 2.60                     | 0.43              |
| 5:AE:610:THR:C | 5:AE:612:GLU:HA | 2.43                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:AK:55:UNK:O  | 11:AK:59:UNK:N  | 2.52                     | 0.43              |
| 7:AM:534:GLU:O  | 7:AM:535:ALA:C  | 2.60                     | 0.43              |
| 2:BK:111:GLN:O  | 2:BK:115:GLU:N  | 2.51                     | 0.43              |
| 4:F:21:UNK:O    | 4:F:25:UNK:N    | 2.52                     | 0.43              |
| 7:O:231:ASP:O   | 7:O:232:THR:C   | 2.61                     | 0.43              |
| 13:T:-7:UNK:O   | 13:T:-6:UNK:C   | 2.67                     | 0.43              |
| 5:9:566:HIS:O   | 5:9:567:GLN:C   | 2.55                     | 0.43              |
| 5:AE:626:LYS:O  | 5:AE:627:HIS:C  | 2.60                     | 0.43              |
| 7:AG:544:TYR:O  | 7:AG:545:SER:C  | 2.57                     | 0.43              |
| 7:AG:553:TYR:O  | 7:AG:557:LEU:N  | 2.52                     | 0.43              |
| 7:Bm:517:THR:O  | 7:Bm:518:TYR:C  | 2.59                     | 0.43              |
| 16:CM:119:ARG:O | 16:CM:120:CYS:C | 2.60                     | 0.43              |
| 2:Ch:297:LYS:O  | 2:Ch:299:LYS:N  | 2.51                     | 0.43              |
| 5:G:786:LEU:O   | 5:G:787:THR:C   | 2.60                     | 0.42              |
| 9:2:123:UNK:O   | 9:2:124:UNK:C   | 2.66                     | 0.42              |
| 3:7:738:LEU:O   | 3:7:742:LEU:N   | 2.52                     | 0.42              |
| 7:AM:163:LYS:O  | 7:AM:164:LYS:C  | 2.62                     | 0.42              |
| 7:4:293:ASP:O   | 7:4:316:ASP:HA  | 2.19                     | 0.42              |
| 14:Am:3:UNK:O   | 14:Am:4:UNK:C   | 2.67                     | 0.42              |
| 4:BZ:16:UNK:O   | 4:BZ:17:UNK:C   | 2.63                     | 0.42              |
| 5:L:442:ILE:O   | 5:L:443:TYR:C   | 2.62                     | 0.42              |
| 7:O:534:GLU:O   | 7:O:535:ALA:C   | 2.55                     | 0.42              |
| 4:d:16:UNK:O    | 4:d:17:UNK:C    | 2.67                     | 0.42              |
| 7:AG:201:ASP:O  | 7:AG:205:GLN:N  | 2.52                     | 0.42              |
| 4:BO:16:UNK:O   | 4:BO:17:UNK:C   | 2.67                     | 0.42              |
| 2:BR:35:VAL:O   | 2:BR:36:ASP:C   | 2.61                     | 0.42              |
| 5:Bf:531:PHE:O  | 5:Bf:532:ALA:C  | 2.60                     | 0.42              |
| 5:G:803:ASP:O   | 5:G:804:LEU:C   | 2.59                     | 0.42              |
| 16:Av:94:PRO:O  | 16:Av:95:ASP:CB | 2.67                     | 0.42              |
| 3:BY:125:THR:O  | 3:BY:126:PHE:CB | 2.67                     | 0.42              |
| 16:CI:44:HIS:O  | 16:CI:45:ALA:C  | 2.60                     | 0.42              |
| 1:i:432:PRO:O   | 1:i:434:ILE:N   | 2.52                     | 0.42              |
| 3:BY:126:PHE:O  | 3:BY:127:LYS:C  | 2.62                     | 0.42              |
| 2:CW:247:VAL:O  | 2:CW:248:HIS:C  | 2.62                     | 0.42              |
| 1:C:201:ASN:O   | 1:C:202:TYR:C   | 2.60                     | 0.42              |
| 2:s:289:TYR:O   | 2:s:290:ASN:CB  | 2.68                     | 0.42              |
| 5:AE:786:LEU:O  | 5:AE:787:THR:C  | 2.60                     | 0.42              |
| 14:AZ:11:UNK:O  | 14:AZ:14:UNK:N  | 2.53                     | 0.42              |
| 7:Bm:553:TYR:O  | 7:Bm:557:LEU:N  | 2.52                     | 0.42              |
| 4:Bw:32:UNK:O   | 4:Bw:33:UNK:C   | 2.68                     | 0.42              |
| 2:CW:331:ASN:O  | 2:CW:332:VAL:C  | 2.62                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:E:608:ASP:C   | 3:E:610:LEU:H   | 2.27                     | 0.42              |
| 2:f:35:VAL:O    | 2:f:36:ASP:C    | 2.62                     | 0.42              |
| 3:7:533:PHE:O   | 3:7:534:CYS:C   | 2.61                     | 0.42              |
| 3:7:593:TRP:O   | 3:7:597:GLN:N   | 2.53                     | 0.42              |
| 5:Bf:626:LYS:O  | 5:Bf:627:HIS:C  | 2.62                     | 0.42              |
| 7:Bm:293:ASP:O  | 7:Bm:316:ASP:HA | 2.20                     | 0.42              |
| 3:E:631:VAL:O   | 3:E:633:TYR:N   | 2.53                     | 0.42              |
| 5:L:626:LYS:O   | 5:L:627:HIS:C   | 2.60                     | 0.42              |
| 5:M:85:LEU:O    | 5:M:96:GLN:HA   | 2.20                     | 0.42              |
| 16:A7:169:PRO:O | 16:A7:170:HIS:C | 2.62                     | 0.42              |
| 4:BO:25:UNK:O   | 4:BO:26:UNK:C   | 2.67                     | 0.42              |
| 3:I:631:VAL:O   | 3:I:633:TYR:N   | 2.52                     | 0.42              |
| 7:AM:138:SER:O  | 7:AM:147:LEU:N  | 2.53                     | 0.42              |
| 4:BZ:33:UNK:CB  | 4:BZ:34:UNK:HA  | 2.49                     | 0.42              |
| 1:C:154:ARG:O   | 1:C:155:ASP:C   | 2.62                     | 0.42              |
| 4:BO:20:UNK:O   | 4:BO:21:UNK:C   | 2.68                     | 0.42              |
| 2:BR:287:GLN:O  | 2:BR:291:TYR:N  | 2.53                     | 0.42              |
| 7:J:554:MET:C   | 7:J:557:LEU:O   | 2.63                     | 0.41              |
| 2:k:5:LEU:O     | 2:k:6:PHE:C     | 2.62                     | 0.41              |
| 5:AU:9:HIS:CB   | 5:AU:279:ARG:H  | 2.33                     | 0.41              |
| 16:Ai:119:ARG:O | 16:Ai:120:CYS:C | 2.60                     | 0.41              |
| 3:BY:307:ASN:O  | 3:BY:308:ILE:C  | 2.60                     | 0.41              |
| 13:Bx:-7:UNK:O  | 13:Bx:-6:UNK:C  | 2.68                     | 0.41              |
| 15:B5:44:UNK:O  | 15:B5:46:UNK:N  | 2.53                     | 0.41              |
| 2:Ch:331:ASN:O  | 2:Ch:332:VAL:C  | 2.63                     | 0.41              |
| 3:I:96:GLY:O    | 3:I:97:TYR:C    | 2.64                     | 0.41              |
| 2:f:41:ASP:O    | 2:f:45:THR:N    | 2.48                     | 0.41              |
| 3:1:732:LEU:C   | 3:1:734:GLU:H   | 2.28                     | 0.41              |
| 3:7:278:ILE:O   | 3:7:292:CYS:HA  | 2.20                     | 0.41              |
| 7:AG:143:GLY:O  | 7:AG:144:GLY:C  | 2.62                     | 0.41              |
| 3:BY:662:ILE:O  | 3:BY:663:GLN:C  | 2.61                     | 0.41              |
| 4:BZ:32:UNK:O   | 4:BZ:33:UNK:C   | 2.68                     | 0.41              |
| 7:Bm:553:TYR:O  | 7:Bm:554:MET:C  | 2.62                     | 0.41              |
| 2:CW:321:SER:O  | 2:CW:322:LYS:C  | 2.63                     | 0.41              |
| 2:q:246:GLN:HA  | 2:q:247:VAL:C   | 2.45                     | 0.41              |
| 7:AM:69:SER:HA  | 7:AM:88:HIS:O   | 2.20                     | 0.41              |
| 14:Am:-20:UNK:O | 14:Am:-16:UNK:N | 2.53                     | 0.41              |
| 16:An:119:ARG:O | 16:An:120:CYS:C | 2.62                     | 0.41              |
| 14:As:11:UNK:O  | 14:As:14:UNK:N  | 2.54                     | 0.41              |
| 5:Bf:597:TRP:O  | 5:Bf:599:GLN:N  | 2.53                     | 0.41              |
| 14:CE:5:UNK:CA  | 14:CE:6:UNK:C   | 2.98                     | 0.41              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 16:CI:73:LEU:O | 16:CI:74:VAL:C  | 2.61                     | 0.41              |
| 1:Ca:201:ASN:O | 1:Ca:202:TYR:C  | 2.63                     | 0.41              |
| 2:Cd:35:VAL:O  | 2:Cd:36:ASP:C   | 2.60                     | 0.41              |
| 5:G:427:PHE:O  | 5:G:431:HIS:N   | 2.52                     | 0.41              |
| 7:J:69:SER:HA  | 7:J:88:HIS:O    | 2.19                     | 0.41              |
| 2:y:286:VAL:O  | 2:y:287:GLN:C   | 2.63                     | 0.41              |
| 5:Bf:794:GLN:O | 5:Bf:795:GLU:C  | 2.62                     | 0.41              |
| 3:E:785:VAL:O  | 3:E:787:GLU:N   | 2.54                     | 0.41              |
| 5:G:597:TRP:O  | 5:G:599:GLN:N   | 2.53                     | 0.41              |
| 2:f:136:GLU:O  | 2:f:137:ASN:C   | 2.64                     | 0.41              |
| 3:n:429:LEU:O  | 3:n:430:ASP:CB  | 2.67                     | 0.41              |
| 2:s:71:ASN:O   | 2:s:75:ALA:N    | 2.46                     | 0.41              |
| 7:4:331:THR:CB | 7:4:339:MET:H   | 2.33                     | 0.41              |
| 5:AE:706:THR:O | 5:AE:707:GLU:C  | 2.63                     | 0.41              |
| 4:BO:-1:UNK:O  | 4:BO:0:UNK:C    | 2.68                     | 0.41              |
| 4:BZ:25:UNK:O  | 4:BZ:26:UNK:C   | 2.68                     | 0.41              |
| 16:CB:30:GLY:O | 16:CB:31:LYS:C  | 2.62                     | 0.41              |
| 2:z:286:VAL:O  | 2:z:287:GLN:C   | 2.63                     | 0.41              |
| 3:E:168:ARG:O  | 3:E:169:TYR:C   | 2.64                     | 0.41              |
| 14:Am:77:UNK:O | 14:Am:78:UNK:C  | 2.69                     | 0.41              |
| 5:Bt:283:ASN:O | 5:Bt:284:LYS:CB | 2.68                     | 0.41              |
| 3:1:96:GLY:O   | 3:1:97:TYR:C    | 2.61                     | 0.41              |
| 7:4:546:ARG:O  | 7:4:547:LEU:C   | 2.62                     | 0.41              |
| 3:7:625:LEU:O  | 3:7:626:LEU:C   | 2.62                     | 0.41              |
| 3:7:732:LEU:C  | 3:7:734:GLU:H   | 2.28                     | 0.41              |
| 5:AE:876:GLN:O | 5:AE:879:ARG:N  | 2.54                     | 0.41              |
| 15:AP:44:UNK:O | 15:AP:46:UNK:N  | 2.54                     | 0.41              |
| 4:BZ:-2:UNK:O  | 4:BZ:-1:UNK:C   | 2.69                     | 0.41              |
| 2:Cd:289:TYR:O | 2:Cd:290:ASN:CB | 2.68                     | 0.41              |
| 2:D:114:THR:O  | 2:D:115:GLU:C   | 2.63                     | 0.41              |
| 2:D:321:SER:O  | 2:D:322:LYS:C   | 2.62                     | 0.41              |
| 7:O:553:TYR:O  | 7:O:554:MET:C   | 2.61                     | 0.41              |
| 4:d:25:UNK:O   | 4:d:26:UNK:C    | 2.68                     | 0.41              |
| 7:AM:243:THR:O | 7:AM:244:CYS:C  | 2.64                     | 0.41              |
| 5:AO:7:SER:O   | 5:AO:9:HIS:N    | 2.54                     | 0.41              |
| 5:AO:323:GLN:O | 5:AO:327:LEU:N  | 2.54                     | 0.41              |
| 16:A7:44:HIS:O | 16:A7:45:ALA:C  | 2.63                     | 0.41              |
| 2:Ch:321:SER:O | 2:Ch:322:LYS:C  | 2.64                     | 0.41              |
| 1:C:364:VAL:O  | 1:C:366:GLY:N   | 2.53                     | 0.41              |
| 3:E:96:GLY:O   | 3:E:97:TYR:C    | 2.61                     | 0.41              |
| 7:J:556:ASN:N  | 7:J:557:LEU:O   | 2.54                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:q:290:ASN:O   | 2:q:291:TYR:C    | 2.63                     | 0.41              |
| 9:AC:117:UNK:HA | 9:AC:118:UNK:CB  | 2.51                     | 0.41              |
| 7:AG:534:GLU:O  | 7:AG:535:ALA:C   | 2.59                     | 0.41              |
| 3:BY:96:GLY:O   | 3:BY:97:TYR:C    | 2.61                     | 0.41              |
| 1:Ca:432:PRO:O  | 1:Ca:434:ILE:N   | 2.53                     | 0.41              |
| 3:I:92:GLU:O    | 3:I:93:LYS:C     | 2.65                     | 0.41              |
| 2:k:10:LYS:O    | 2:k:11:TYR:C     | 2.64                     | 0.41              |
| 3:n:528:GLY:O   | 3:n:529:THR:C    | 2.62                     | 0.41              |
| 3:7:152:ASN:O   | 3:7:156:TYR:N    | 2.53                     | 0.41              |
| 1:Ca:243:TYR:HA | 1:Ca:320:GLY:HA2 | 2.03                     | 0.41              |
| 1:Ca:374:ASN:O  | 1:Ca:375:ASN:C   | 2.64                     | 0.41              |
| 2:Cd:328:SER:O  | 2:Cd:330:ALA:N   | 2.54                     | 0.41              |
| 3:E:152:ASN:O   | 3:E:156:TYR:N    | 2.53                     | 0.40              |
| 7:AM:536:ILE:O  | 7:AM:537:ALA:C   | 2.61                     | 0.40              |
| 2:Cd:330:ALA:H  | 2:Cd:332:VAL:N   | 2.12                     | 0.40              |
| 3:I:152:ASN:O   | 3:I:156:TYR:N    | 2.54                     | 0.40              |
| 3:I:560:TYR:H   | 3:I:683:ALA:CB   | 2.35                     | 0.40              |
| 4:d:34:UNK:O    | 4:d:35:UNK:C     | 2.65                     | 0.40              |
| 3:n:732:LEU:C   | 3:n:734:GLU:N    | 2.79                     | 0.40              |
| 16:Az:62:GLU:O  | 16:Az:63:LYS:C   | 2.62                     | 0.40              |
| 7:Bm:69:SER:HA  | 7:Bm:88:HIS:O    | 2.21                     | 0.40              |
| 2:CW:91:ILE:O   | 2:CW:95:SER:N    | 2.55                     | 0.40              |
| 3:I:307:ASN:O   | 3:I:308:ILE:C    | 2.61                     | 0.40              |
| 2:f:289:TYR:O   | 2:f:290:ASN:CB   | 2.70                     | 0.40              |
| 7:4:45:GLY:O    | 7:4:46:HIS:C     | 2.64                     | 0.40              |
| 5:9:617:ILE:O   | 5:9:618:THR:C    | 2.64                     | 0.40              |
| 3:BY:799:GLU:O  | 3:BY:800:SER:C   | 2.62                     | 0.40              |
| 7:Bm:138:SER:O  | 7:Bm:147:LEU:N   | 2.54                     | 0.40              |
| 2:Ch:290:ASN:O  | 2:Ch:291:TYR:C   | 2.62                     | 0.40              |
| 1:A:362:ASN:O   | 1:A:363:PRO:C    | 2.65                     | 0.40              |
| 2:D:247:VAL:O   | 2:D:248:HIS:C    | 2.64                     | 0.40              |
| 4:o:32:UNK:O    | 4:o:33:UNK:C     | 2.69                     | 0.40              |
| 3:7:307:ASN:O   | 3:7:308:ILE:C    | 2.61                     | 0.40              |
| 2:BK:30:GLU:O   | 2:BK:31:SER:CB   | 2.69                     | 0.40              |
| 3:BY:631:VAL:O  | 3:BY:632:ALA:C   | 2.65                     | 0.40              |
| 1:CP:70:SER:O   | 1:CP:71:ASN:C    | 2.64                     | 0.40              |
| 7:J:342:LYS:O   | 7:J:343:THR:C    | 2.59                     | 0.40              |
| 2:k:35:VAL:O    | 2:k:36:ASP:C     | 2.64                     | 0.40              |
| 7:AG:553:TYR:O  | 7:AG:554:MET:C   | 2.58                     | 0.40              |
| 7:AM:553:TYR:O  | 7:AM:556:ASN:N   | 2.52                     | 0.40              |
| 14:Am:91:UNK:O  | 14:Am:92:UNK:C   | 2.69                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 16:Aq:176:ILE:O | 16:Aq:177:ARG:C | 2.63                     | 0.40              |
| 5:Bt:266:ALA:O  | 5:Bt:275:ALA:N  | 2.53                     | 0.40              |
| 2:Cd:86:ASN:O   | 2:Cd:89:SER:N   | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 425/452 (94%) | 373 (88%) | 41 (10%) | 11 (3%)  | 4           | 28 |
| 1   | BD    | 425/452 (94%) | 374 (88%) | 37 (9%)  | 14 (3%)  | 3           | 24 |
| 1   | C     | 425/452 (94%) | 369 (87%) | 44 (10%) | 12 (3%)  | 4           | 27 |
| 1   | CP    | 425/452 (94%) | 369 (87%) | 43 (10%) | 13 (3%)  | 3           | 25 |
| 1   | Ca    | 425/452 (94%) | 375 (88%) | 40 (9%)  | 10 (2%)  | 5           | 29 |
| 1   | i     | 425/452 (94%) | 371 (87%) | 45 (11%) | 9 (2%)   | 5           | 32 |
| 2   | BK    | 278/380 (73%) | 269 (97%) | 5 (2%)   | 4 (1%)   | 9           | 37 |
| 2   | BR    | 252/380 (66%) | 244 (97%) | 7 (3%)   | 1 (0%)   | 30          | 63 |
| 2   | CW    | 278/380 (73%) | 262 (94%) | 12 (4%)  | 4 (1%)   | 9           | 37 |
| 2   | Cd    | 252/380 (66%) | 243 (96%) | 3 (1%)   | 6 (2%)   | 5           | 29 |
| 2   | Ch    | 278/380 (73%) | 263 (95%) | 12 (4%)  | 3 (1%)   | 12          | 42 |
| 2   | D     | 278/380 (73%) | 266 (96%) | 8 (3%)   | 4 (1%)   | 9           | 37 |
| 2   | f     | 252/380 (66%) | 244 (97%) | 6 (2%)   | 2 (1%)   | 16          | 49 |
| 2   | k     | 278/380 (73%) | 262 (94%) | 12 (4%)  | 4 (1%)   | 9           | 37 |
| 2   | q     | 278/380 (73%) | 266 (96%) | 8 (3%)   | 4 (1%)   | 9           | 37 |
| 2   | s     | 252/380 (66%) | 244 (97%) | 6 (2%)   | 2 (1%)   | 16          | 49 |
| 2   | y     | 252/380 (66%) | 244 (97%) | 6 (2%)   | 2 (1%)   | 16          | 49 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 2   | z     | 252/380 (66%)  | 244 (97%) | 6 (2%)   | 2 (1%)   | 16          | 49 |
| 3   | 1     | 615/937 (66%)  | 577 (94%) | 23 (4%)  | 15 (2%)  | 5           | 29 |
| 3   | 7     | 805/937 (86%)  | 761 (94%) | 28 (4%)  | 16 (2%)  | 6           | 32 |
| 3   | BY    | 767/937 (82%)  | 724 (94%) | 27 (4%)  | 16 (2%)  | 5           | 32 |
| 3   | E     | 718/937 (77%)  | 677 (94%) | 25 (4%)  | 16 (2%)  | 5           | 30 |
| 3   | I     | 805/937 (86%)  | 765 (95%) | 26 (3%)  | 14 (2%)  | 7           | 34 |
| 3   | n     | 659/937 (70%)  | 620 (94%) | 25 (4%)  | 14 (2%)  | 5           | 32 |
| 5   | 9     | 299/1202 (25%) | 272 (91%) | 23 (8%)  | 4 (1%)   | 10          | 39 |
| 5   | AB    | 352/1202 (29%) | 332 (94%) | 17 (5%)  | 3 (1%)   | 14          | 45 |
| 5   | AE    | 514/1202 (43%) | 479 (93%) | 27 (5%)  | 8 (2%)   | 8           | 36 |
| 5   | AO    | 352/1202 (29%) | 335 (95%) | 13 (4%)  | 4 (1%)   | 12          | 42 |
| 5   | AU    | 352/1202 (29%) | 334 (95%) | 15 (4%)  | 3 (1%)   | 14          | 45 |
| 5   | Bf    | 464/1202 (39%) | 432 (93%) | 27 (6%)  | 5 (1%)   | 12          | 42 |
| 5   | Bt    | 352/1202 (29%) | 330 (94%) | 20 (6%)  | 2 (1%)   | 22          | 55 |
| 5   | G     | 410/1202 (34%) | 382 (93%) | 26 (6%)  | 2 (0%)   | 25          | 58 |
| 5   | L     | 514/1202 (43%) | 484 (94%) | 25 (5%)  | 5 (1%)   | 13          | 44 |
| 5   | M     | 352/1202 (29%) | 326 (93%) | 23 (6%)  | 3 (1%)   | 14          | 45 |
| 5   | R     | 352/1202 (29%) | 329 (94%) | 19 (5%)  | 4 (1%)   | 12          | 42 |
| 5   | v     | 355/1202 (30%) | 327 (92%) | 22 (6%)  | 6 (2%)   | 7           | 34 |
| 7   | 4     | 359/634 (57%)  | 315 (88%) | 38 (11%) | 6 (2%)   | 7           | 34 |
| 7   | AG    | 359/634 (57%)  | 316 (88%) | 35 (10%) | 8 (2%)   | 5           | 30 |
| 7   | AM    | 359/634 (57%)  | 319 (89%) | 36 (10%) | 4 (1%)   | 12          | 42 |
| 7   | Bm    | 359/634 (57%)  | 317 (88%) | 37 (10%) | 5 (1%)   | 9           | 37 |
| 7   | J     | 359/634 (57%)  | 317 (88%) | 34 (10%) | 8 (2%)   | 5           | 30 |
| 7   | O     | 359/634 (57%)  | 317 (88%) | 36 (10%) | 6 (2%)   | 7           | 34 |
| 16  | A7    | 154/230 (67%)  | 143 (93%) | 9 (6%)   | 2 (1%)   | 10          | 39 |
| 16  | Ai    | 147/230 (64%)  | 133 (90%) | 10 (7%)  | 4 (3%)   | 4           | 27 |
| 16  | An    | 147/230 (64%)  | 133 (90%) | 9 (6%)   | 5 (3%)   | 3           | 24 |
| 16  | Aq    | 154/230 (67%)  | 141 (92%) | 12 (8%)  | 1 (1%)   | 22          | 55 |
| 16  | Av    | 154/230 (67%)  | 143 (93%) | 7 (4%)   | 4 (3%)   | 4           | 28 |
| 16  | Az    | 147/230 (64%)  | 129 (88%) | 13 (9%)  | 5 (3%)   | 3           | 24 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| 16  | CB    | 147/230 (64%)     | 130 (88%)   | 13 (9%)   | 4 (3%)   | 4           | 27 |
| 16  | CI    | 154/230 (67%)     | 144 (94%)   | 9 (6%)    | 1 (1%)   | 22          | 55 |
| 16  | CM    | 147/230 (64%)     | 127 (86%)   | 15 (10%)  | 5 (3%)   | 3           | 24 |
| 16  | CT    | 154/230 (67%)     | 142 (92%)   | 11 (7%)   | 1 (1%)   | 22          | 55 |
| 16  | Z     | 147/230 (64%)     | 133 (90%)   | 10 (7%)   | 4 (3%)   | 4           | 27 |
| 16  | c     | 154/230 (67%)     | 143 (93%)   | 9 (6%)    | 2 (1%)   | 10          | 39 |
| All | All   | 18727/33882 (55%) | 17310 (92%) | 1095 (6%) | 322 (2%) | 10          | 34 |

All (322) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | SER  |
| 1   | A     | 101 | PRO  |
| 1   | C     | 68  | SER  |
| 1   | C     | 101 | PRO  |
| 2   | D     | 234 | LYS  |
| 3   | E     | 72  | ASP  |
| 3   | E     | 295 | LEU  |
| 3   | E     | 430 | ASP  |
| 3   | E     | 704 | PRO  |
| 3   | I     | 72  | ASP  |
| 3   | I     | 295 | LEU  |
| 3   | I     | 430 | ASP  |
| 3   | I     | 704 | PRO  |
| 3   | I     | 838 | GLU  |
| 7   | J     | 325 | SER  |
| 5   | M     | 110 | HIS  |
| 7   | O     | 325 | SER  |
| 5   | R     | 110 | HIS  |
| 16  | Z     | 141 | LYS  |
| 16  | c     | 40  | GLN  |
| 1   | i     | 68  | SER  |
| 2   | k     | 234 | LYS  |
| 3   | n     | 72  | ASP  |
| 3   | n     | 295 | LEU  |
| 3   | n     | 430 | ASP  |
| 3   | n     | 755 | ALA  |
| 2   | s     | 45  | THR  |
| 3   | 1     | 72  | ASP  |
| 3   | 1     | 253 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1     | 430 | ASP  |
| 7   | 4     | 167 | CYS  |
| 7   | 4     | 325 | SER  |
| 3   | 7     | 72  | ASP  |
| 3   | 7     | 430 | ASP  |
| 5   | AE    | 583 | PHE  |
| 5   | AE    | 598 | LEU  |
| 7   | AG    | 143 | GLY  |
| 7   | AG    | 259 | ILE  |
| 7   | AG    | 325 | SER  |
| 7   | AM    | 325 | SER  |
| 5   | AO    | 8   | THR  |
| 5   | AO    | 110 | HIS  |
| 5   | AU    | 110 | HIS  |
| 16  | An    | 141 | LYS  |
| 16  | Aq    | 40  | GLN  |
| 16  | Av    | 27  | THR  |
| 16  | Az    | 141 | LYS  |
| 16  | A7    | 40  | GLN  |
| 16  | A7    | 95  | ASP  |
| 1   | BD    | 68  | SER  |
| 1   | BD    | 101 | PRO  |
| 1   | BD    | 259 | THR  |
| 2   | BK    | 234 | LYS  |
| 3   | BY    | 72  | ASP  |
| 3   | BY    | 253 | ASN  |
| 3   | BY    | 295 | LEU  |
| 3   | BY    | 430 | ASP  |
| 3   | BY    | 557 | PRO  |
| 5   | Bf    | 598 | LEU  |
| 7   | Bm    | 325 | SER  |
| 5   | Bt    | 110 | HIS  |
| 16  | CB    | 141 | LYS  |
| 16  | CM    | 141 | LYS  |
| 16  | CM    | 172 | ASP  |
| 1   | CP    | 68  | SER  |
| 1   | CP    | 101 | PRO  |
| 1   | CP    | 364 | VAL  |
| 16  | CT    | 40  | GLN  |
| 2   | CW    | 234 | LYS  |
| 1   | Ca    | 68  | SER  |
| 1   | Ca    | 101 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ca    | 316 | SER  |
| 2   | Cd    | 328 | SER  |
| 2   | Cd    | 355 | TYR  |
| 1   | A     | 236 | ASN  |
| 1   | C     | 265 | ALA  |
| 2   | D     | 247 | VAL  |
| 3   | E     | 480 | ASN  |
| 3   | E     | 560 | TYR  |
| 3   | E     | 747 | LYS  |
| 3   | E     | 804 | ILE  |
| 5   | G     | 454 | ASP  |
| 5   | G     | 465 | TYR  |
| 3   | I     | 480 | ASN  |
| 3   | I     | 560 | TYR  |
| 3   | I     | 747 | LYS  |
| 7   | J     | 232 | THR  |
| 7   | J     | 512 | ASN  |
| 5   | L     | 454 | ASP  |
| 5   | L     | 465 | TYR  |
| 5   | L     | 650 | VAL  |
| 7   | O     | 244 | CYS  |
| 5   | R     | 54  | ASN  |
| 16  | Z     | 142 | ASN  |
| 16  | Z     | 172 | ASP  |
| 1   | i     | 101 | PRO  |
| 1   | i     | 316 | SER  |
| 3   | n     | 480 | ASN  |
| 3   | n     | 704 | PRO  |
| 2   | q     | 247 | VAL  |
| 2   | s     | 290 | ASN  |
| 5   | v     | 454 | ASP  |
| 5   | v     | 588 | PHE  |
| 5   | v     | 650 | VAL  |
| 5   | v     | 707 | GLU  |
| 3   | 1     | 480 | ASN  |
| 3   | 1     | 704 | PRO  |
| 3   | 7     | 295 | LEU  |
| 3   | 7     | 480 | ASN  |
| 3   | 7     | 560 | TYR  |
| 3   | 7     | 709 | ASP  |
| 5   | 9     | 454 | ASP  |
| 5   | 9     | 465 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AB    | 80  | ILE  |
| 5   | AB    | 110 | HIS  |
| 5   | AE    | 454 | ASP  |
| 5   | AE    | 650 | VAL  |
| 5   | AE    | 901 | TYR  |
| 7   | AG    | 232 | THR  |
| 7   | AG    | 244 | CYS  |
| 7   | AM    | 512 | ASN  |
| 16  | Ai    | 141 | LYS  |
| 16  | Ai    | 142 | ASN  |
| 16  | Ai    | 172 | ASP  |
| 16  | An    | 142 | ASN  |
| 16  | An    | 172 | ASP  |
| 16  | Az    | 142 | ASN  |
| 16  | Az    | 172 | ASP  |
| 1   | BD    | 236 | ASN  |
| 1   | BD    | 432 | PRO  |
| 2   | BR    | 290 | ASN  |
| 3   | BY    | 116 | LYS  |
| 3   | BY    | 480 | ASN  |
| 3   | BY    | 704 | PRO  |
| 5   | Bf    | 454 | ASP  |
| 7   | Bm    | 117 | GLN  |
| 16  | CB    | 142 | ASN  |
| 16  | CB    | 172 | ASP  |
| 16  | CM    | 142 | ASN  |
| 16  | CM    | 173 | ILE  |
| 1   | CP    | 236 | ASN  |
| 1   | CP    | 258 | ILE  |
| 1   | CP    | 265 | ALA  |
| 2   | Cd    | 29  | ILE  |
| 2   | Cd    | 45  | THR  |
| 2   | Cd    | 329 | GLN  |
| 2   | Ch    | 234 | LYS  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 316 | SER  |
| 1   | C     | 171 | VAL  |
| 7   | J     | 171 | GLY  |
| 5   | R     | 309 | LYS  |
| 2   | f     | 45  | THR  |
| 2   | k     | 247 | VAL  |
| 3   | n     | 116 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | q     | 280 | ILE  |
| 5   | v     | 465 | TYR  |
| 2   | y     | 290 | ASN  |
| 3   | 1     | 116 | LYS  |
| 3   | 1     | 560 | TYR  |
| 3   | 1     | 709 | ASP  |
| 7   | 4     | 512 | ASN  |
| 3   | 7     | 116 | LYS  |
| 3   | 7     | 286 | ASN  |
| 3   | 7     | 704 | PRO  |
| 5   | AE    | 465 | TYR  |
| 5   | AE    | 642 | ILE  |
| 7   | AG    | 158 | TRP  |
| 7   | AM    | 158 | TRP  |
| 7   | AM    | 232 | THR  |
| 5   | AO    | 167 | SER  |
| 5   | AO    | 192 | GLU  |
| 1   | BD    | 156 | ILE  |
| 1   | BD    | 316 | SER  |
| 2   | BK    | 247 | VAL  |
| 3   | BY    | 126 | PHE  |
| 3   | BY    | 683 | ALA  |
| 3   | BY    | 804 | ILE  |
| 5   | Bf    | 465 | TYR  |
| 7   | Bm    | 232 | THR  |
| 7   | Bm    | 249 | SER  |
| 5   | Bt    | 282 | LYS  |
| 1   | CP    | 156 | ILE  |
| 2   | CW    | 247 | VAL  |
| 2   | CW    | 280 | ILE  |
| 1   | Ca    | 171 | VAL  |
| 2   | Cd    | 290 | ASN  |
| 2   | Ch    | 247 | VAL  |
| 2   | z     | 290 | ASN  |
| 1   | A     | 124 | LYS  |
| 1   | A     | 336 | LYS  |
| 1   | C     | 39  | LEU  |
| 1   | C     | 373 | SER  |
| 2   | D     | 280 | ILE  |
| 3   | E     | 116 | LYS  |
| 3   | E     | 286 | ASN  |
| 3   | E     | 709 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 838 | GLU  |
| 3   | I     | 39  | LYS  |
| 3   | I     | 116 | LYS  |
| 3   | I     | 123 | TRP  |
| 3   | I     | 709 | ASP  |
| 3   | I     | 804 | ILE  |
| 7   | J     | 158 | TRP  |
| 7   | J     | 160 | LEU  |
| 5   | M     | 5   | HIS  |
| 7   | O     | 153 | LYS  |
| 7   | O     | 158 | TRP  |
| 2   | f     | 290 | ASN  |
| 1   | i     | 124 | LYS  |
| 1   | i     | 373 | SER  |
| 2   | k     | 280 | ILE  |
| 2   | k     | 351 | ILE  |
| 3   | n     | 39  | LYS  |
| 2   | q     | 246 | GLN  |
| 2   | y     | 45  | THR  |
| 3   | 1     | 39  | LYS  |
| 3   | 1     | 123 | TRP  |
| 3   | 1     | 286 | ASN  |
| 7   | 4     | 232 | THR  |
| 7   | 4     | 249 | SER  |
| 3   | 7     | 39  | LYS  |
| 3   | 7     | 123 | TRP  |
| 3   | 7     | 784 | GLN  |
| 3   | 7     | 804 | ILE  |
| 7   | AG    | 249 | SER  |
| 5   | AU    | 309 | LYS  |
| 16  | Ai    | 69  | THR  |
| 16  | An    | 69  | THR  |
| 16  | Az    | 41  | ASP  |
| 16  | Az    | 69  | THR  |
| 3   | BY    | 39  | LYS  |
| 3   | BY    | 599 | VAL  |
| 3   | BY    | 604 | LEU  |
| 3   | BY    | 838 | GLU  |
| 16  | CB    | 69  | THR  |
| 16  | CM    | 69  | THR  |
| 1   | CP    | 124 | LYS  |
| 1   | Ca    | 124 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ca    | 156 | ILE  |
| 2   | Ch    | 280 | ILE  |
| 2   | z     | 45  | THR  |
| 1   | C     | 124 | LYS  |
| 1   | C     | 291 | ASP  |
| 1   | C     | 362 | ASN  |
| 1   | C     | 432 | PRO  |
| 3   | E     | 39  | LYS  |
| 3   | E     | 126 | PHE  |
| 3   | I     | 126 | PHE  |
| 7   | J     | 249 | SER  |
| 5   | L     | 587 | PHE  |
| 7   | O     | 117 | GLN  |
| 16  | Z     | 69  | THR  |
| 16  | c     | 133 | ASN  |
| 3   | n     | 126 | PHE  |
| 3   | n     | 604 | LEU  |
| 3   | n     | 683 | ALA  |
| 2   | q     | 31  | SER  |
| 5   | v     | 649 | SER  |
| 3   | 1     | 126 | PHE  |
| 3   | 1     | 604 | LEU  |
| 3   | 1     | 683 | ALA  |
| 3   | 7     | 126 | PHE  |
| 3   | 7     | 747 | LYS  |
| 5   | AE    | 649 | SER  |
| 5   | AU    | 153 | ALA  |
| 16  | Av    | 95  | ASP  |
| 16  | Av    | 133 | ASN  |
| 1   | BD    | 59  | ASP  |
| 1   | BD    | 124 | LYS  |
| 1   | BD    | 265 | ALA  |
| 1   | BD    | 356 | TYR  |
| 3   | BY    | 709 | ASP  |
| 16  | CI    | 133 | ASN  |
| 1   | Ca    | 131 | ASN  |
| 1   | Ca    | 236 | ASN  |
| 1   | A     | 235 | PRO  |
| 1   | A     | 407 | VAL  |
| 1   | A     | 432 | PRO  |
| 1   | C     | 407 | VAL  |
| 2   | D     | 324 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 604 | LEU  |
| 5   | L     | 649 | SER  |
| 1   | i     | 59  | ASP  |
| 3   | n     | 560 | TYR  |
| 3   | n     | 599 | VAL  |
| 7   | 4     | 117 | GLN  |
| 5   | 9     | 587 | PHE  |
| 1   | BD    | 235 | PRO  |
| 1   | BD    | 291 | ASP  |
| 2   | BK    | 31  | SER  |
| 5   | Bf    | 587 | PHE  |
| 7   | Bm    | 158 | TRP  |
| 1   | CP    | 235 | PRO  |
| 1   | CP    | 291 | ASP  |
| 1   | CP    | 336 | LYS  |
| 1   | Ca    | 407 | VAL  |
| 1   | Ca    | 432 | PRO  |
| 7   | O     | 49  | ILE  |
| 1   | i     | 407 | VAL  |
| 1   | BD    | 407 | VAL  |
| 1   | CP    | 407 | VAL  |
| 1   | C     | 156 | ILE  |
| 1   | i     | 432 | PRO  |
| 3   | 1     | 295 | LEU  |
| 3   | 7     | 599 | VAL  |
| 16  | Av    | 128 | ILE  |
| 1   | CP    | 432 | PRO  |
| 5   | M     | 343 | GLY  |
| 5   | 9     | 650 | VAL  |
| 2   | BK    | 280 | ILE  |
| 3   | E     | 599 | VAL  |
| 5   | R     | 341 | LYS  |
| 1   | i     | 156 | ILE  |
| 3   | n     | 558 | VAL  |
| 5   | AB    | 78  | VAL  |
| 7   | AG    | 49  | ILE  |
| 16  | An    | 37  | ILE  |
| 5   | Bf    | 650 | VAL  |
| 2   | CW    | 318 | ILE  |
| 1   | A     | 156 | ILE  |
| 7   | J     | 49  | ILE  |



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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

There are no chain breaks in this entry.



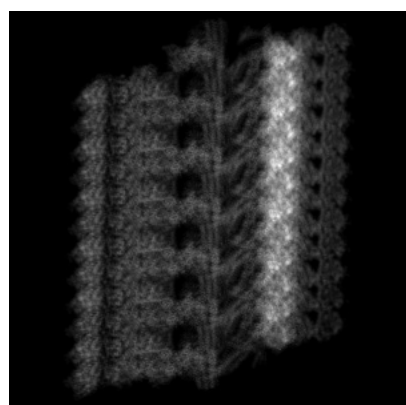
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53471. These allow visual inspection of the internal detail of the map and identification of artifacts.

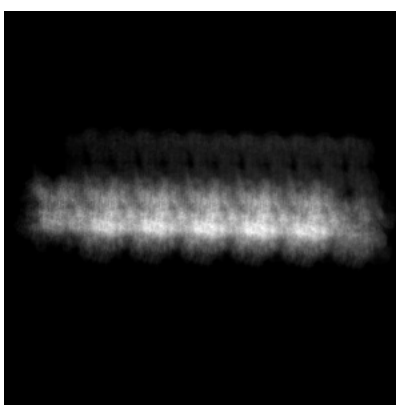
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

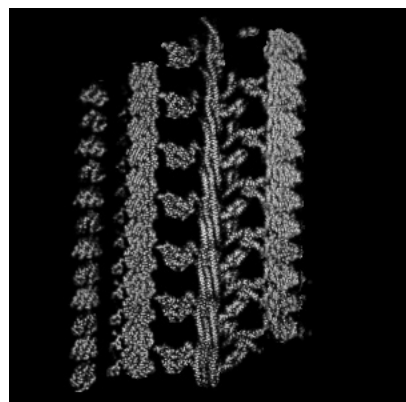


Z

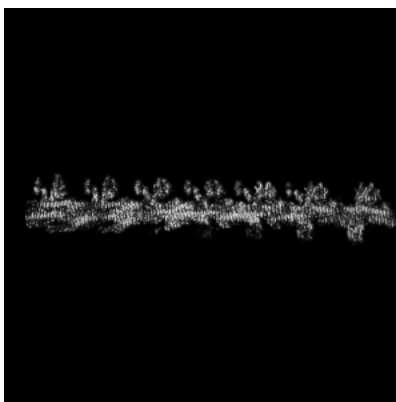
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 240



Y Index: 240



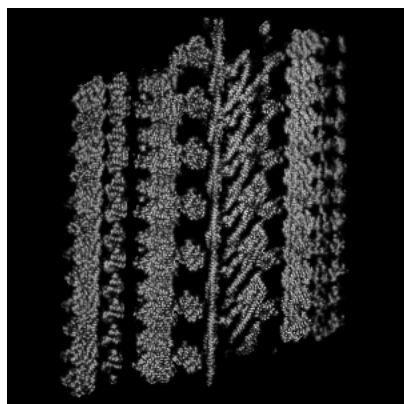
Z Index: 240



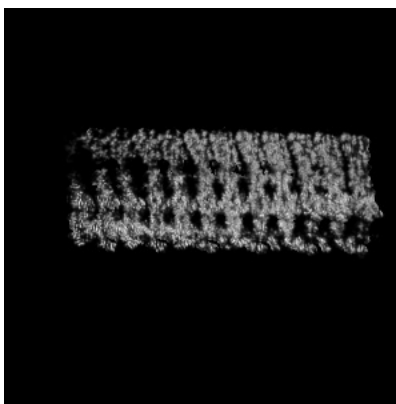
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

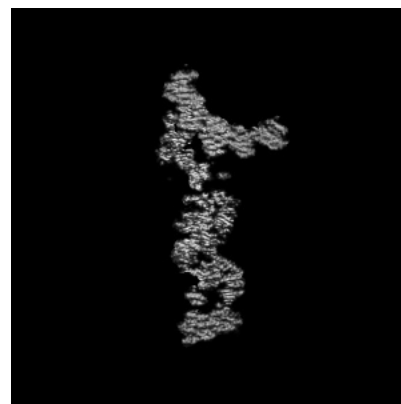
### 6.3.1 Primary map



X Index: 218



Y Index: 335

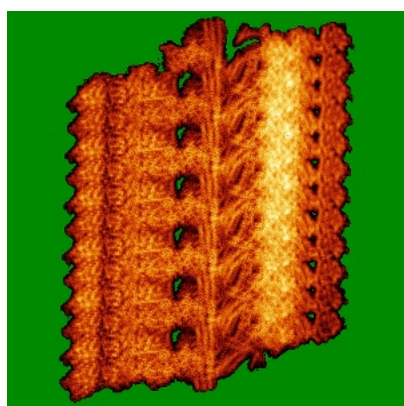


Z Index: 311

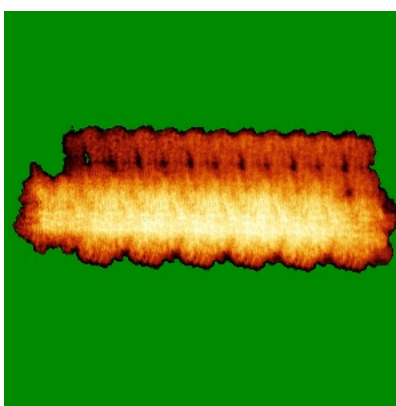
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

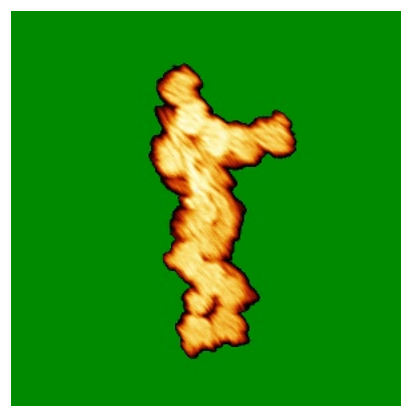
### 6.4.1 Primary map



X



Y



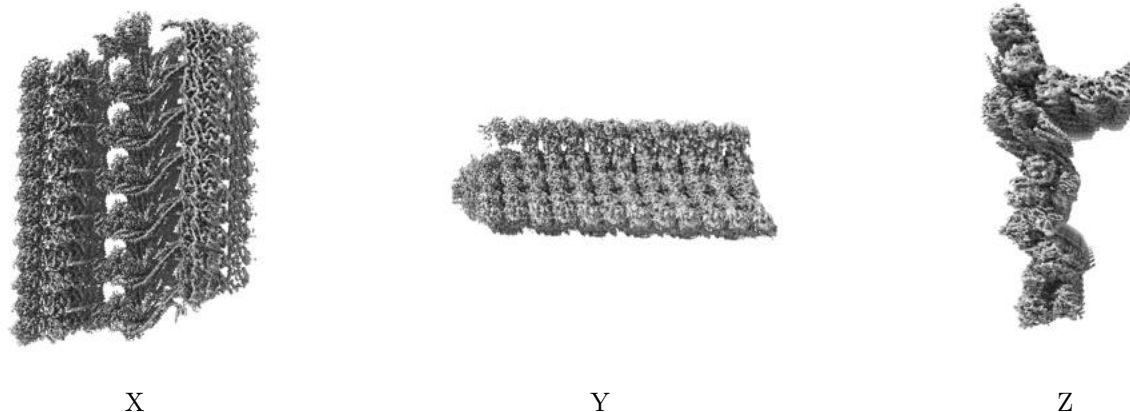
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

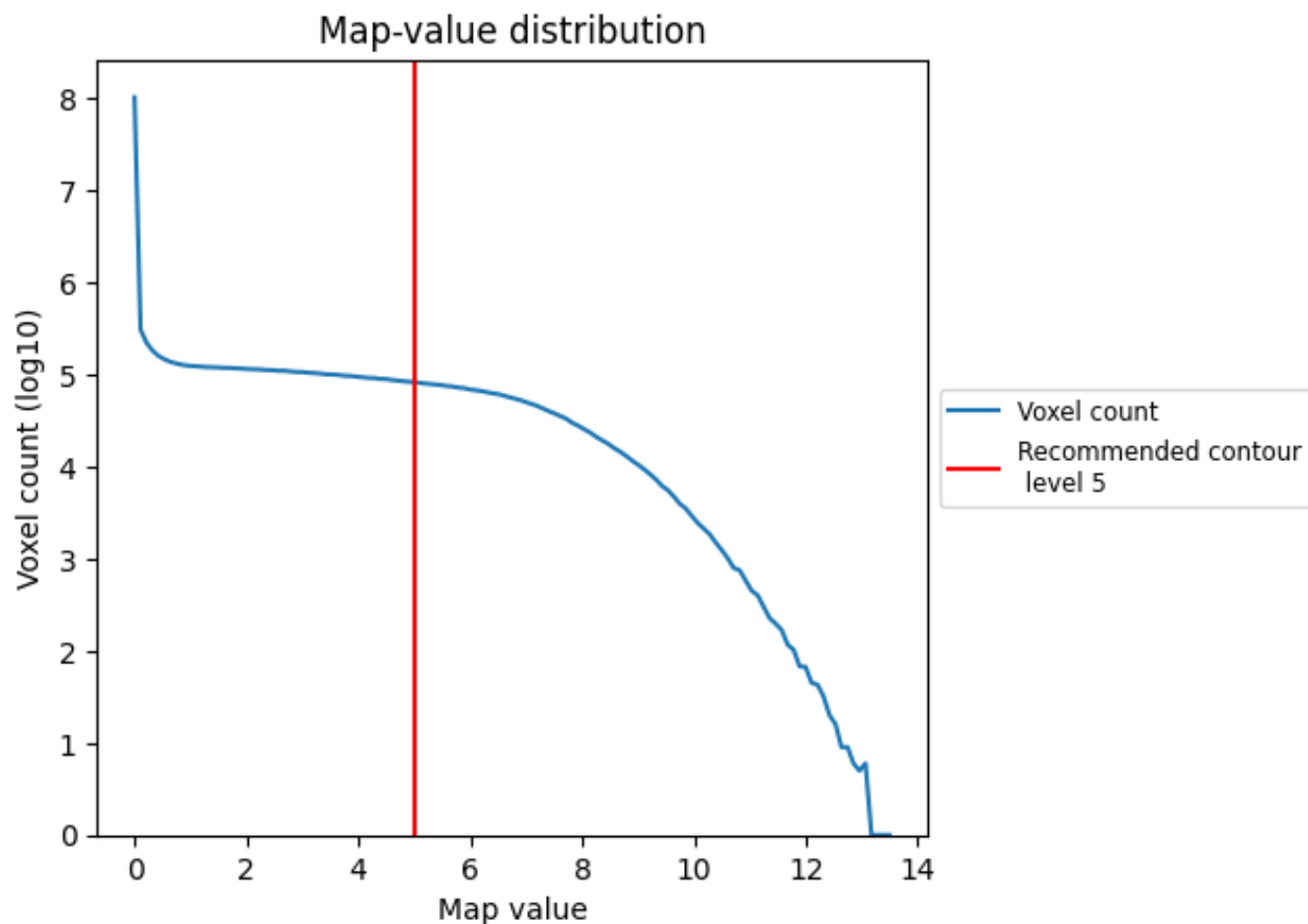
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

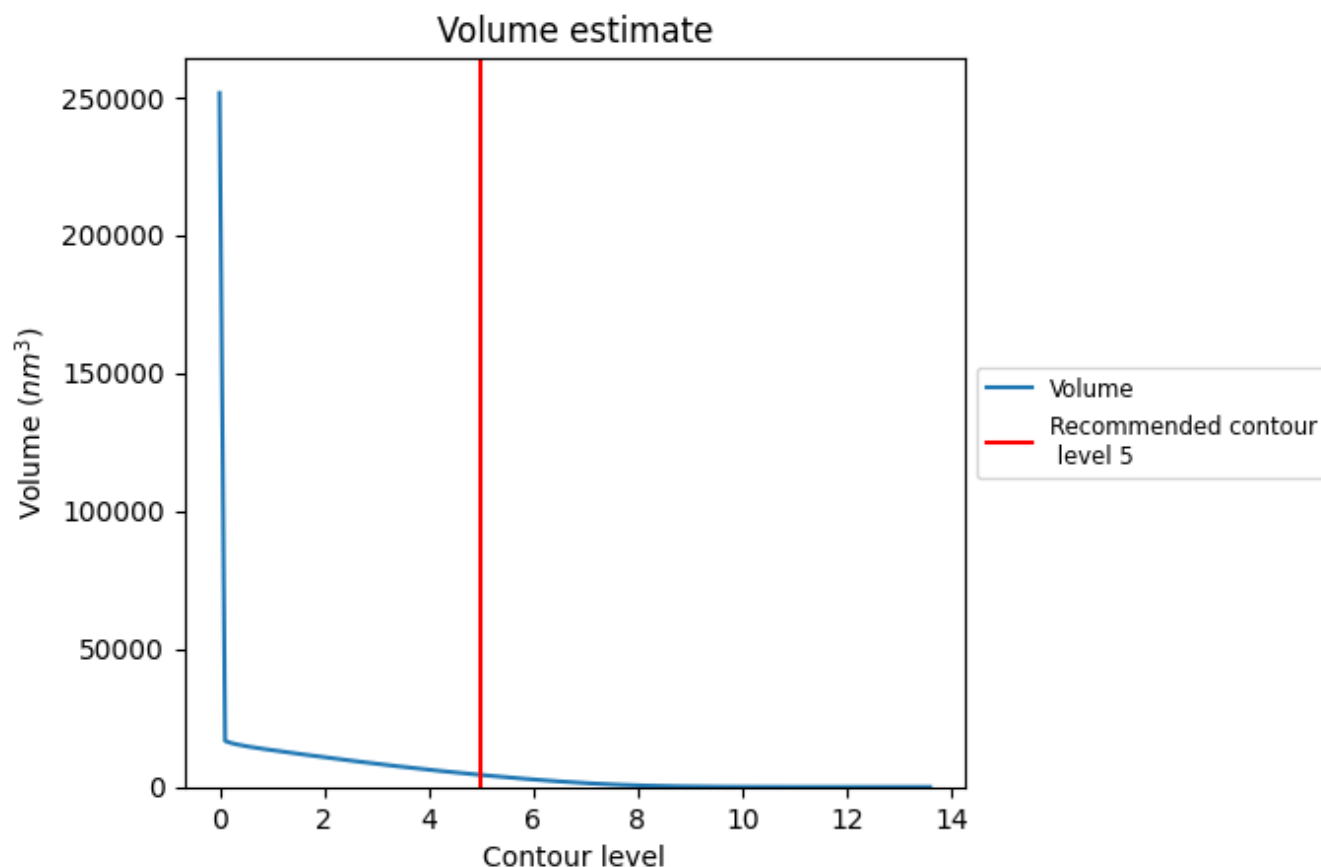
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate [i](#)

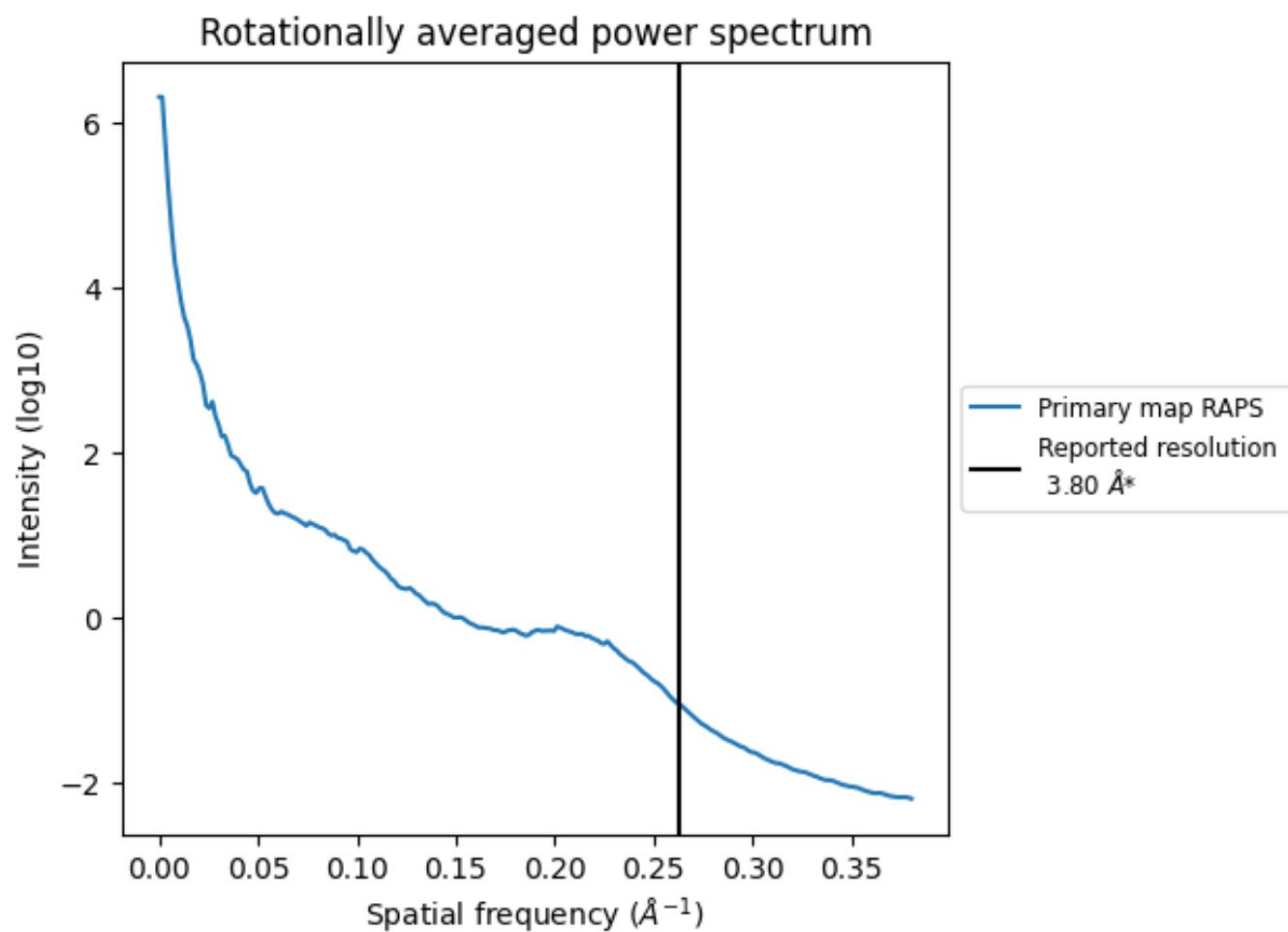


The volume at the recommended contour level is  $4355 \text{ nm}^3$ ; this corresponds to an approximate mass of 3934 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

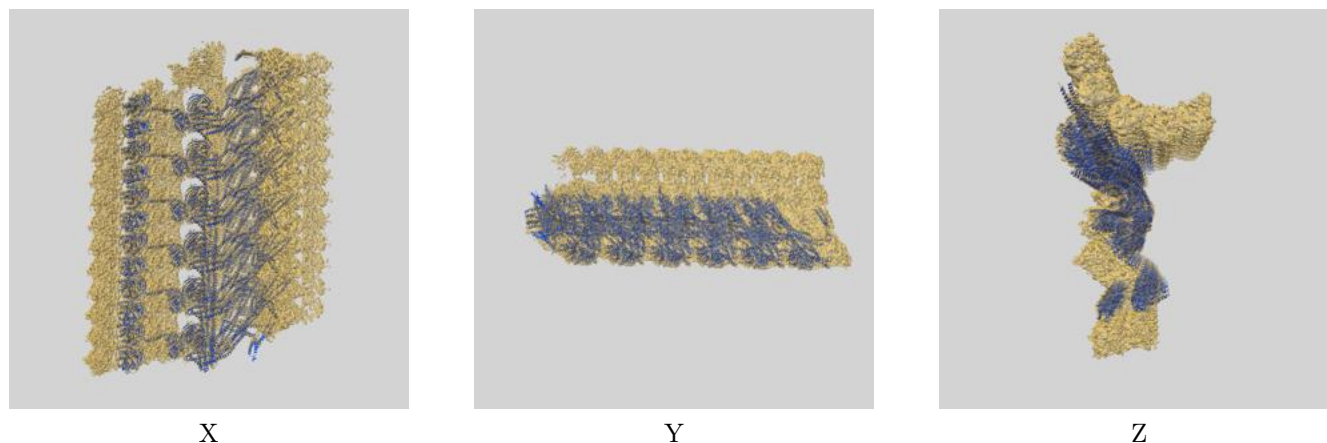
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53471 and PDB model 9QZF. Per-residue inclusion information can be found in section 3 on page 15.

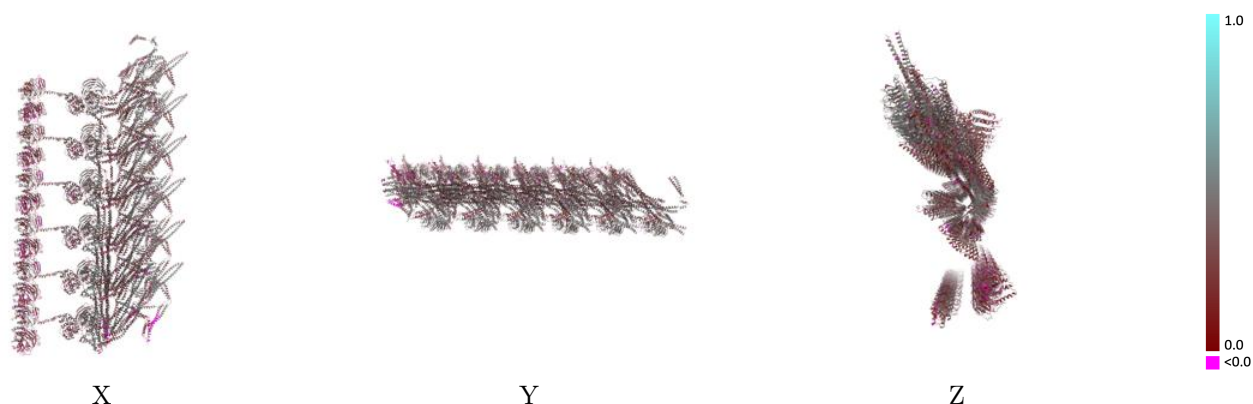
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

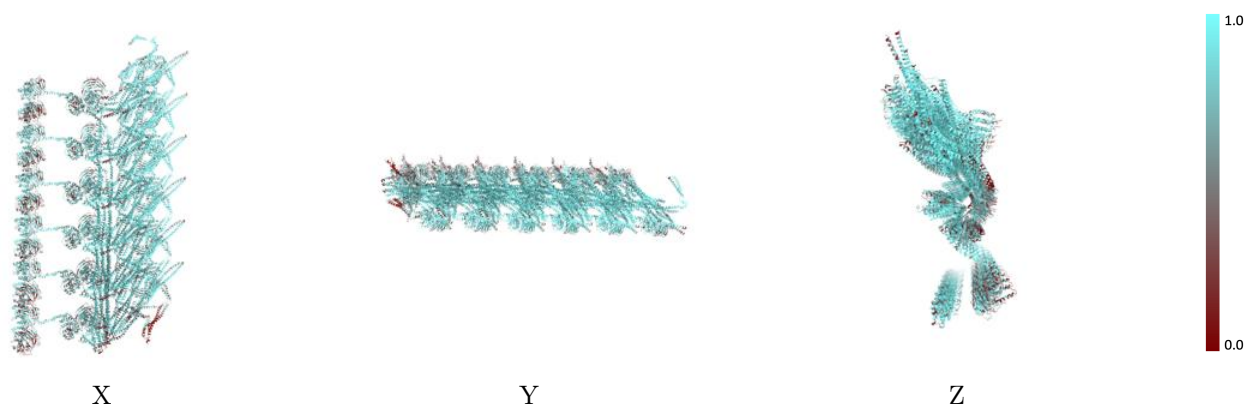


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

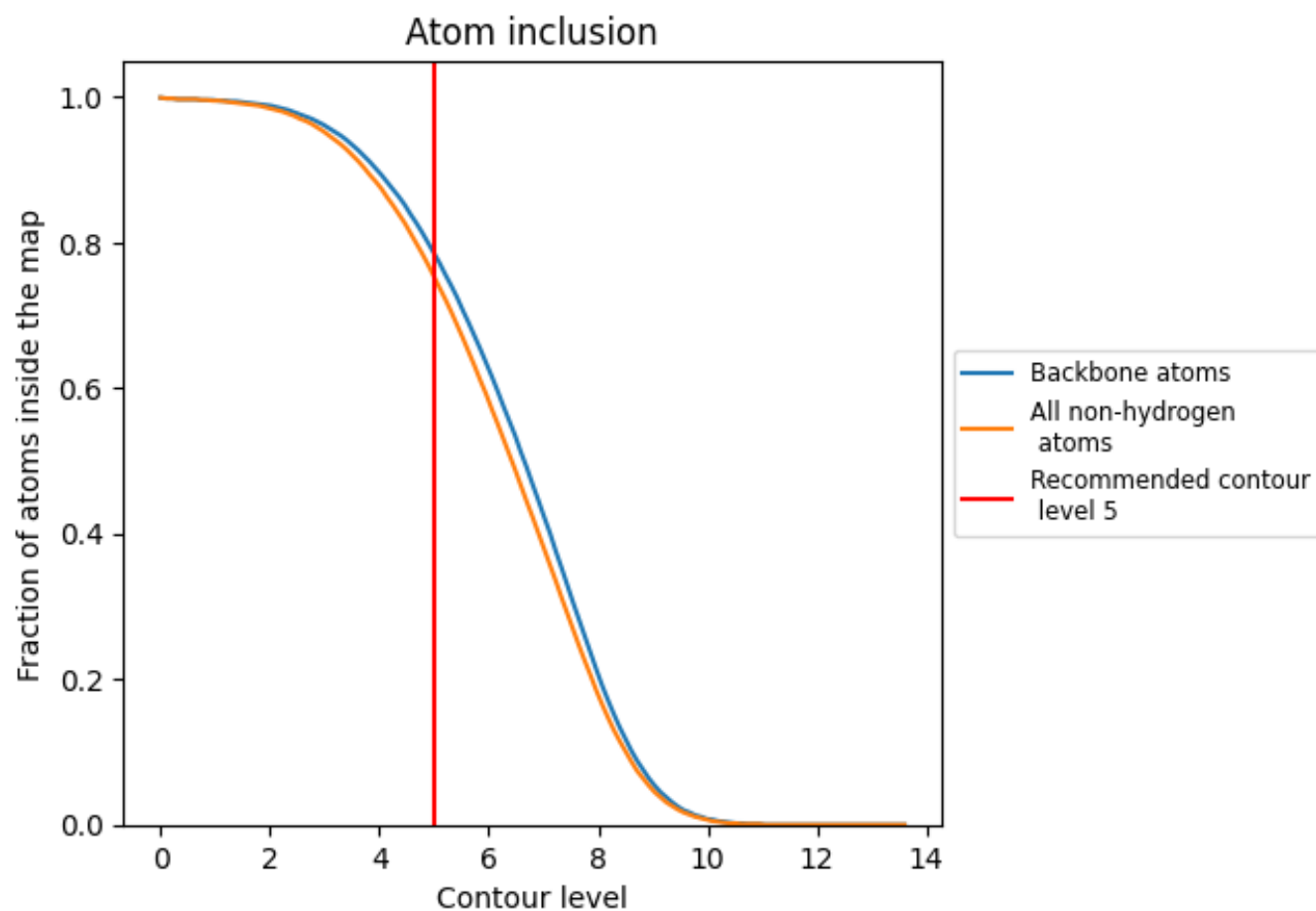
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).



## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 78% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.





















































































| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7530   |  0.3370   |
| 0     |  0.8930   |  0.3640   |
| 1     |  0.5950   |  0.3520   |
| 2     |  0.9020   |  0.3790   |
| 4     |  0.6570   |  0.2890   |
| 5     |  0.7290   |  0.4000   |
| 7     |  0.7440   |  0.3410   |
| 9     |  0.7150   |  0.3350   |
| A     |  0.7590   |  0.3960   |
| A7    |  0.7940   |  0.3400   |
| AB    |  0.4420   |  0.2140   |
| AC    |  0.8560   |  0.4000   |
| AE    |  0.8500   |  0.3580   |
| AG    |  0.6470   |  0.2890   |
| AH    |  0.8900  |  0.3500  |
| AJ    |  0.7690 |  0.4220 |
| AK    |  0.8020 |  0.3780 |
| AM    |  0.7320 |  0.2870 |
| AO    |  0.4300 |  0.2210 |
| AP    |  0.8800 |  0.3710 |
| AR    |  0.8490 |  0.3760 |
| AS    |  0.6830 |  0.3720 |
| AU    |  0.5010 |  0.2150 |
| AW    |  0.7810 |  0.4480 |
| AZ    |  0.8180 |  0.3400 |
| Aa    |  0.7060 |  0.3870 |
| Ac    |  0.8440 |  0.4140 |
| Ae    |  0.7880 |  0.3640 |
| Ai    |  0.7740 |  0.3300 |
| Ak    |  0.7880 |  0.3420 |
| Am    |  0.5520 |  0.2930 |
| An    |  0.7430 |  0.3270 |
| Aq    |  0.7230 |  0.3400 |
| As    |  0.8990 |  0.3380 |
| Av    |  0.6900 |  0.3360 |



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

























































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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Az    |  0.7940   |  0.3240   |
| B1    |  0.8500   |  0.4240   |
| B2    |  0.9330   |  0.3680   |
| B4    |  0.8520   |  0.3670   |
| B5    |  0.9250   |  0.3690   |
| B8    |  0.8730   |  0.3710   |
| B9    |  0.9180   |  0.3590   |
| BD    |  0.8410   |  0.3990   |
| BK    |  0.8620   |  0.3480   |
| BO    |  0.9420   |  0.3710   |
| BR    |  0.8200   |  0.3130   |
| BV    |  0.8540   |  0.3530   |
| BY    |  0.7140   |  0.3540   |
| BZ    |  0.9010   |  0.3710   |
| Bc    |  0.8380   |  0.3660   |
| Bf    |  0.8210   |  0.3570   |
| Bg    |  0.8460   |  0.3710   |
| Bj    |  0.9580   |  0.3760   |
| Bm    |  0.6990   |  0.2870   |
| Bn    |  0.8480  |  0.3750  |
| Bq    |  0.9390 |  0.3630 |
| Bt    |  0.4650 |  0.1940 |
| Bu    |  0.9490 |  0.3970 |
| Bw    |  0.9430 |  0.3710 |
| Bx    |  0.9290 |  0.3460 |
| C     |  0.7660 |  0.4030 |
| CA    |  0.8520 |  0.3760 |
| CB    |  0.8010 |  0.3260 |
| CE    |  0.8850 |  0.3430 |
| CF    |  0.9120 |  0.3650 |
| CH    |  0.9430 |  0.3910 |
| CI    |  0.7480 |  0.3350 |
| CM    |  0.8050 |  0.3230 |
| CO    |  0.9330 |  0.3750 |
| CP    |  0.8500 |  0.3950 |
| CT    |  0.8050 |  0.3370 |
| CV    |  0.9200 |  0.3590 |
| CW    |  0.8710 |  0.3560 |
| Ca    |  0.7740 |  0.3950 |
| Cc    |  0.9250 |  0.3730 |
| Cd    |  0.8200 |  0.3150 |
| Ch    |  0.8010 |  0.3510 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| D     |  0.8070   |  0.3360   |
| E     |  0.7170   |  0.3540   |
| F     |  0.8720   |  0.3760   |
| G     |  0.8170   |  0.3510   |
| H     |  0.7910   |  0.3620   |
| I     |  0.6590   |  0.3400   |
| J     |  0.7180   |  0.2830   |
| K     |  0.7750   |  0.3750   |
| L     |  0.8080   |  0.3430   |
| M     |  0.5110   |  0.2000   |
| N     |  0.9200   |  0.3900   |
| O     |  0.6220   |  0.2700   |
| P     |  0.8250   |  0.4210   |
| Q     |  0.8910   |  0.3580   |
| R     |  0.4080   |  0.2080   |
| S     |  0.8610   |  0.3590   |
| T     |  0.8740   |  0.3600   |
| U     |  0.7810   |  0.4140   |
| V     |  0.8690  |  0.3470  |
| W     |  0.8760 |  0.3700 |
| X     |  0.7390 |  0.3470 |
| Z     |  0.8210 |  0.3170 |
| a     |  0.8520 |  0.3460 |
| c     |  0.7330 |  0.3350 |
| d     |  0.8910 |  0.3640 |
| f     |  0.7520 |  0.3050 |
| i     |  0.8760 |  0.3990 |
| k     |  0.7040 |  0.3330 |
| l     |  0.7910 |  0.3620 |
| n     |  0.5920 |  0.3350 |
| o     |  0.4950 |  0.2440 |
| q     |  0.8820 |  0.3490 |
| s     |  0.6480 |  0.2900 |
| t     |  0.7750 |  0.3690 |
| v     |  0.7590 |  0.3600 |
| w     |  0.7290 |  0.3830 |
| y     |  0.8370 |  0.3210 |
| z     |  0.7550 |  0.3040 |