



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 06:27 PM EDT

PDB ID : 9OP9 / pdb_00009op9
EMDB ID : EMD-70685
Title : Two Component Protein Nano-Particle (T=3). De Novo Design, Computationally Relaxed into Low Resolution Subtomogram Averaged CryoEM Map with Icosahedral Symmetry Applied
Authors : DiMaio, F.; Chmielewski, D.; Weidle, C.
Deposited on : 2025-05-17
Resolution : 31.60 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

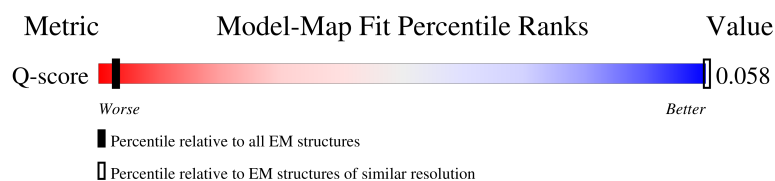
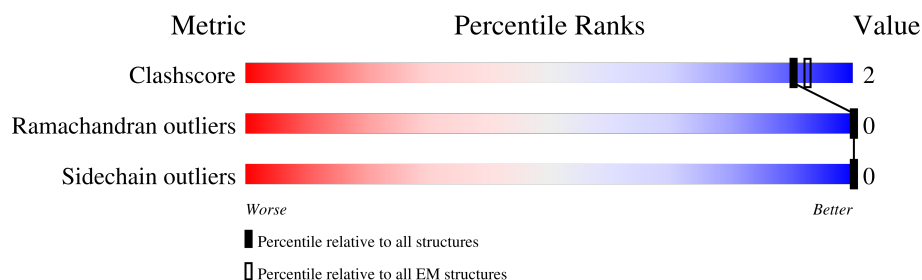
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 31.60 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.





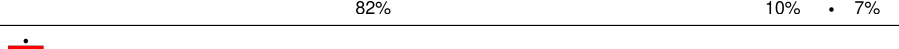
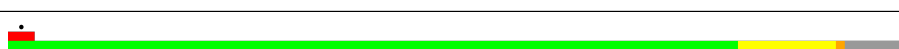



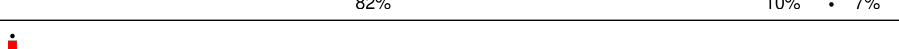



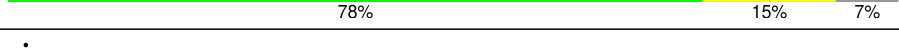

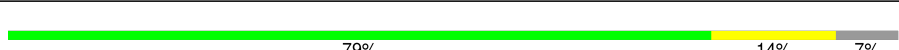


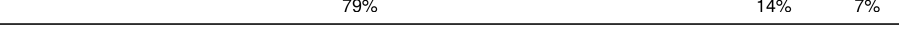







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 1 (31.60 - 31.60) |

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 ≥ 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 | AA | 114 |  82% 10% • 7% |
| 1 | AC | 114 |  83% 9% • 7% |
| 1 | AE | 114 |  79% 14% 7% |
| 1 | AG | 114 |  82% 10% • 7% |














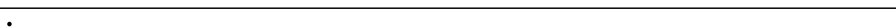











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | AI | 114 |  |
| 1 | AK | 114 |  |
| 1 | AM | 114 |  |
| 1 | AP | 114 |  |
| 1 | AR | 114 |  |
| 1 | AS | 114 |  |
| 1 | AU | 114 |  |
| 1 | AW | 114 |  |
| 1 | AY | 114 |  |
| 1 | BA | 114 |  |
| 1 | BC | 114 |  |
| 1 | BE | 114 |  |
| 1 | BG | 114 |  |
| 1 | BI | 114 |  |
| 1 | BK | 114 |  |
| 1 | BM | 114 |  |
| 1 | BO | 114 |  |
| 1 | BQ | 114 |  |
| 1 | BS | 114 |  |
| 1 | BU | 114 |  |
| 1 | BW | 114 |  |
| 1 | BY | 114 |  |
| 1 | CA | 114 |  |
| 1 | CC | 114 |  |
| 1 | CE | 114 | |



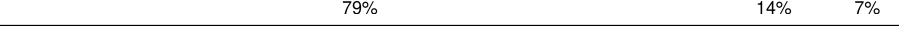
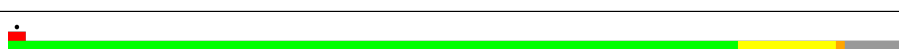



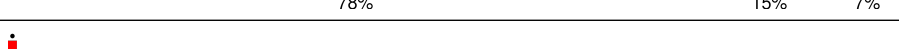



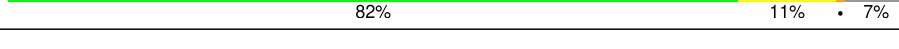

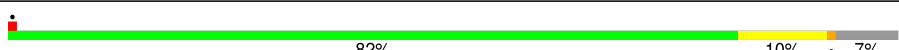


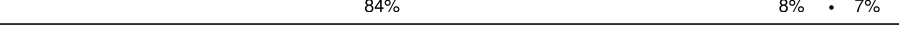







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | CG | 114 |  |
| 1 | CI | 114 |  |
| 1 | CK | 114 |  |
| 1 | CM | 114 |  |
| 1 | CO | 114 |  |
| 1 | CQ | 114 |  |
| 1 | CS | 114 |  |
| 1 | CU | 114 |  |
| 1 | CW | 114 |  |
| 1 | CY | 114 |  |
| 1 | DA | 114 |  |
| 1 | DC | 114 |  |
| 1 | DE | 114 |  |
| 1 | DG | 114 |  |
| 1 | DI | 114 |  |
| 1 | DK | 114 |  |
| 1 | DM | 114 |  |
| 1 | DO | 114 |  |
| 1 | DQ | 114 |  |
| 1 | DS | 114 |  |
| 1 | DU | 114 |  |
| 1 | DX | 114 |  |
| 1 | DZ | 114 |  |
| 1 | EB | 114 |  |
| 1 | ED | 114 |  |













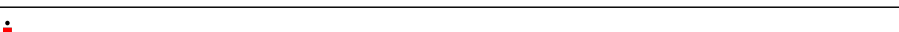

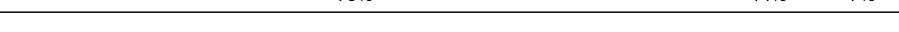

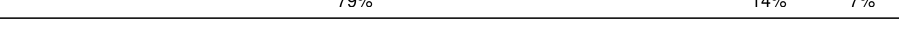








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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | EF | 114 |  |
| 1 | EH | 114 |  |
| 1 | EJ | 114 |  |
| 1 | EL | 114 |  |
| 1 | EN | 114 |  |
| 1 | EP | 114 |  |
| 1 | ER | 114 |  |
| 1 | ET | 114 |  |
| 1 | EV | 114 |  |
| 1 | EX | 114 |  |
| 1 | EZ | 114 |  |
| 1 | FB | 114 |  |
| 1 | FD | 114 |  |
| 1 | FF | 114 |  |
| 1 | FH | 114 |  |
| 1 | FJ | 114 |  |
| 1 | FL | 114 |  |
| 1 | FN | 114 |  |
| 1 | FP | 114 |  |
| 1 | FR | 114 |  |
| 1 | FT | 114 |  |
| 1 | FV | 114 |  |
| 1 | FX | 114 |  |
| 1 | FZ | 114 |  |
| 1 | GB | 114 | |







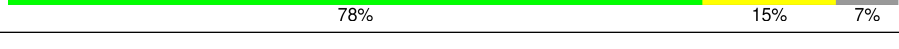
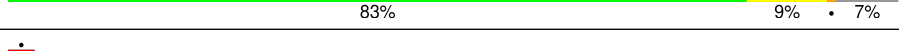
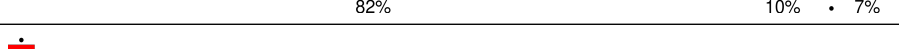
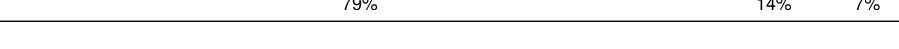
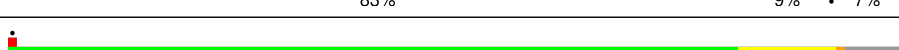

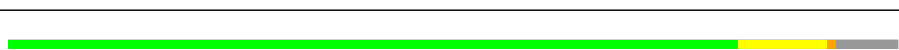

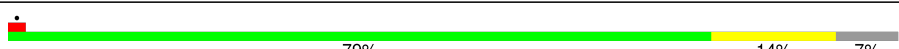





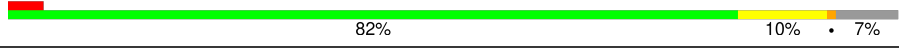
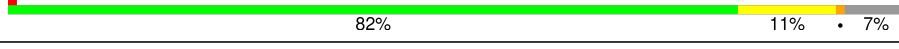



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | GD | 114 |  82%11% • 7% |
| 1 | GF | 114 |  79%14%7% |
| 1 | GH | 114 |  82%10% • 7% |
| 1 | GJ | 114 |  82%11% • 7% |
| 1 | GL | 114 |  78%15%7% |
| 1 | GN | 114 |  82%10% • 7% |
| 1 | GP | 114 |  82%10% • 7% |
| 1 | GR | 114 |  79%14%7% |
| 1 | GT | 114 |  82%10% • 7% |
| 1 | GV | 114 |  82%11% • 7% |
| 1 | GX | 114 |  79%14%7% |
| 1 | GZ | 114 |  82%10% • 7% |
| 1 | HB | 114 |  84%8% • 7% |
| 1 | HD | 114 |  79%14%7% |
| 1 | HG | 114 |  82%11% • 7% |
| 1 | HI | 114 |  79%14%7% |
| 1 | HL | 114 |  83%9% • 7% |
| 1 | HN | 114 |  79%14%7% |
| 1 | HP | 114 |  82%10% • 7% |
| 1 | HR | 114 |  82%11% • 7% |
| 1 | HT | 114 |  79%14%7% |
| 1 | HV | 114 |  82%10% • 7% |
| 1 | HX | 114 |  83%9% • 7% |
| 1 | HZ | 114 |  79%14%7% |
| 1 | IC | 114 |  84%8% • 7% |







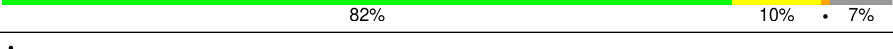
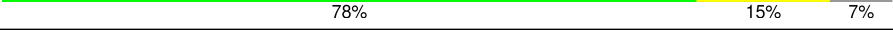
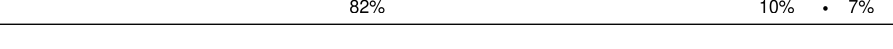
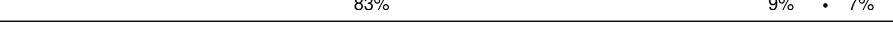
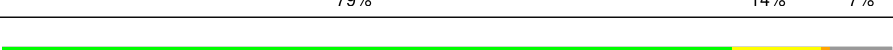

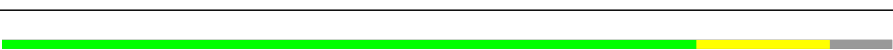

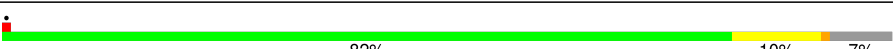





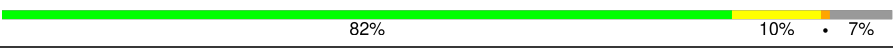
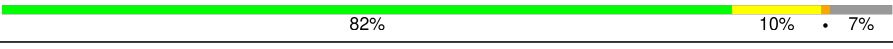



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | IE | 114 |  |
| 1 | IH | 114 |  |
| 1 | II | 114 |  |
| 1 | IK | 114 |  |
| 1 | IM | 114 |  |
| 1 | IO | 114 |  |
| 1 | IQ | 114 |  |
| 1 | IS | 114 |  |
| 1 | IU | 114 |  |
| 1 | IW | 114 |  |
| 1 | IY | 114 |  |
| 1 | JA | 114 |  |
| 1 | JC | 114 |  |
| 1 | JE | 114 |  |
| 1 | JG | 114 |  |
| 1 | JI | 114 |  |
| 1 | JK | 114 |  |
| 1 | JM | 114 |  |
| 1 | JO | 114 |  |
| 1 | JQ | 114 |  |
| 1 | JS | 114 |  |
| 1 | JV | 114 |  |
| 1 | JX | 114 |  |
| 1 | JZ | 114 |  |
| 1 | KB | 114 |  |














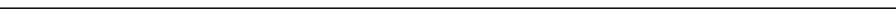











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | KD | 114 |  |
| 1 | KF | 114 |  |
| 1 | KH | 114 |  |
| 1 | KJ | 114 |  |
| 1 | KL | 114 |  |
| 1 | KN | 114 |  |
| 1 | KP | 114 |  |
| 1 | KR | 114 |  |
| 1 | KT | 114 |  |
| 1 | KV | 114 |  |
| 1 | KX | 114 |  |
| 1 | KZ | 114 |  |
| 1 | LB | 114 |  |
| 1 | LD | 114 |  |
| 1 | LF | 114 |  |
| 1 | LH | 114 |  |
| 1 | LJ | 114 |  |
| 1 | LL | 114 |  |
| 1 | LN | 114 |  |
| 1 | LP | 114 |  |
| 1 | LR | 114 |  |
| 1 | WA | 114 |  |
| 1 | WB | 114 |  |
| 1 | WC | 114 |  |
| 1 | WD | 114 |  |


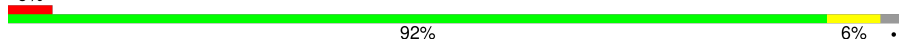
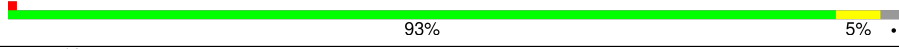
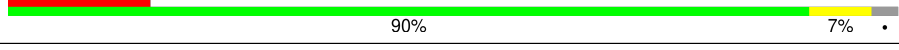
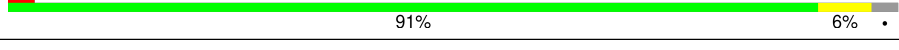
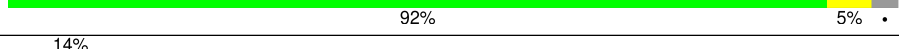
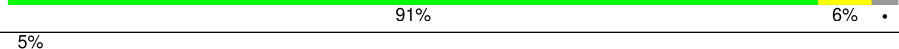
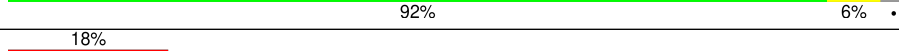
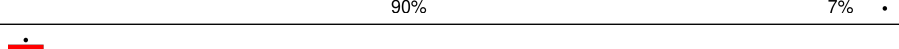
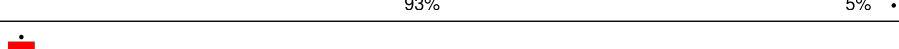
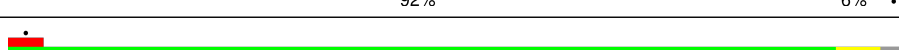
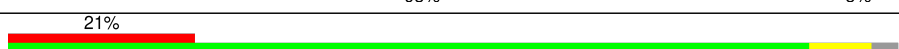
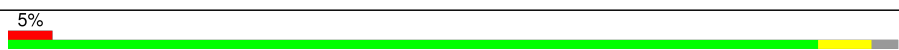
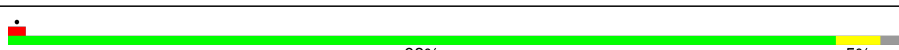
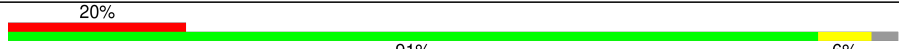

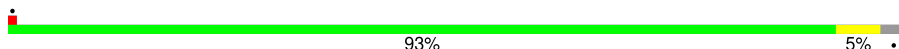

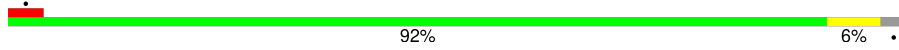
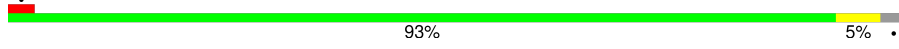
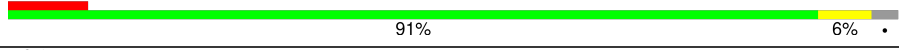
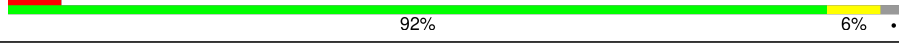
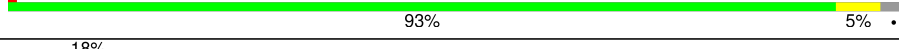
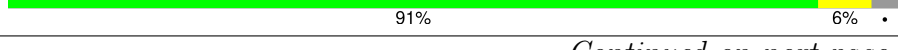

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | YA | 114 |  |
| 1 | YC | 114 |  |
| 1 | YE | 114 |  |
| 1 | YG | 114 |  |
| 1 | YI | 114 |  |
| 1 | YK | 114 |  |
| 1 | YM | 114 |  |
| 1 | YO | 114 |  |
| 1 | YQ | 114 |  |
| 1 | YS | 114 |  |
| 1 | YU | 114 |  |
| 1 | YW | 114 |  |
| 1 | YY | 114 |  |
| 1 | ZA | 114 |  |
| 1 | ZC | 114 |  |
| 1 | ZE | 114 |  |
| 1 | ZG | 114 |  |
| 1 | ZI | 114 |  |
| 1 | ZK | 114 |  |
| 1 | ZM | 114 |  |
| 1 | ZO | 114 |  |
| 1 | ZQ | 114 |  |
| 1 | ZS | 114 |  |
| 1 | ZU | 114 |  |
| 1 | ZW | 114 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | ZY | 114 |  |
| 2 | AB | 300 |  |
| 2 | AD | 300 |  |
| 2 | AF | 300 |  |
| 2 | AH | 300 |  |
| 2 | AJ | 300 |  |
| 2 | AL | 300 |  |
| 2 | AN | 300 |  |
| 2 | AO | 300 |  |
| 2 | AQ | 300 |  |
| 2 | AT | 300 |  |
| 2 | AV | 300 |  |
| 2 | AX | 300 |  |
| 2 | AZ | 300 |  |
| 2 | BB | 300 |  |
| 2 | BD | 300 |  |
| 2 | BF | 300 |  |
| 2 | BH | 300 |  |
| 2 | BJ | 300 |  |
| 2 | BL | 300 |  |
| 2 | BN | 300 |  |
| 2 | BP | 300 |  |
| 2 | BR | 300 |  |
| 2 | BT | 300 |  |
| 2 | BV | 300 |  |




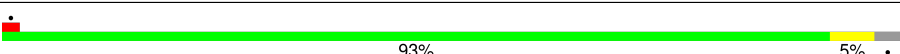
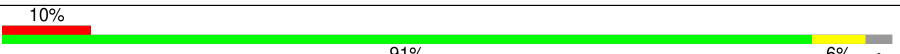
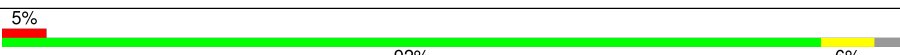
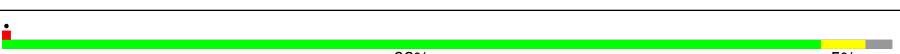
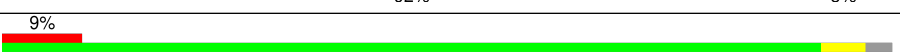

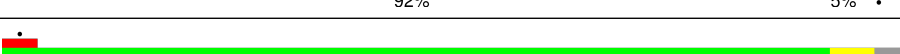
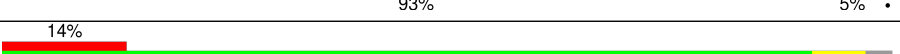
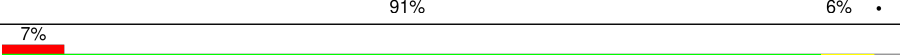
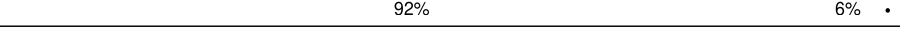
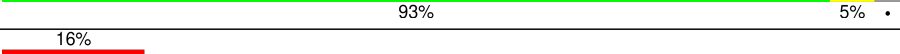

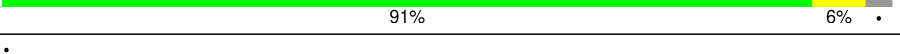
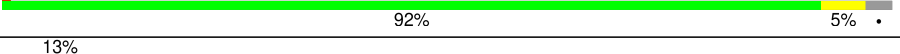
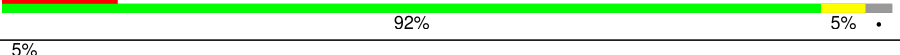
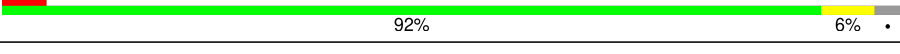
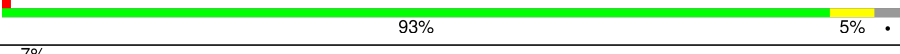
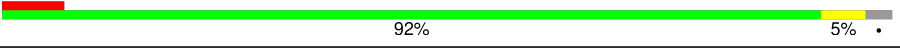
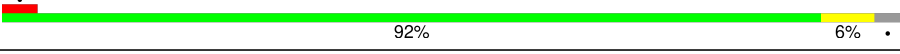
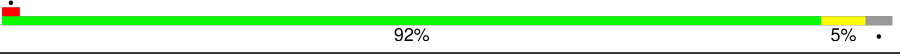


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | BX | 300 | |
| 2 | BZ | 300 | |
| 2 | CB | 300 | |
| 2 | CD | 300 | |
| 2 | CF | 300 | |
| 2 | CH | 300 | |
| 2 | CJ | 300 | |
| 2 | CL | 300 | |
| 2 | CN | 300 | |
| 2 | CP | 300 | |
| 2 | CR | 300 | |
| 2 | CT | 300 | |
| 2 | CV | 300 | |
| 2 | CX | 300 | |
| 2 | CZ | 300 | |
| 2 | DB | 300 | |
| 2 | DD | 300 | |
| 2 | DF | 300 | |
| 2 | DH | 300 | |
| 2 | DJ | 300 | |
| 2 | DL | 300 | |
| 2 | DN | 300 | |
| 2 | DP | 300 | |
| 2 | DR | 300 | |
| 2 | DT | 300 | |

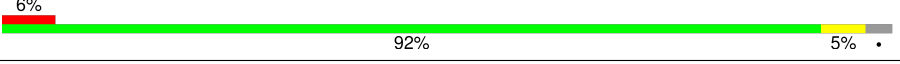
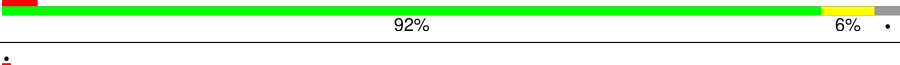
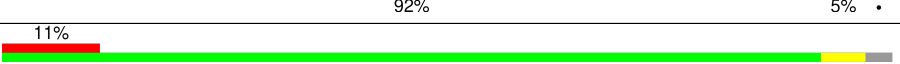
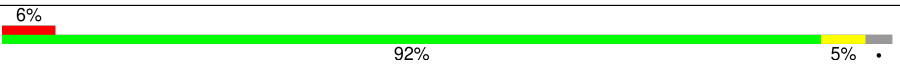
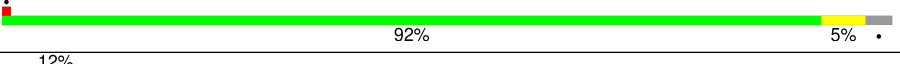
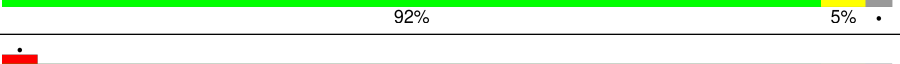
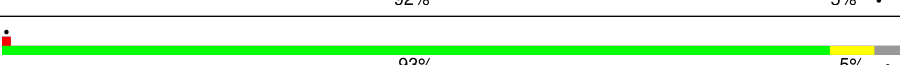
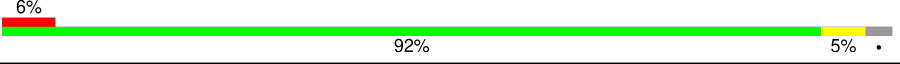
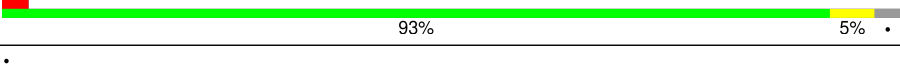

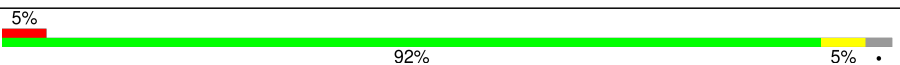
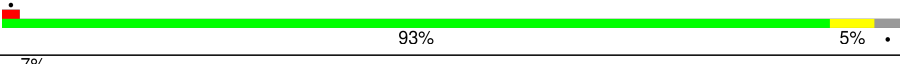
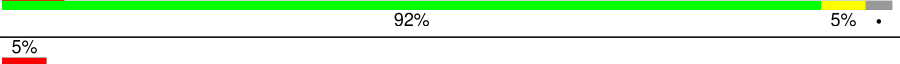
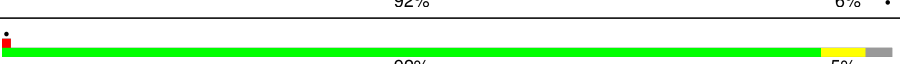
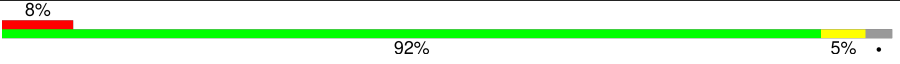
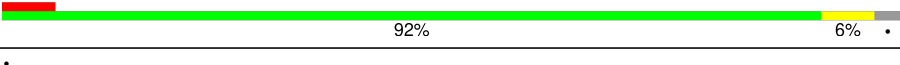
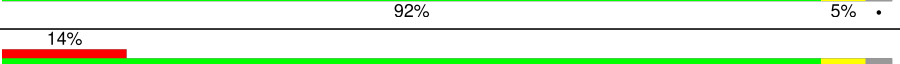
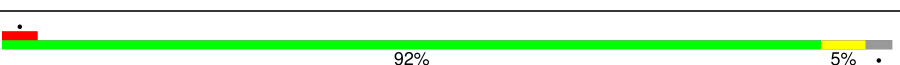
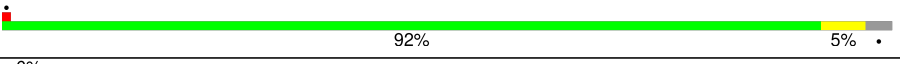
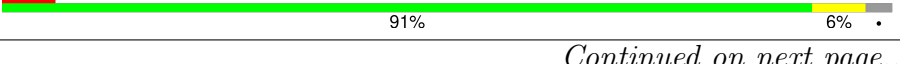



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | DW | 300 |  |
| 2 | DY | 300 |  |
| 2 | EA | 300 |  |
| 2 | EC | 300 |  |
| 2 | EE | 300 |  |
| 2 | EG | 300 |  |
| 2 | EI | 300 |  |
| 2 | EK | 300 |  |
| 2 | EM | 300 |  |
| 2 | EO | 300 |  |
| 2 | EQ | 300 |  |
| 2 | ES | 300 |  |
| 2 | EU | 300 |  |
| 2 | EW | 300 |  |
| 2 | EY | 300 |  |
| 2 | FA | 300 |  |
| 2 | FC | 300 |  |
| 2 | FE | 300 |  |
| 2 | FG | 300 |  |
| 2 | FI | 300 |  |
| 2 | FK | 300 |  |
| 2 | FM | 300 |  |
| 2 | FO | 300 |  |
| 2 | FQ | 300 |  |
| 2 | FS | 300 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | FU | 300 |  |
| 2 | FW | 300 |  |
| 2 | FY | 300 |  |
| 2 | GA | 300 |  |
| 2 | GC | 300 |  |
| 2 | GE | 300 |  |
| 2 | GG | 300 |  |
| 2 | GI | 300 |  |
| 2 | GK | 300 |  |
| 2 | GM | 300 |  |
| 2 | GO | 300 |  |
| 2 | GQ | 300 |  |
| 2 | GS | 300 |  |
| 2 | GU | 300 |  |
| 2 | GW | 300 |  |
| 2 | GY | 300 |  |
| 2 | HA | 300 |  |
| 2 | HC | 300 |  |
| 2 | HE | 300 |  |
| 2 | HF | 300 |  |
| 2 | HH | 300 |  |
| 2 | HJ | 300 |  |
| 2 | HK | 300 |  |
| 2 | HM | 300 | |
| 2 | HO | 300 | |

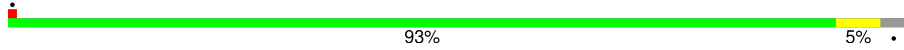

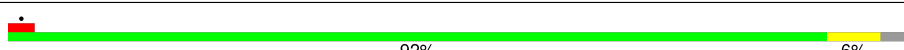
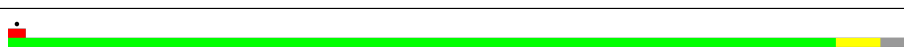
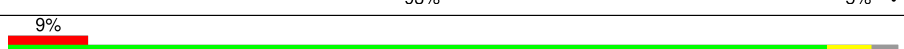
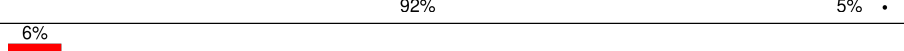
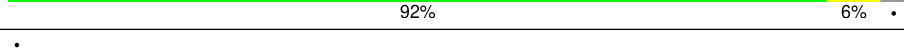
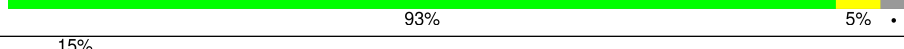

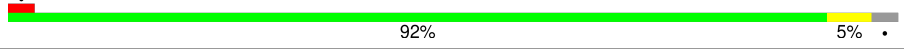
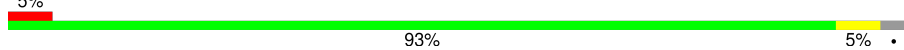
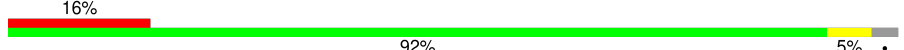
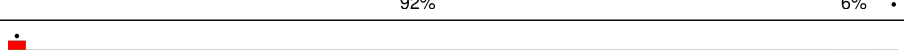


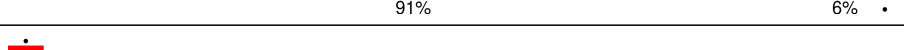
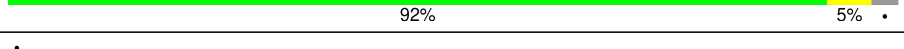
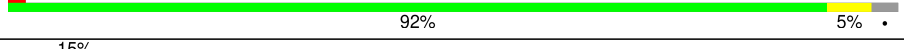
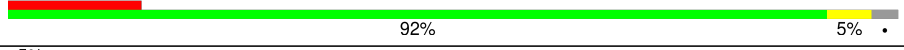
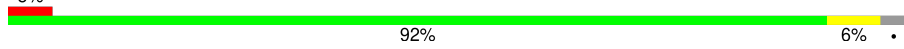
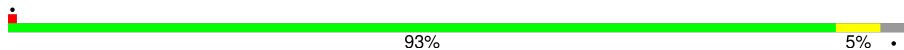
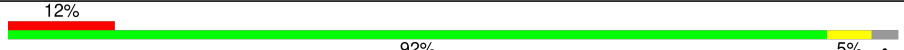

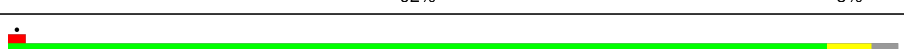
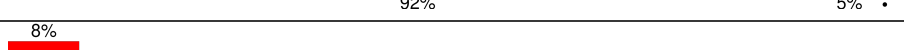
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | HQ | 300 | |
| 2 | HS | 300 | |
| 2 | HU | 300 | |
| 2 | HW | 300 | |
| 2 | HY | 300 | |
| 2 | IA | 300 | |
| 2 | IB | 300 | |
| 2 | ID | 300 | |
| 2 | IF | 300 | |
| 2 | IG | 300 | |
| 2 | IJ | 300 | |
| 2 | IL | 300 | |
| 2 | IN | 300 | |
| 2 | IP | 300 | |
| 2 | IR | 300 | |
| 2 | IT | 300 | |
| 2 | IV | 300 | |
| 2 | IX | 300 | |
| 2 | IZ | 300 | |
| 2 | JB | 300 | |
| 2 | JD | 300 | |
| 2 | JF | 300 | |
| 2 | JH | 300 | |
| 2 | JJ | 300 | |
| 2 | JL | 300 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | JN | 300 |  |
| 2 | JP | 300 |  |
| 2 | JR | 300 |  |
| 2 | JT | 300 |  |
| 2 | JU | 300 |  |
| 2 | JW | 300 |  |
| 2 | JY | 300 |  |
| 2 | KA | 300 |  |
| 2 | KC | 300 |  |
| 2 | KE | 300 |  |
| 2 | KG | 300 |  |
| 2 | KI | 300 |  |
| 2 | KK | 300 |  |
| 2 | KM | 300 |  |
| 2 | KO | 300 |  |
| 2 | KQ | 300 |  |
| 2 | KS | 300 |  |
| 2 | KU | 300 |  |
| 2 | KW | 300 |  |
| 2 | KY | 300 |  |
| 2 | LA | 300 |  |
| 2 | LC | 300 |  |
| 2 | LE | 300 |  |
| 2 | LG | 300 |  |
| 2 | LI | 300 |  |

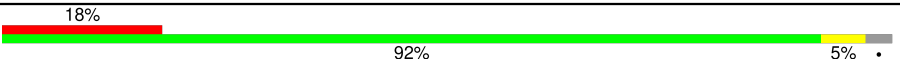
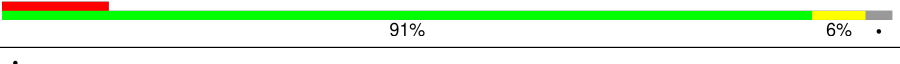
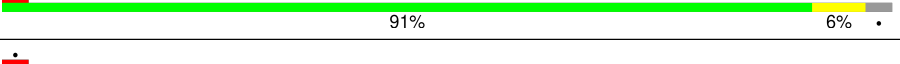
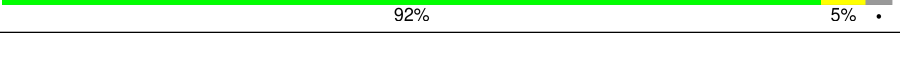
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | LK | 300 | |
| 2 | LM | 300 | |
| 2 | LO | 300 | |
| 2 | LQ | 300 | |
| 2 | LS | 300 | |
| 2 | YB | 300 | |
| 2 | YD | 300 | |
| 2 | YF | 300 | |
| 2 | YH | 300 | |
| 2 | YJ | 300 | |
| 2 | YL | 300 | |
| 2 | YN | 300 | |
| 2 | YP | 300 | |
| 2 | YR | 300 | |
| 2 | YT | 300 | |
| 2 | YV | 300 | |
| 2 | YX | 300 | |
| 2 | YZ | 300 | |
| 2 | ZB | 300 | |
| 2 | ZD | 300 | |
| 2 | ZF | 300 | |
| 2 | ZH | 300 | |
| 2 | ZJ | 300 | |
| 2 | ZL | 300 | |
| 2 | ZN | 300 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | ZP | 300 |  |
| 2 | ZR | 300 |  |
| 2 | ZT | 300 |  |
| 2 | ZV | 300 |  |
| 2 | ZX | 300 |  |
| 2 | ZZ | 300 |  |

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 553500 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 C2-B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | ZA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YW | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | YY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | AG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AR | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AW | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | AY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | BU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BW | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | BY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CW | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | CY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | DI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | DZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ED | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EF | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EH | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EJ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EL | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EN | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ER | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ET | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | EX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | EZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FD | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FF | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FH | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FJ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FL | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FN | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FR | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FT | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | FZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GD | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GF | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GH | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GJ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GL | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | GN | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GR | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GT | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | GZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HD | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | WB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | WA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HL | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HN | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HR | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HT | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | HX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | HZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | WC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IH | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | II | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IU | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IW | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | IY | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JA | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | ZK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JC | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JE | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JG | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JI | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JK | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1 | JM | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JO | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JQ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JS | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | WD | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | JZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KB | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KD | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KF | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KH | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KJ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KL | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KN | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KP | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KR | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KT | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KV | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KX | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |
| 1 | KZ | 106 | Total 808 | C 506 | N 149 | O 152 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | ZM | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LB | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LD | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LF | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LH | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LJ | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LL | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LN | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LP | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | LR | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | ZO | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | ZQ | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | ZS | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | ZU | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | ZW | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |
| 1 | YA | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 506 | 149 | 152 | 1 | | |

- Molecule 2 is a protein called C3-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | YD | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2267 | 1421 | 413 | 430 | 3 | | |
| 2 | ZZ | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2267 | 1421 | 413 | 430 | 3 | | |
| 2 | YF | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2267 | 1421 | 413 | 430 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | YH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YZ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | AV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | AZ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | BZ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | CJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | CZ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | DY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | EA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EI | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ES | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | EY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FI | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | FO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FS | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | FY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GI | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GS | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | GY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | HC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HS | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | HY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ID | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | IN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | IZ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JD | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JF | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JH | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JJ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | JY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | ZL | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KI | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KS | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KU | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KW | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | KY | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LA | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LC | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LE | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LG | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LI | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LK | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LM | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LO | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

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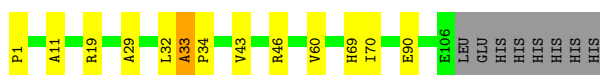
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2 | LQ | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | LS | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZN | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZP | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZR | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZT | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZV | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | ZX | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |
| 2 | YB | 292 | Total 2267 | C 1421 | N 413 | O 430 | S 3 | 0 | 0 |

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

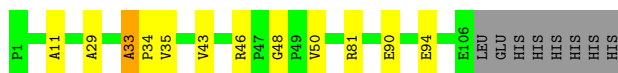
- Molecule 1: C2-B

Chain ZA: 




- Molecule 1: C2-B

Chain YC: 




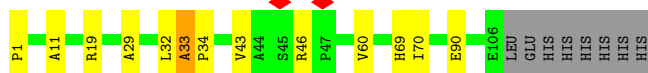
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Chain ZY: 




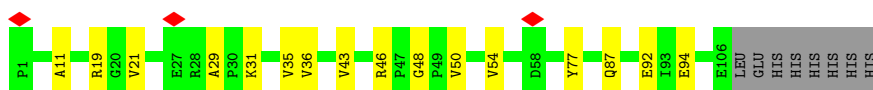
- Molecule 1: C2-B

Chain YE: 

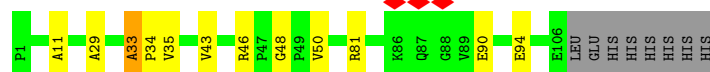
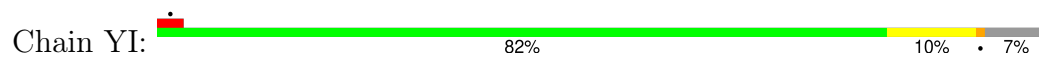


- Molecule 1: C2-B

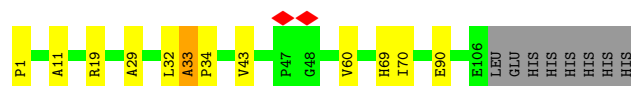
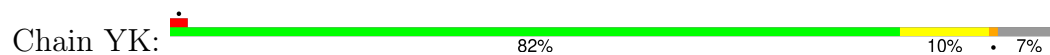
Chain YG: 



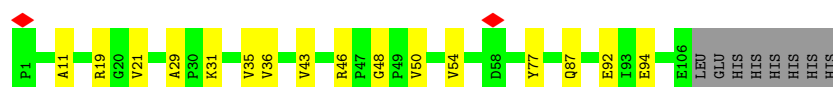
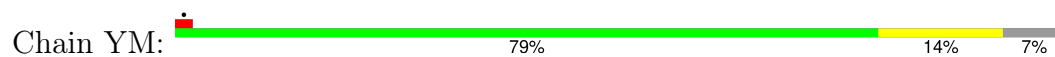
- Molecule 1: C2-B



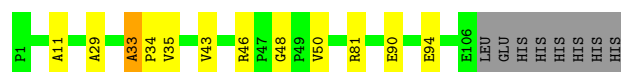
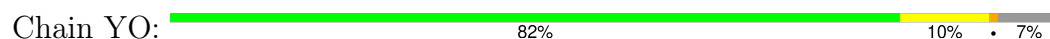
- Molecule 1: C2-B



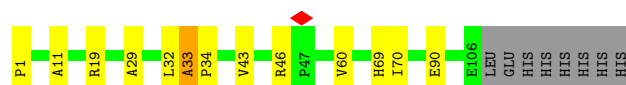
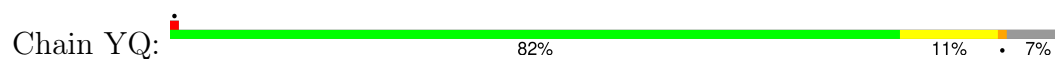
- Molecule 1: C2-B



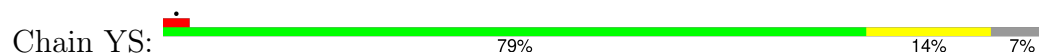
- Molecule 1: C2-B



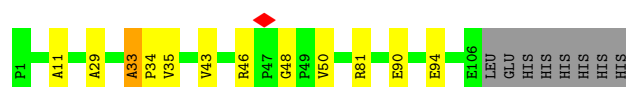
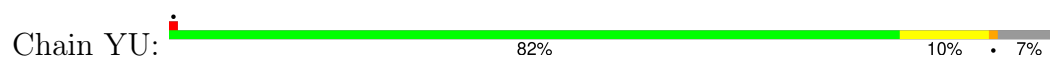
- Molecule 1: C2-B




- Molecule 1: C2-B



- Molecule 1: C2-B




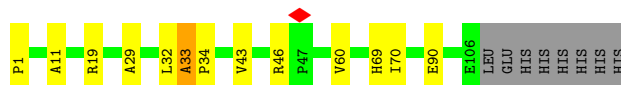
- Molecule 1: C2-B

Chain AA:  82% 10% • 7%




- Molecule 1: C2-B

Chain YW:  82% 11% • 7%




- Molecule 1: C2-B

Chain YY:  79% 14% 7%




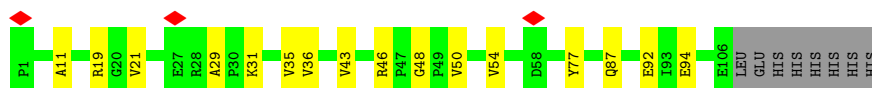
- Molecule 1: C2-B

Chain AC:  83% 9% • 7%




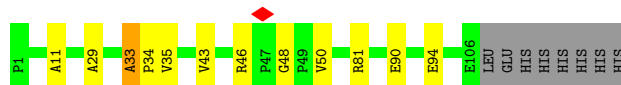
- Molecule 1: C2-B

Chain AE:  79% 14% 7%




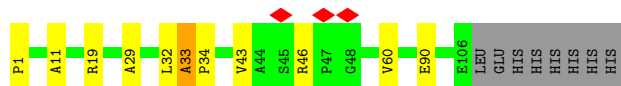
- Molecule 1: C2-B

Chain AG:  82% 10% • 7%


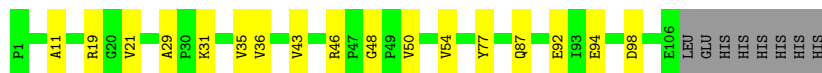


- Molecule 1: C2-B


Chain AI:  83% 9% • 7%




• Molecule 1: C2-B

Chain AK:  78% 15% 7%


• Molecule 1: C2-B

Chain AM:  82% 10% 7%


• Molecule 1: C2-B

Chain AP:  79% 14% 7%


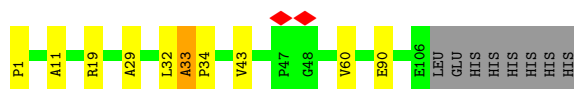
• Molecule 1: C2-B

Chain AR:  82% 11% 7%


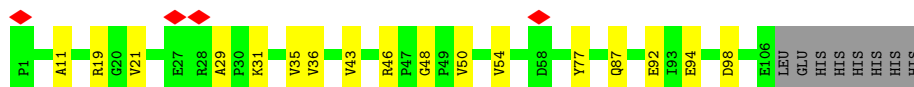
• Molecule 1: C2-B

Chain AS:  82% 10% 7%


• Molecule 1: C2-B

Chain AU:  84% 8% 7%

• Molecule 1: C2-B


Chain AW:  78% 15% 7%

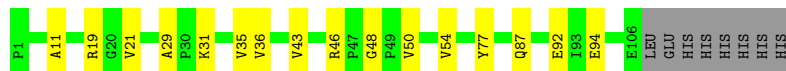
- Molecule 1: C2-B

Chain AY:  82% 10% • 7%




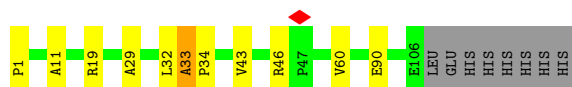
- Molecule 1: C2-B

Chain ZC:  79% 14% 7%




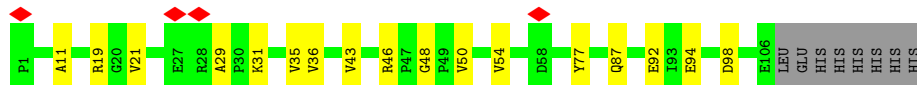
- Molecule 1: C2-B

Chain BA:  83% 9% • 7%




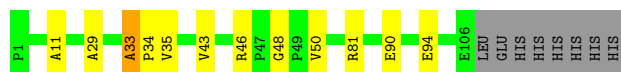
- Molecule 1: C2-B

Chain BC:  78% 15% 7%




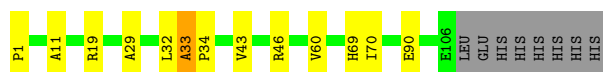
- Molecule 1: C2-B

Chain BE:  82% 10% • 7%




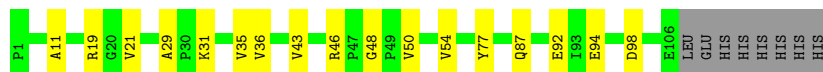
- Molecule 1: C2-B

Chain BG:  82% 11% • 7%

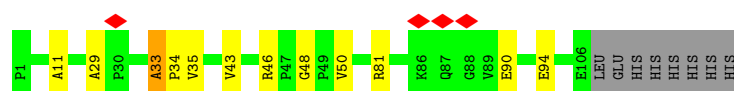
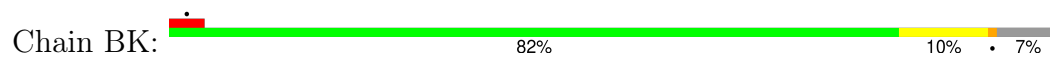


- Molecule 1: C2-B

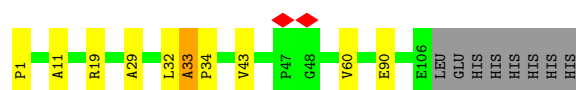
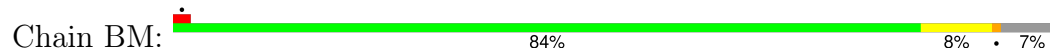
Chain BI:  78% 15% 7%



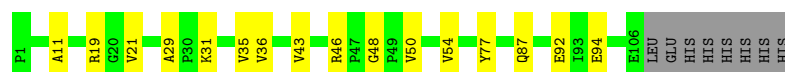
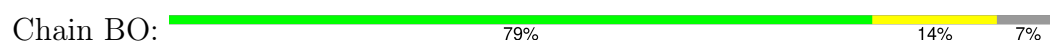
- Molecule 1: C2-B



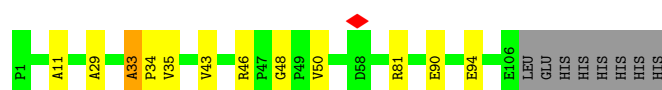
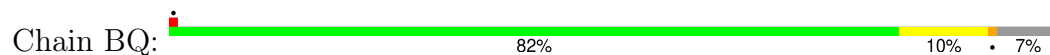
- Molecule 1: C2-B



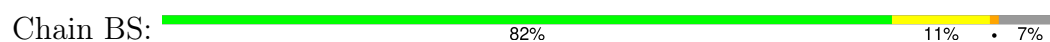
- Molecule 1: C2-B



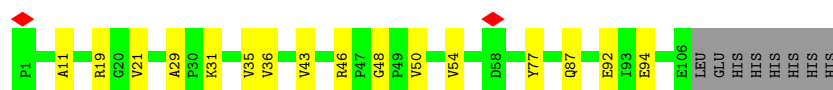
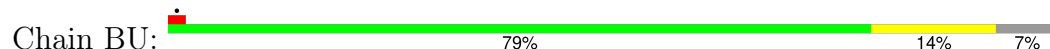
- Molecule 1: C2-B



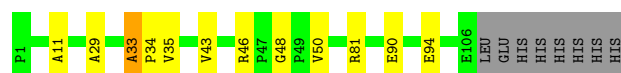
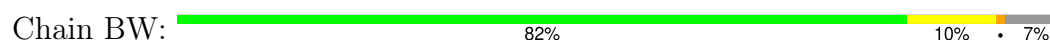
- Molecule 1: C2-B




- Molecule 1: C2-B



- Molecule 1: C2-B




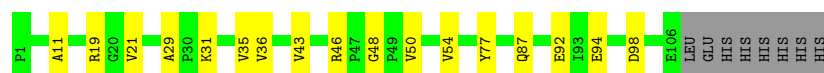
- Molecule 1: C2-B

Chain BY:  82% 11% • 7%




• Molecule 1: C2-B

Chain CA:  78% 15% 7%




• Molecule 1: C2-B

Chain CC:  82% 10% • 7%




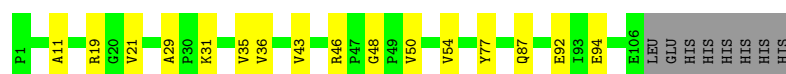
• Molecule 1: C2-B

Chain CE:  82% 11% • 7%




• Molecule 1: C2-B

Chain CG:  79% 14% 7%




• Molecule 1: C2-B

Chain CI:  82% 10% • 7%




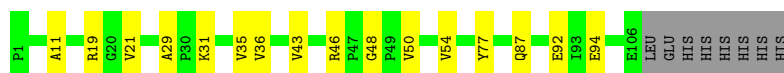
• Molecule 1: C2-B

Chain CK:  82% 11% • 7%

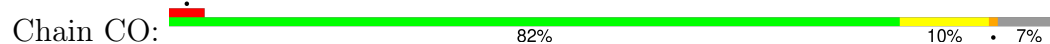


• Molecule 1: C2-B

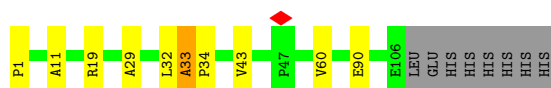
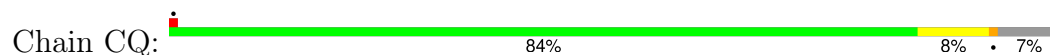
Chain CM:  79% 14% 7%



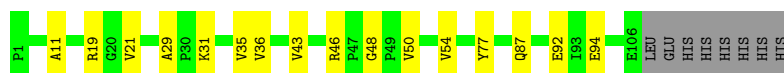
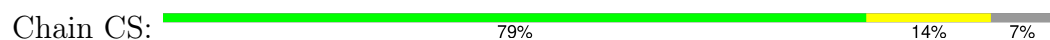
- Molecule 1: C2-B



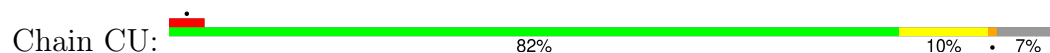
- Molecule 1: C2-B



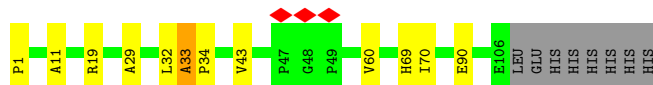
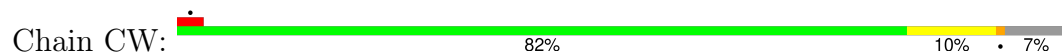
- Molecule 1: C2-B



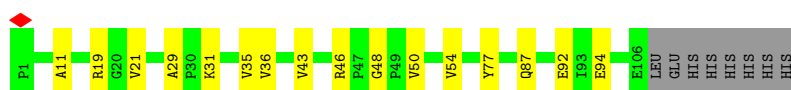
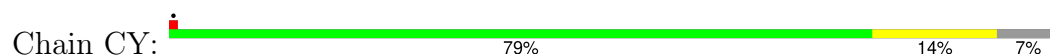
- Molecule 1: C2-B



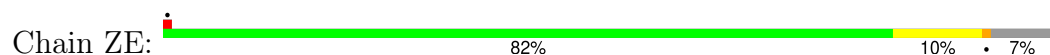
- Molecule 1: C2-B



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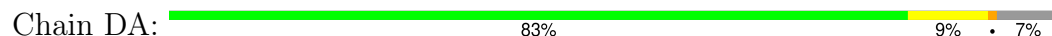


- Molecule 1: C2-B

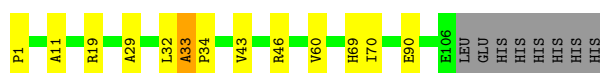
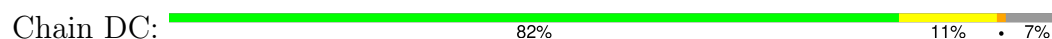




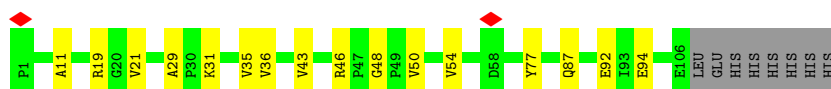
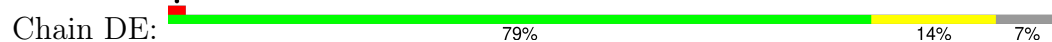
- Molecule 1: C2-B



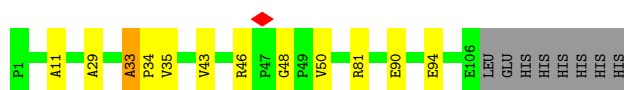
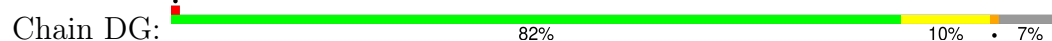
- Molecule 1: C2-B



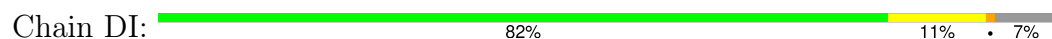
- Molecule 1: C2-B



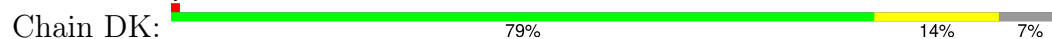
- Molecule 1: C2-B



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- Molecule 1: C2-B

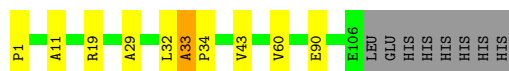
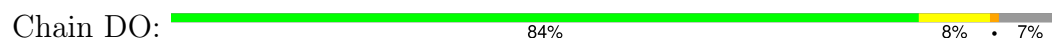


- Molecule 1: C2-B

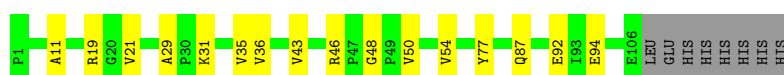
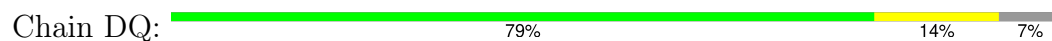




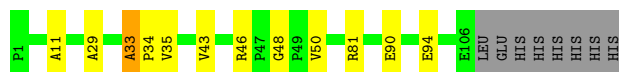
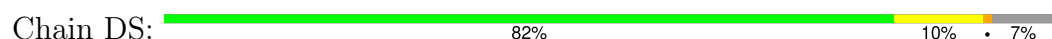
- Molecule 1: C2-B



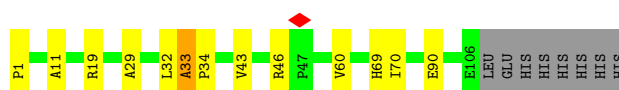
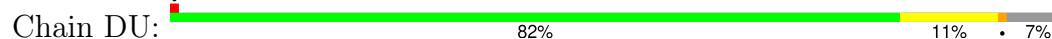
- Molecule 1: C2-B



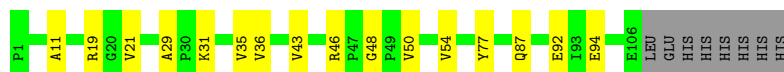
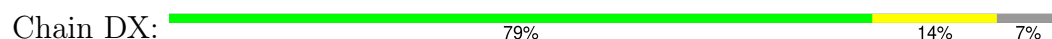
- Molecule 1: C2-B



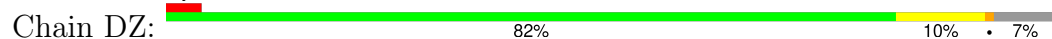
- Molecule 1: C2-B



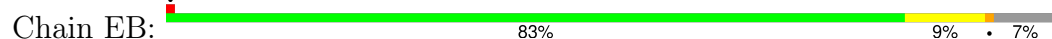
- Molecule 1: C2-B



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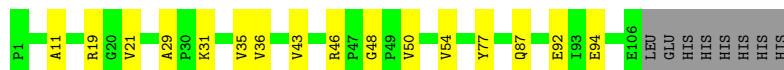
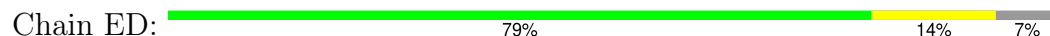


- Molecule 1: C2-B

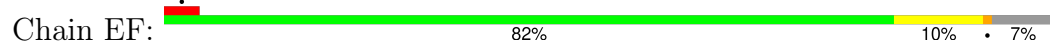




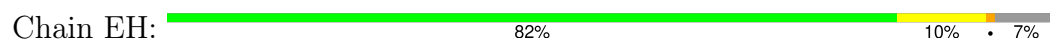
- Molecule 1: C2-B



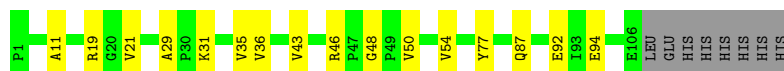
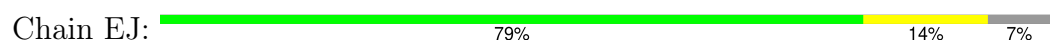
- Molecule 1: C2-B



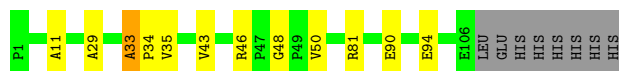
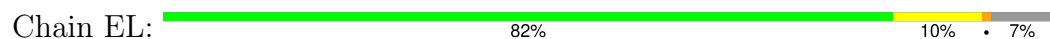
- Molecule 1: C2-B



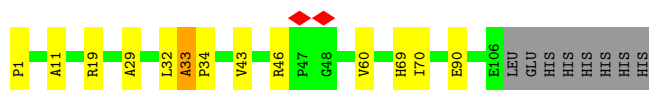
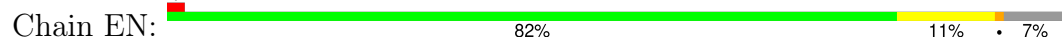
- Molecule 1: C2-B



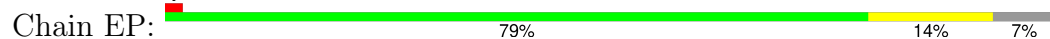
- Molecule 1: C2-B



- Molecule 1: C2-B



- Molecule 1: C2-B





- Molecule 1: C2-B

Chain ER: 82% 10% 7%



- Molecule 1: C2-B

Chain ET: 83% 9% 7%



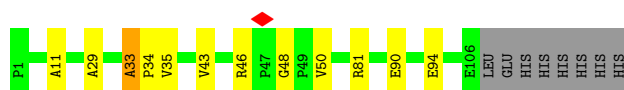
- Molecule 1: C2-B

Chain EV: 78% 15% 7%



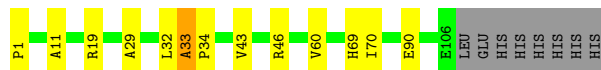
- Molecule 1: C2-B

Chain EX: 82% 10% 7%



- Molecule 1: C2-B

Chain EZ: 82% 11% 7%



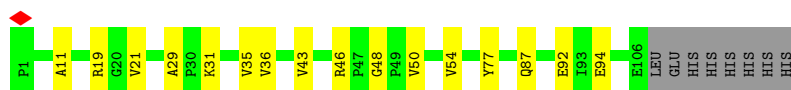
- Molecule 1: C2-B

Chain ZG: 82% 10% 7%



- Molecule 1: C2-B

Chain FB: 79% 14% 7%



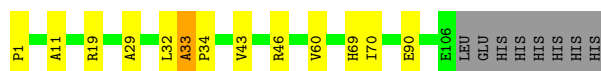
- Molecule 1: C2-B

Chain FD: 82% 10% • 7%



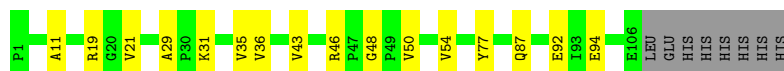
- Molecule 1: C2-B

Chain FF: 82% 11% • 7%



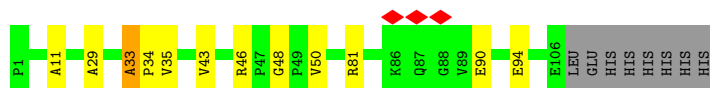
- Molecule 1: C2-B

Chain FH: 79% 14% 7%



- Molecule 1: C2-B

Chain FJ: 82% 10% • 7%



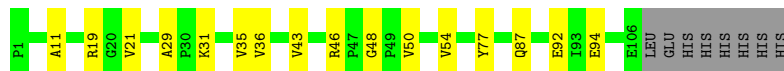
- Molecule 1: C2-B

Chain FL: 82% 10% • 7%



- Molecule 1: C2-B

Chain FN: 79% 14% 7%

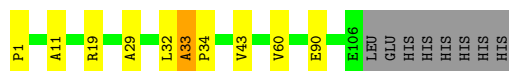
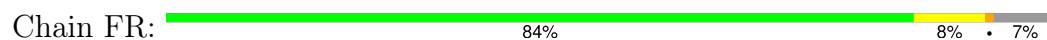


- Molecule 1: C2-B

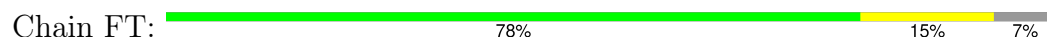
Chain FP: 82% 10% • 7%



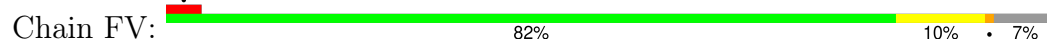
- Molecule 1: C2-B



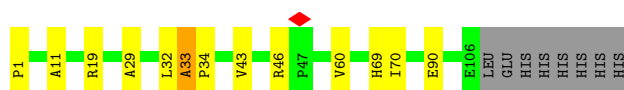
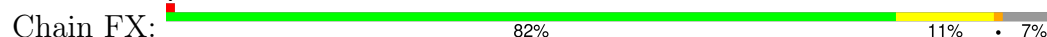
- Molecule 1: C2-B



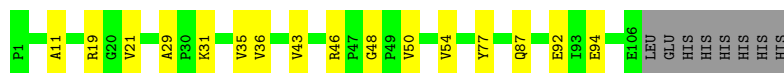
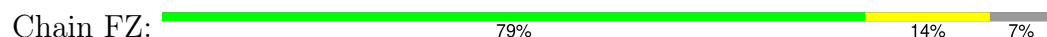
- Molecule 1: C2-B



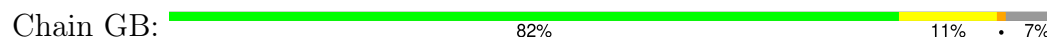
- Molecule 1: C2-B



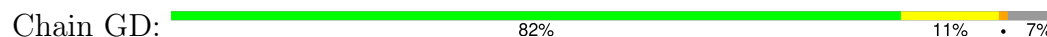
- Molecule 1: C2-B

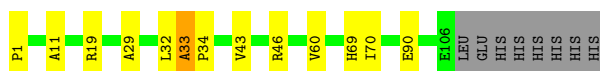


- Molecule 1: C2-B

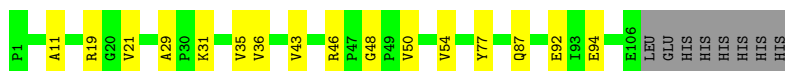
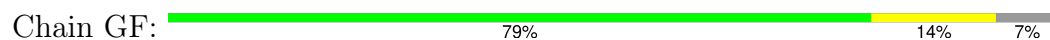


- Molecule 1: C2-B

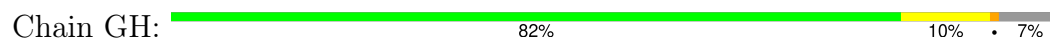




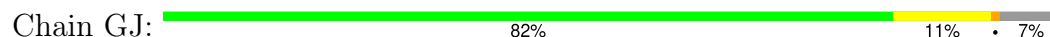
- Molecule 1: C2-B



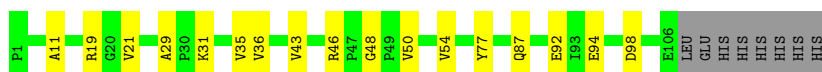
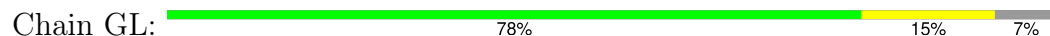
- Molecule 1: C2-B



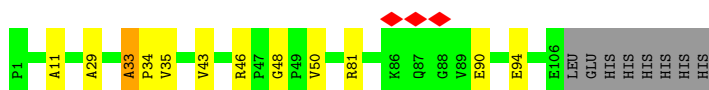
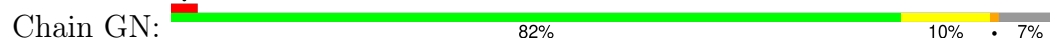
- Molecule 1: C2-B



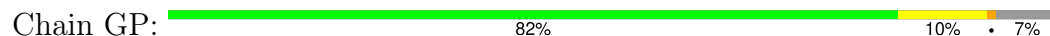
- Molecule 1: C2-B



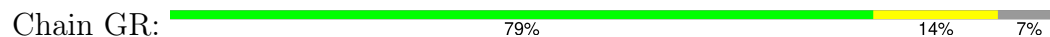
- Molecule 1: C2-B

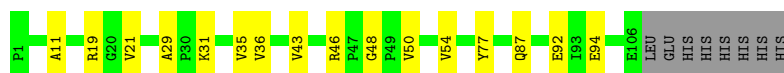


- Molecule 1: C2-B

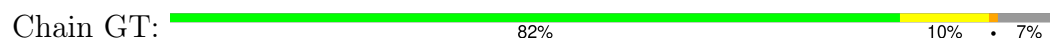


- Molecule 1: C2-B

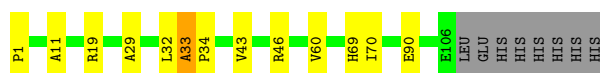
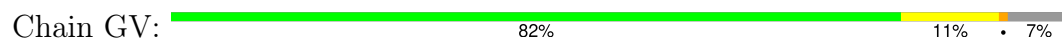




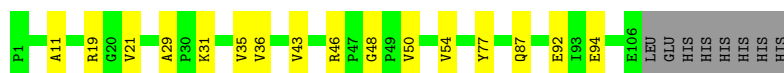
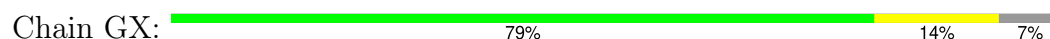
- Molecule 1: C2-B



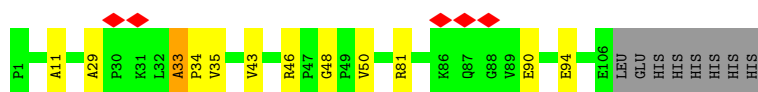
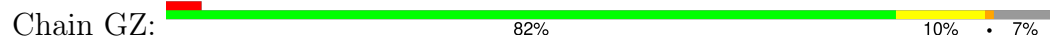
- Molecule 1: C2-B



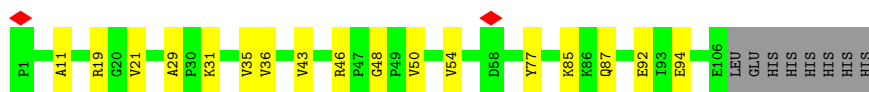
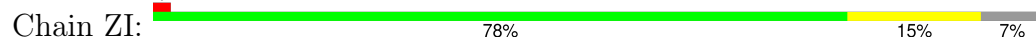
- Molecule 1: C2-B



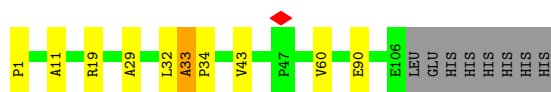
- Molecule 1: C2-B



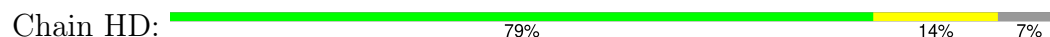
- Molecule 1: C2-B

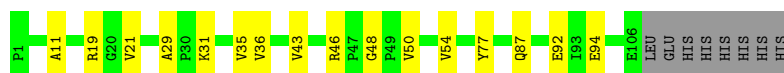


- Molecule 1: C2-B

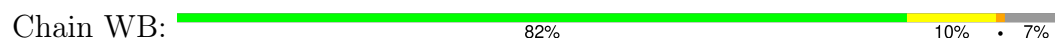


- Molecule 1: C2-B

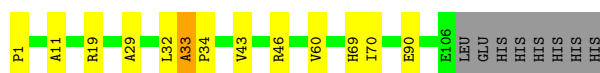
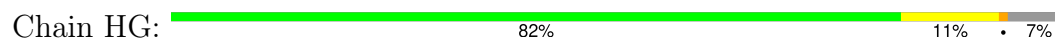




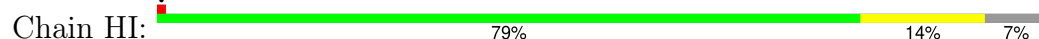
- Molecule 1: C2-B



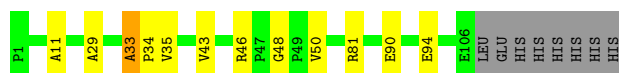
- Molecule 1: C2-B



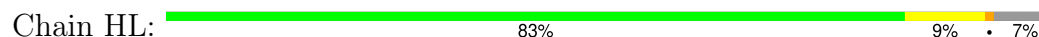
- Molecule 1: C2-B



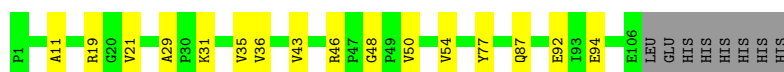
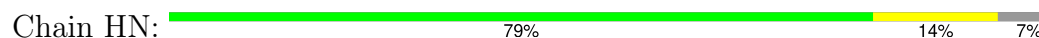
- Molecule 1: C2-B



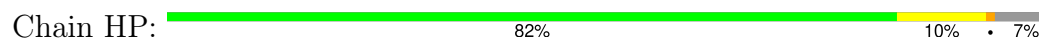
- Molecule 1: C2-B



- Molecule 1: C2-B

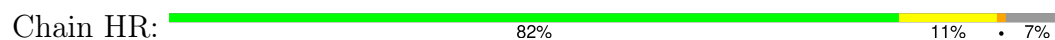


- Molecule 1: C2-B

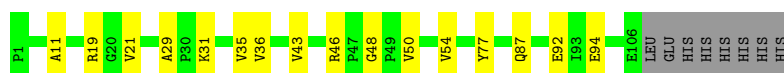
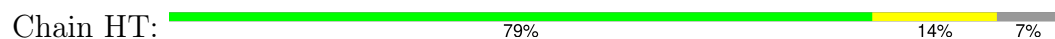




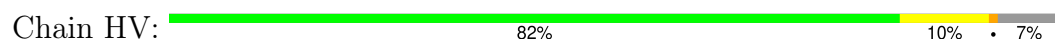
- Molecule 1: C2-B



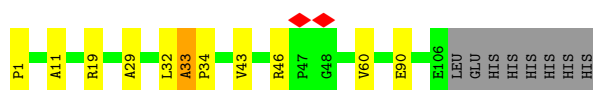
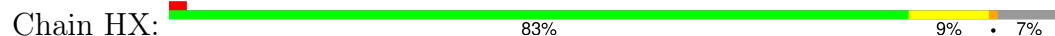
- Molecule 1: C2-B



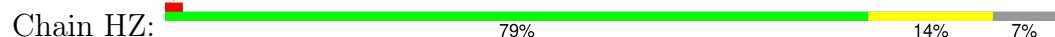
- Molecule 1: C2-B



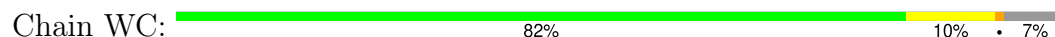
- Molecule 1: C2-B



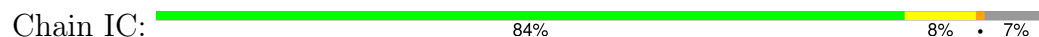
- Molecule 1: C2-B

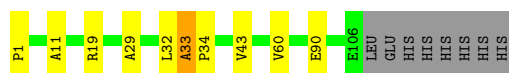


- Molecule 1: C2-B

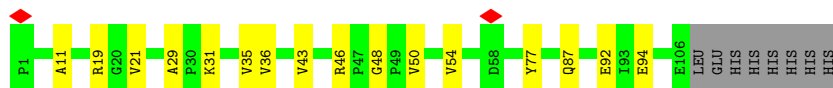
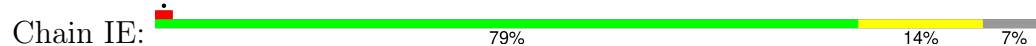


- Molecule 1: C2-B

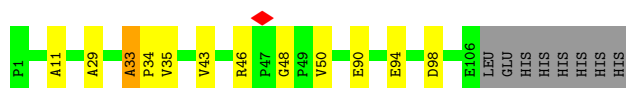
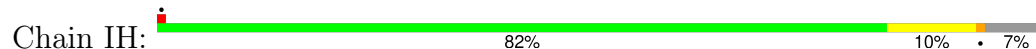




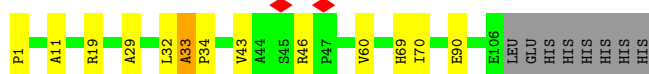
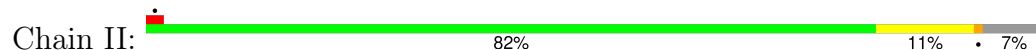
- Molecule 1: C2-B



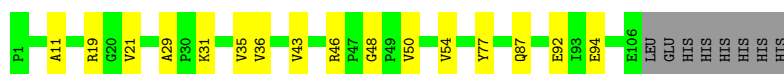
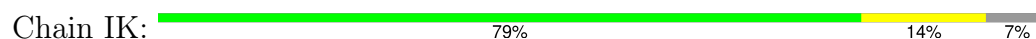
- Molecule 1: C2-B



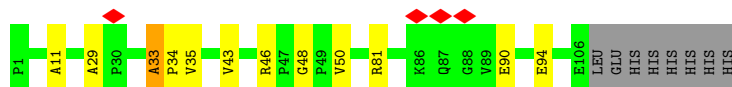
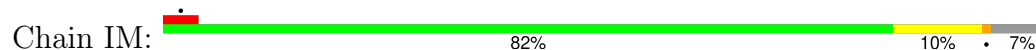
- Molecule 1: C2-B



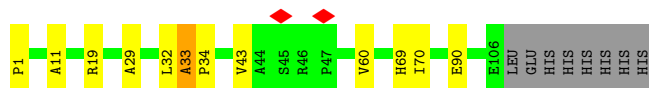
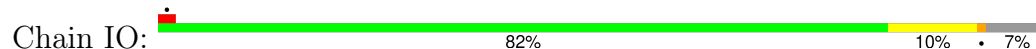
- Molecule 1: C2-B



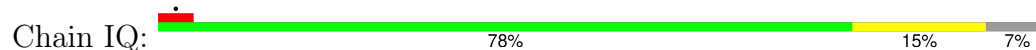
- Molecule 1: C2-B



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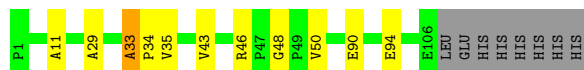
- Molecule 1: C2-B





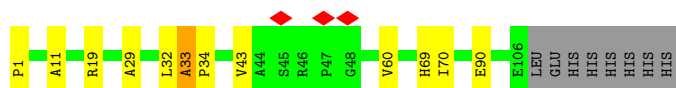
• Molecule 1: C2-B

Chain IS: 83% 9% • 7%



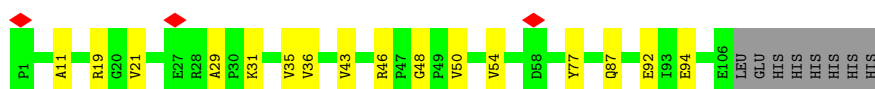
• Molecule 1: C2-B

Chain IU: 82% 10% • 7%



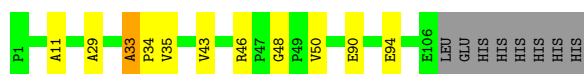
• Molecule 1: C2-B

Chain IW: 79% 14% 7%



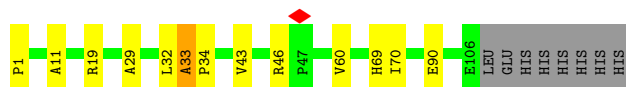
• Molecule 1: C2-B

Chain IY: 83% 9% • 7%



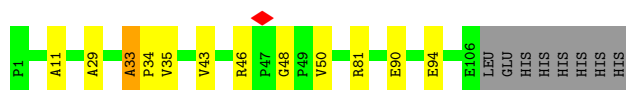
• Molecule 1: C2-B

Chain JA: 82% 11% • 7%



• Molecule 1: C2-B

Chain ZK: 82% 10% • 7%

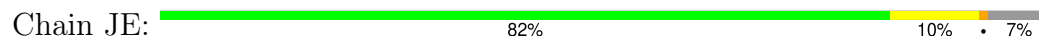


• Molecule 1: C2-B

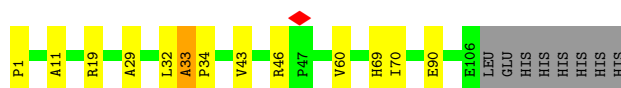
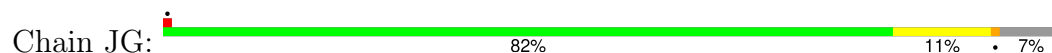
Chain JC: 79% 14% 7%



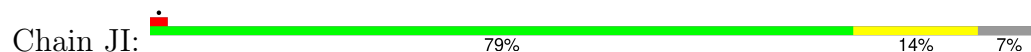
• Molecule 1: C2-B



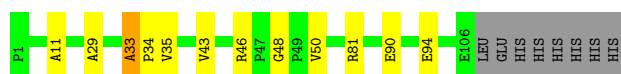
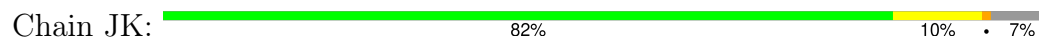
• Molecule 1: C2-B



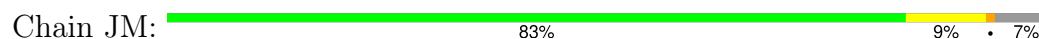
• Molecule 1: C2-B



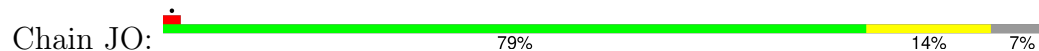
• Molecule 1: C2-B



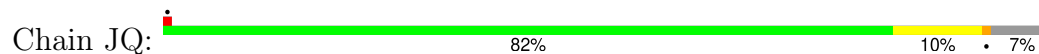
• Molecule 1: C2-B

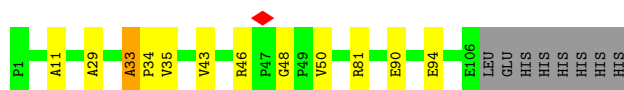


• Molecule 1: C2-B

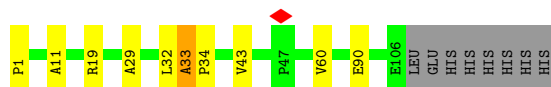
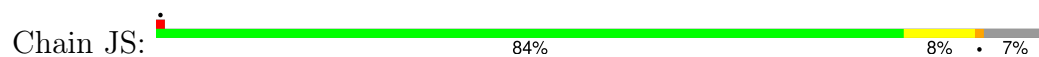


• Molecule 1: C2-B

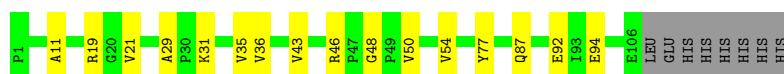
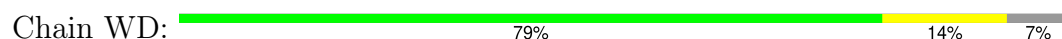




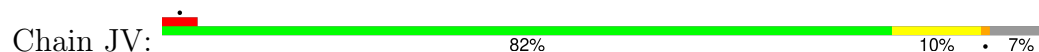
- Molecule 1: C2-B



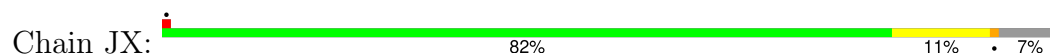
- Molecule 1: C2-B



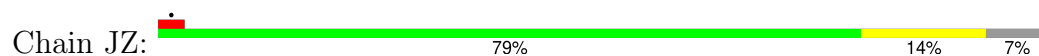
- Molecule 1: C2-B



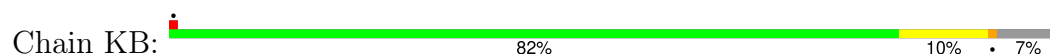
- Molecule 1: C2-B



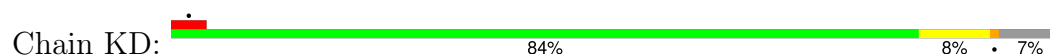
- Molecule 1: C2-B

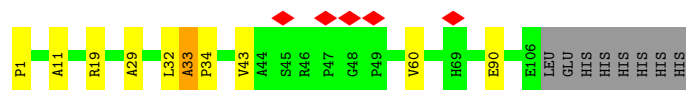


- Molecule 1: C2-B

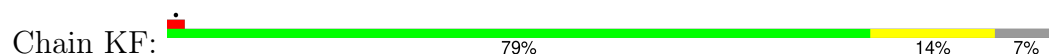


- Molecule 1: C2-B

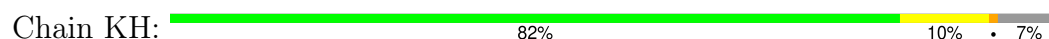




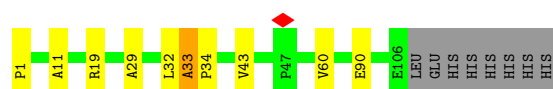
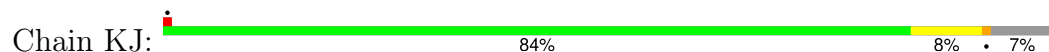
- Molecule 1: C2-B



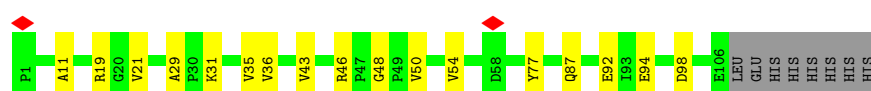
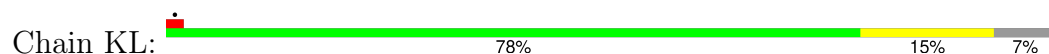
- Molecule 1: C2-B



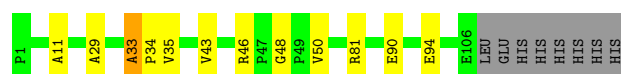
- Molecule 1: C2-B



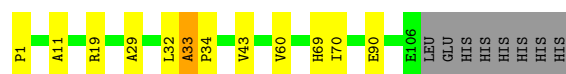
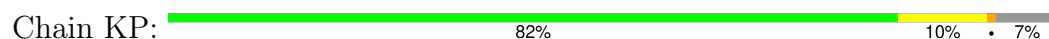
- Molecule 1: C2-B



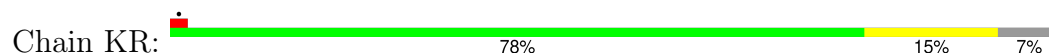
- Molecule 1: C2-B

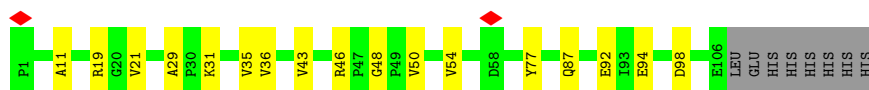


- Molecule 1: C2-B



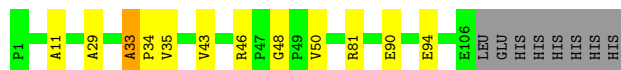
- Molecule 1: C2-B





- Molecule 1: C2-B

Chain KT: 82% 10% • 7%



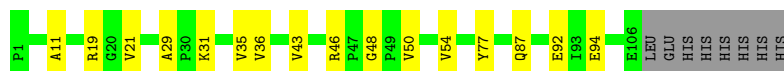
- Molecule 1: C2-B

Chain KV: 83% 9% • 7%



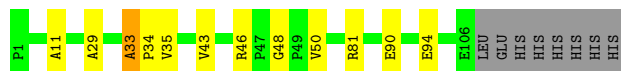
- Molecule 1: C2-B

Chain KX: 79% 14% 7%



- Molecule 1: C2-B

Chain KZ: 82% 10% • 7%



- Molecule 1: C2-B

Chain ZM: 82% 10% • 7%



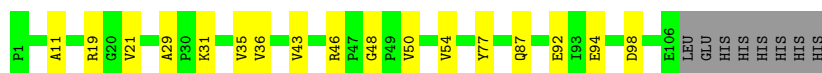
- Molecule 1: C2-B

Chain LB: 82% 10% • 7%

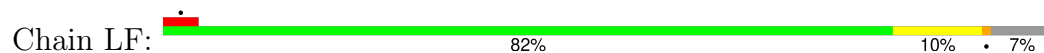


- Molecule 1: C2-B

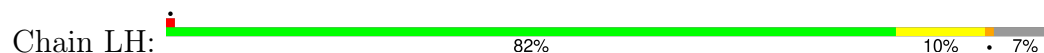
Chain LD: 78% 15% 7%



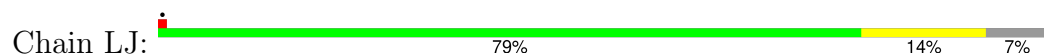
- Molecule 1: C2-B



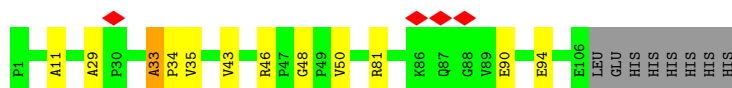
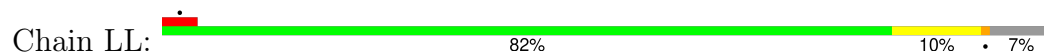
- Molecule 1: C2-B



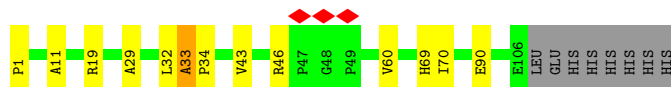
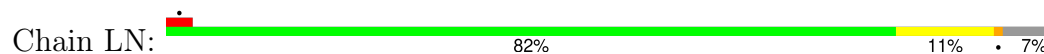
- Molecule 1: C2-B



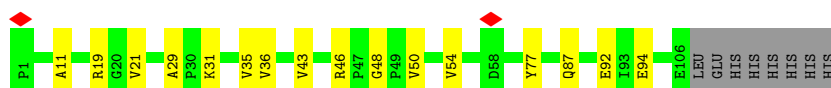
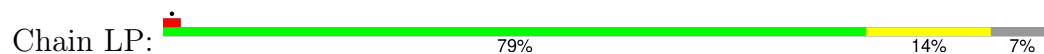
- Molecule 1: C2-B



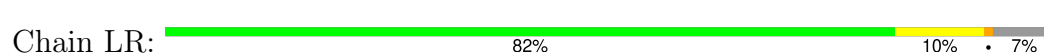
- Molecule 1: C2-B

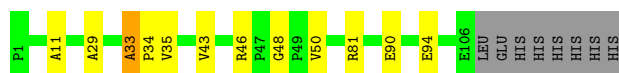


- Molecule 1: C2-B

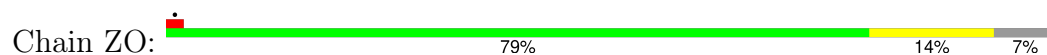


- Molecule 1: C2-B

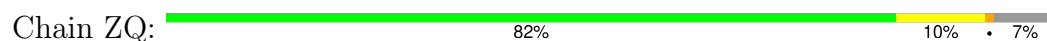




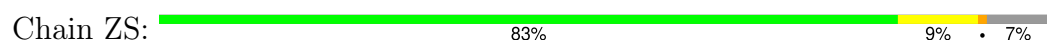
- Molecule 1: C2-B



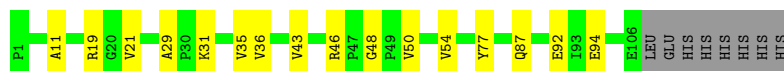
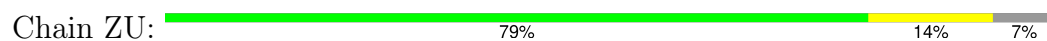
- Molecule 1: C2-B



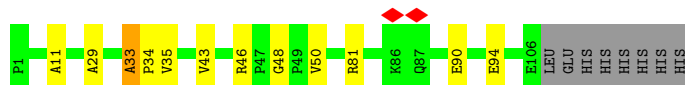
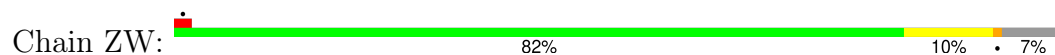
- Molecule 1: C2-B



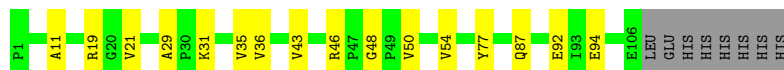
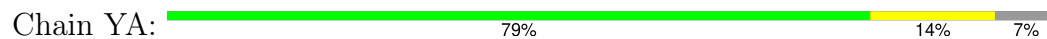
- Molecule 1: C2-B



- Molecule 1: C2-B

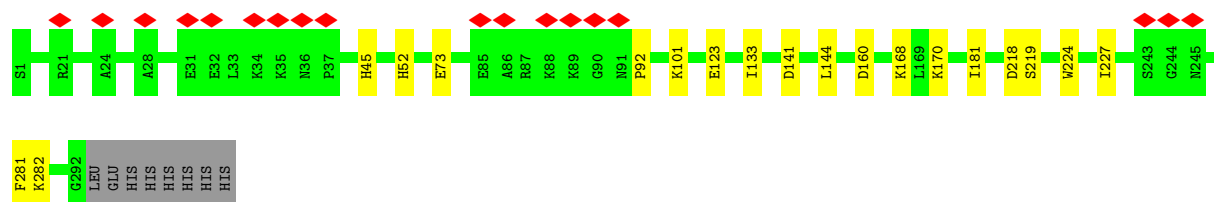


- Molecule 1: C2-B

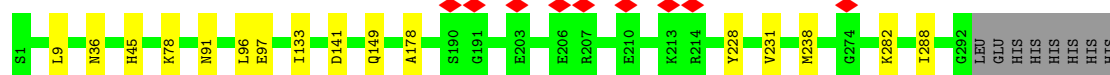


- Molecule 2: C3-A

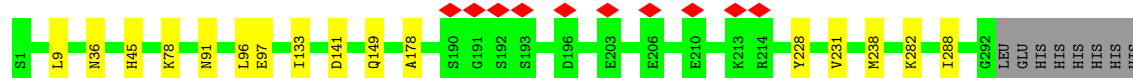




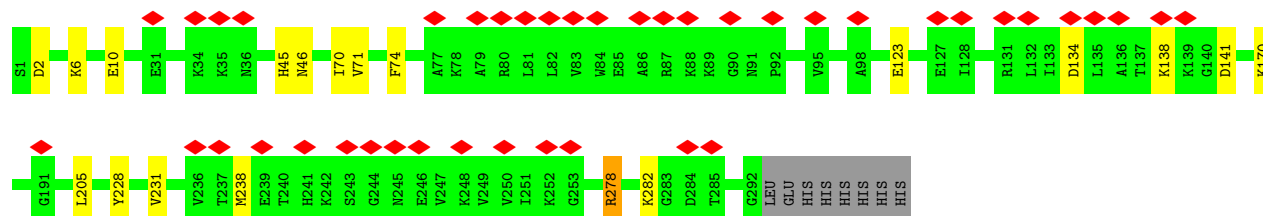
- Molecule 2: C3-A



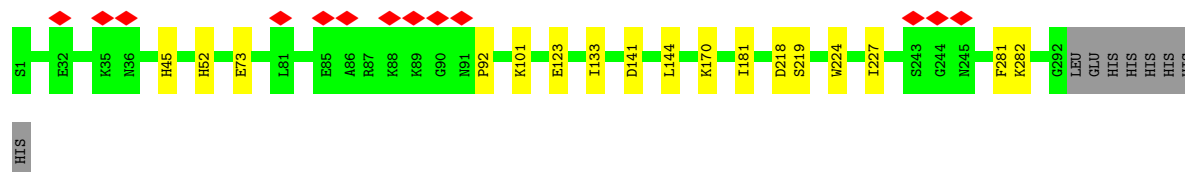
- Molecule 2: C3-A



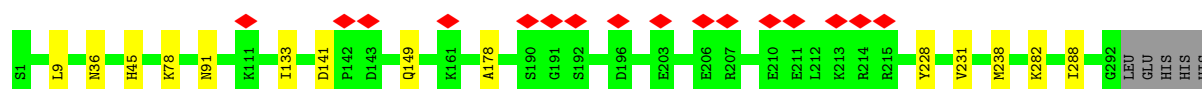
- Molecule 2: C3-A



- Molecule 2: C3-A



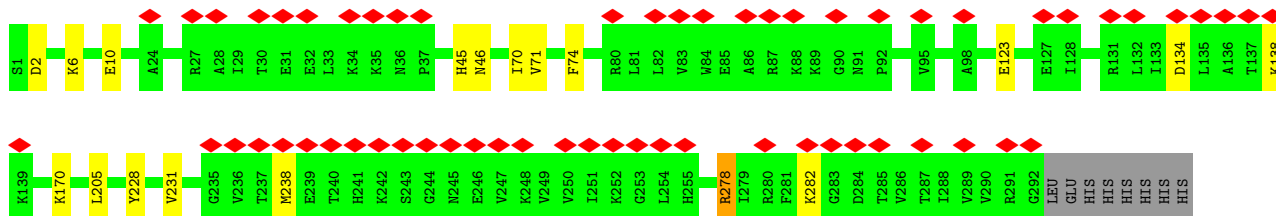
- Molecule 2: C3-A



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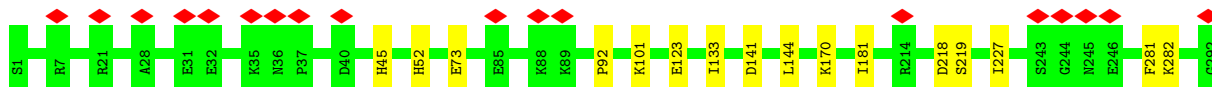
• Molecule 2: C3-A

Chain YN: 20% 91% 6% .



• Molecule 2: C3-A

Chain YP: 6% 92% 5% .



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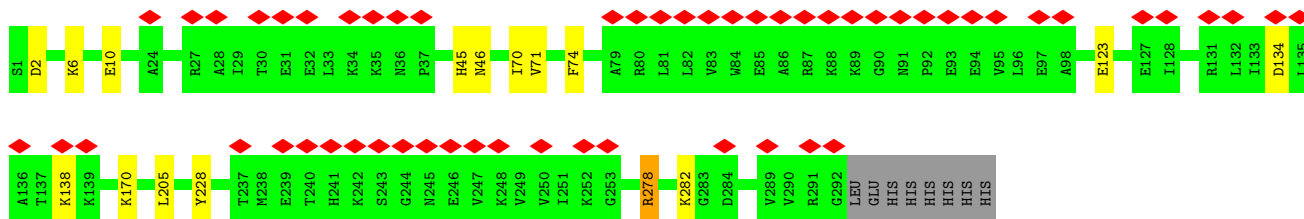
• Molecule 2: C3-A

Chain YR: 92% 5% .



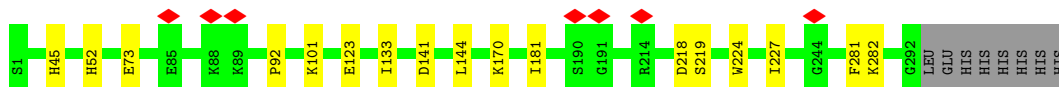
• Molecule 2: C3-A

Chain YT: 19% 92% 5% .

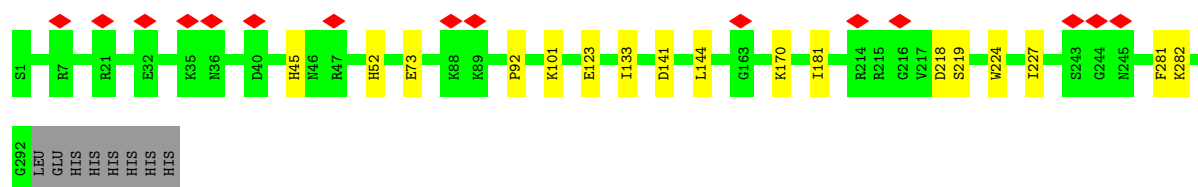


• Molecule 2: C3-A

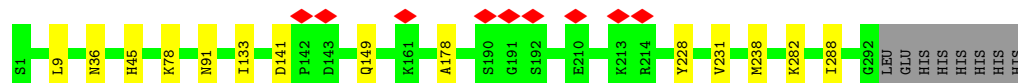
Chain YV: 92% 6% .



• Molecule 2: C3-A



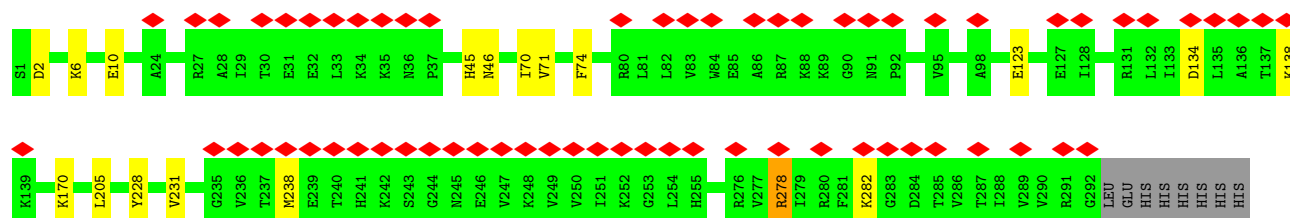
• Molecule 2: C3-A



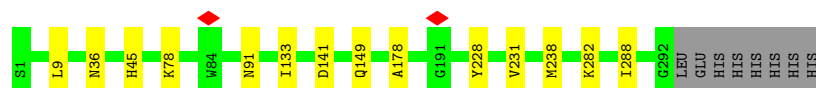
• Molecule 2: C3-A



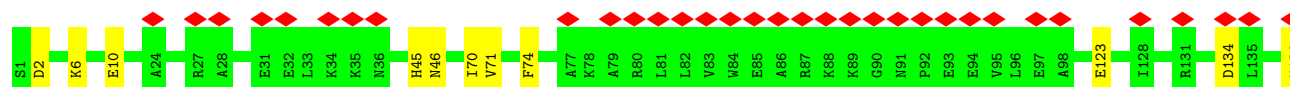
• Molecule 2: C3-A

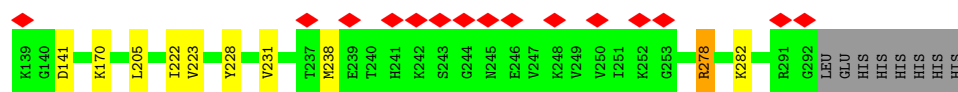


• Molecule 2: C3-A

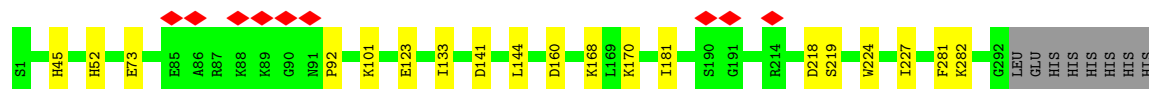


• Molecule 2: C3-A

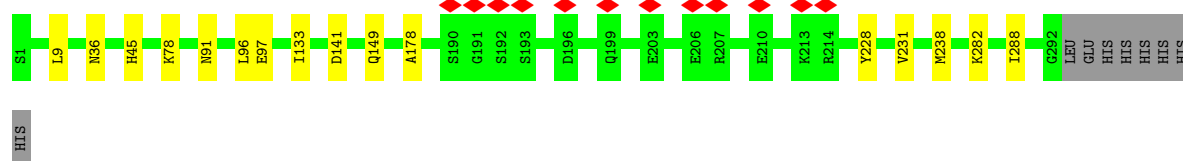




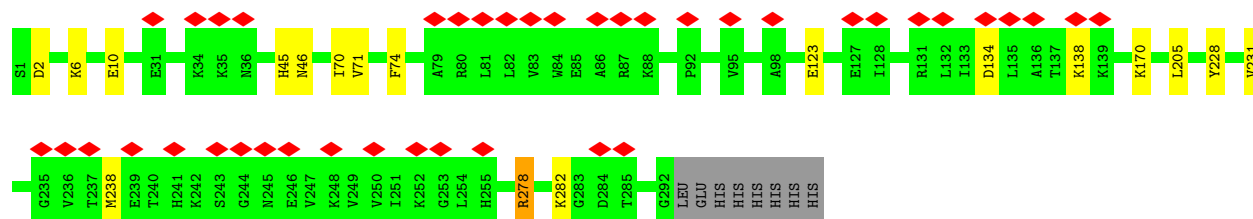
• Molecule 2: C3-A



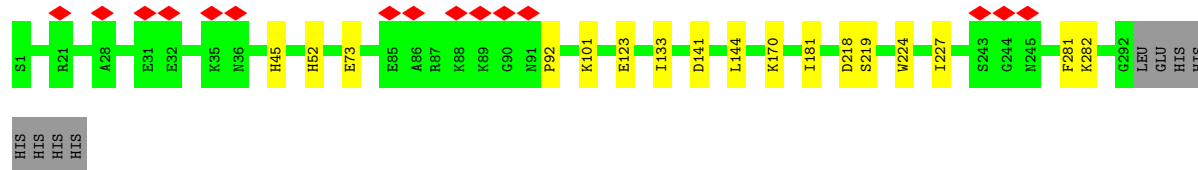
• Molecule 2: C3-A



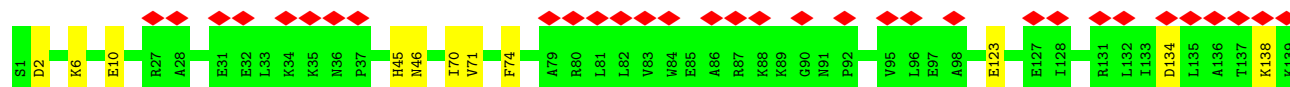
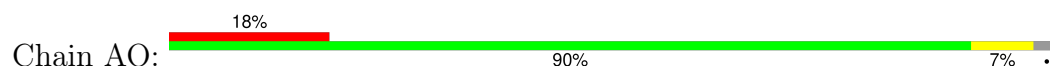
• Molecule 2: C3-A

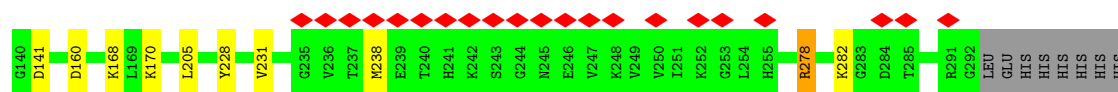


• Molecule 2: C3-A

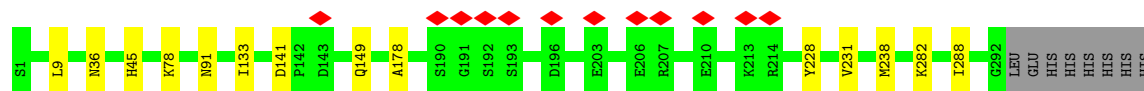


• Molecule 2: C3-A





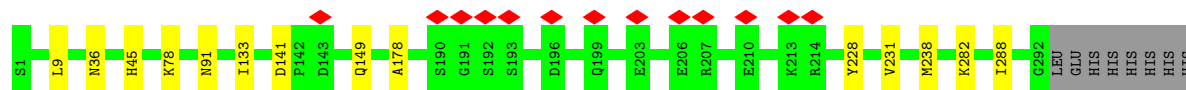
• Molecule 2: C3-A



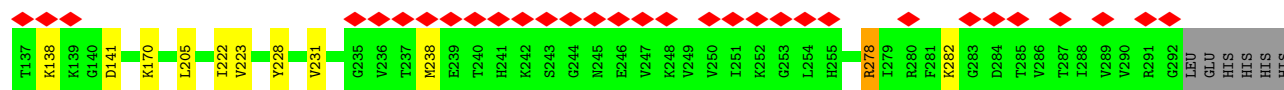
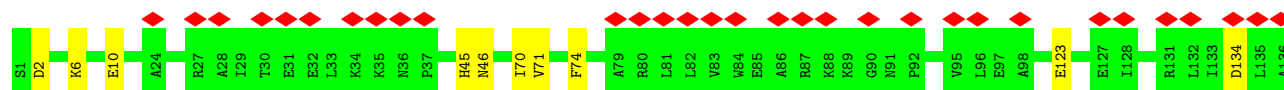
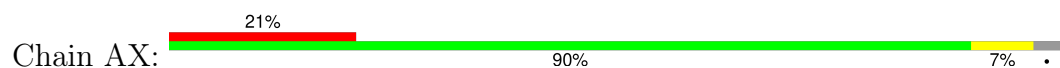
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



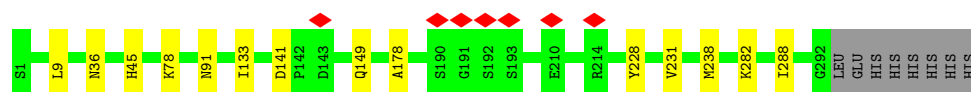
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• Molecule 2: C3-A

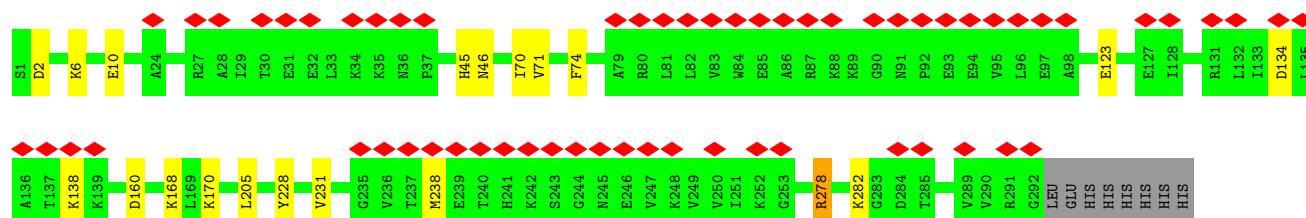


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HIS
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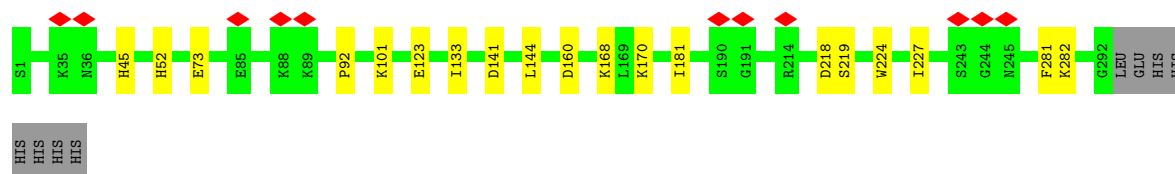
• Molecule 2: C3-A

Chain BB:  93% 5% .

• Molecule 2: C3-A

Chain BD:  20% 91% 6% .


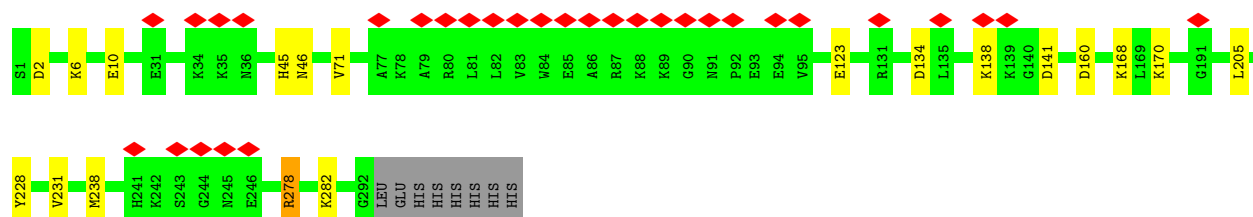
• Molecule 2: C3-A

Chain BF:  91% 6% .

• Molecule 2: C3-A

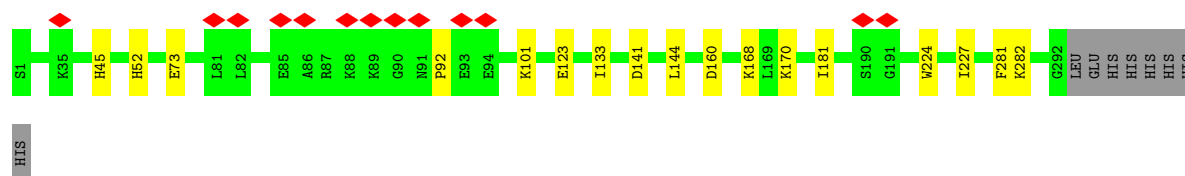
Chain BH:  93% 5% .

• Molecule 2: C3-A

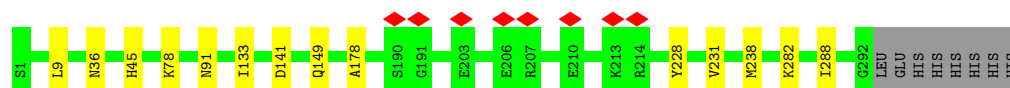
Chain BJ:  10% 91% 6% .

• Molecule 2: C3-A

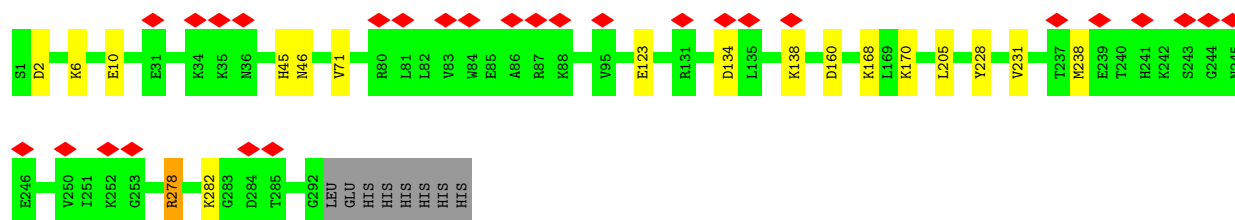
Chain BL:  92% 6% .



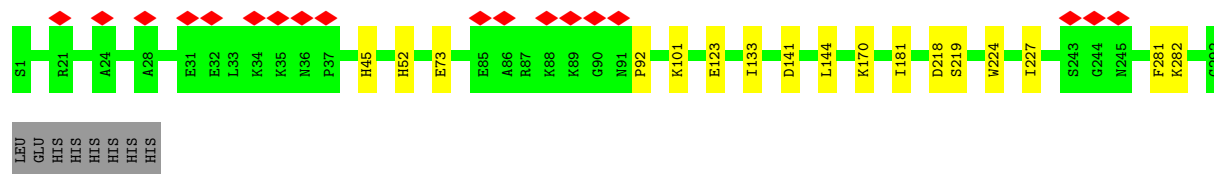
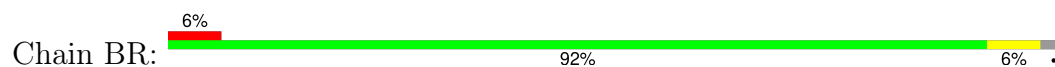
• Molecule 2: C3-A



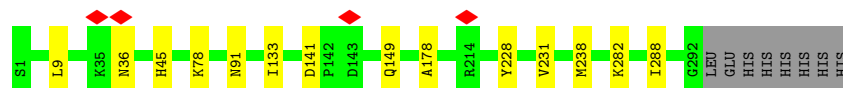
• Molecule 2: C3-A



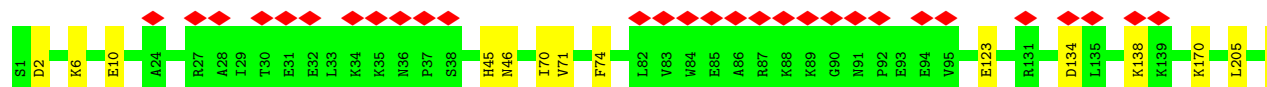
• Molecule 2: C3-A

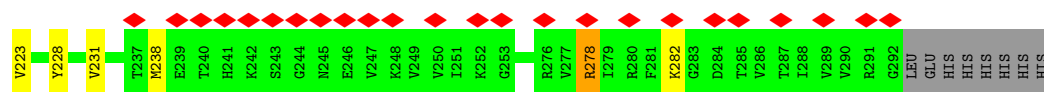


• Molecule 2: C3-A

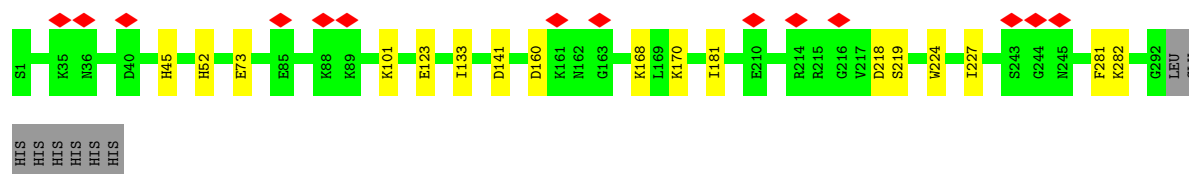


• Molecule 2: C3-A

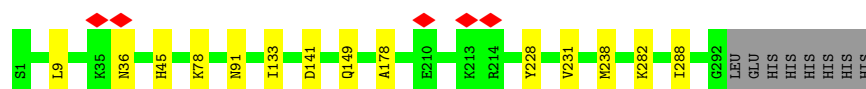




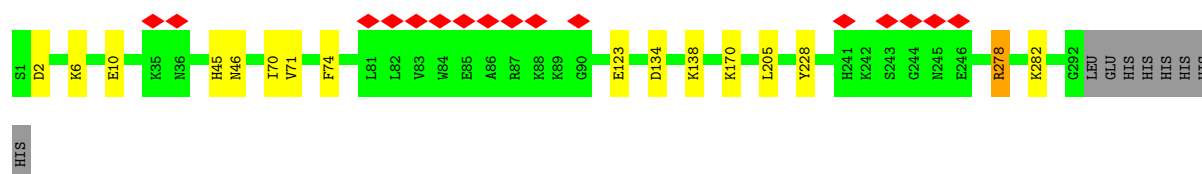
• Molecule 2: C3-A



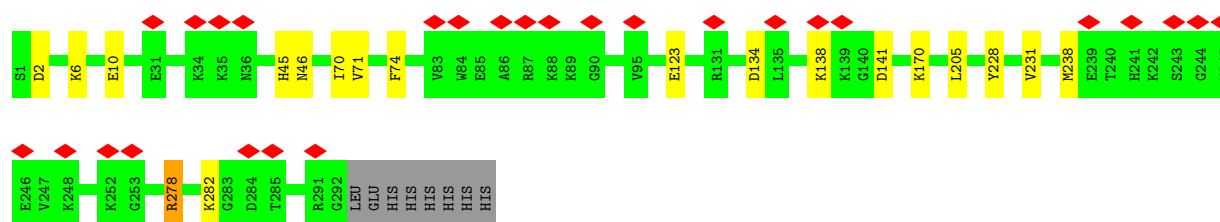
• Molecule 2: C3-A



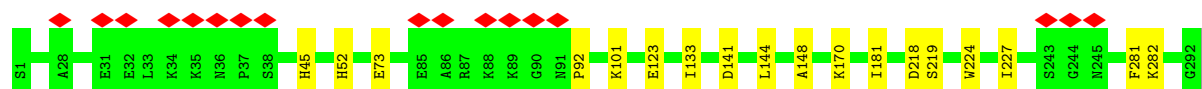
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



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• Molecule 2: C3-A

Chain CF:  92% 5%



• Molecule 2: C3-A

Chain CH:  10% 90% 7%



• Molecule 2: C3-A

Chain CJ:  92% 6%



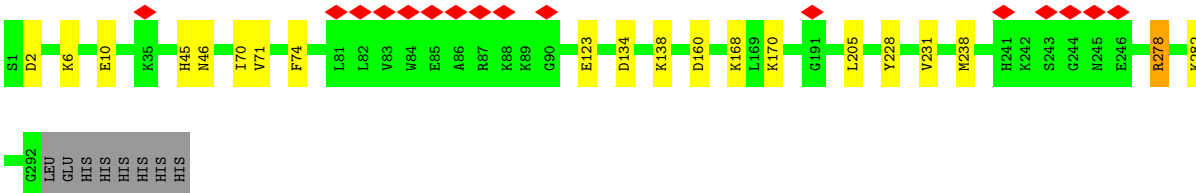
• Molecule 2: C3-A

Chain CL:  93% 5%



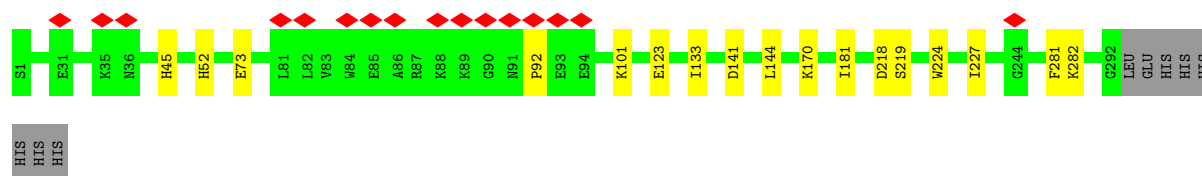
• Molecule 2: C3-A

Chain CN:  5% 91% 6%



• Molecule 2: C3-A

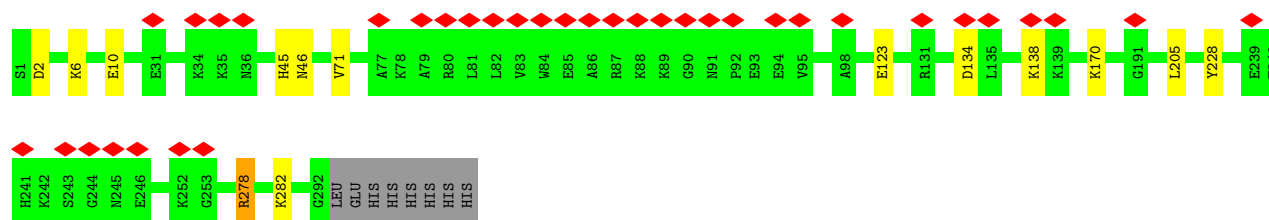
Chain CP:  5% 92% 6%



• Molecule 2: C3-A



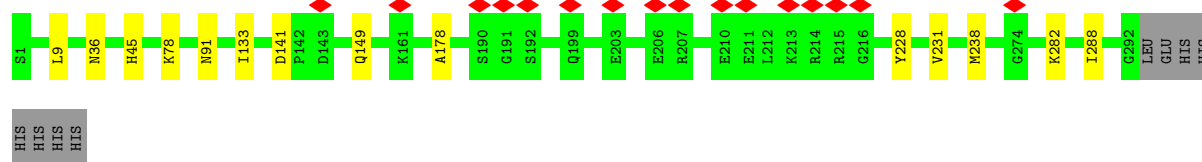
• Molecule 2: C3-A



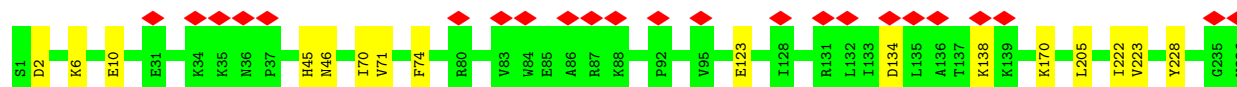
• Molecule 2: C3-A

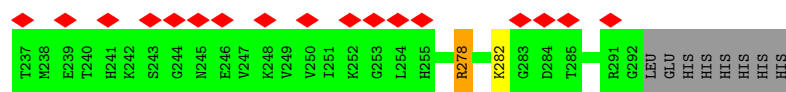


• Molecule 2: C3-A

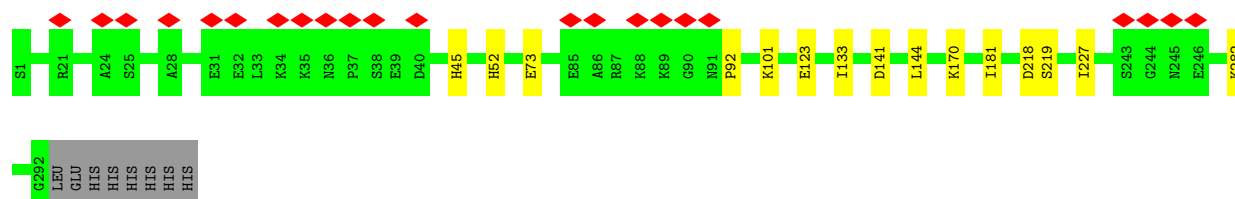


• Molecule 2: C3-A





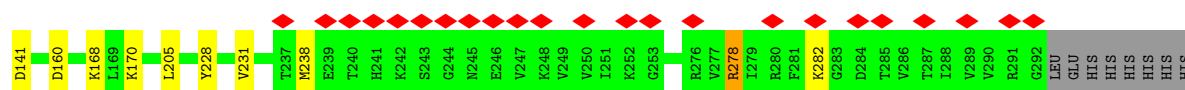
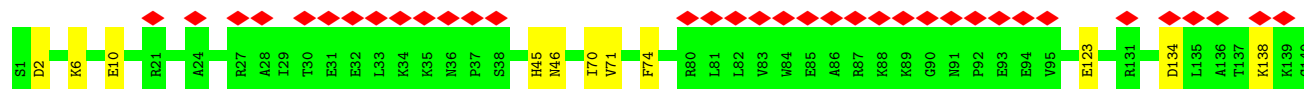
• Molecule 2: C3-A



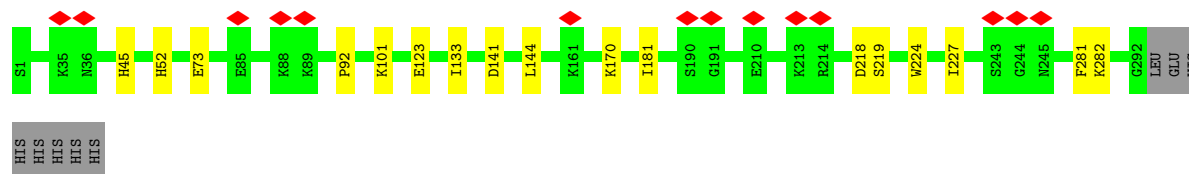
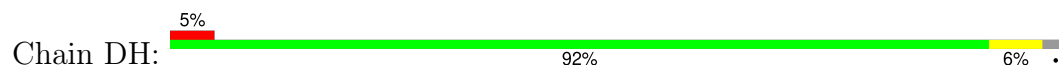
• Molecule 2: C3-A



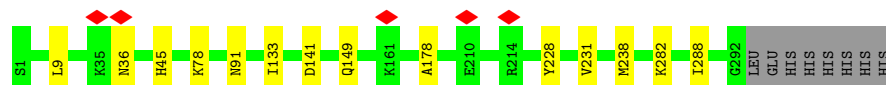
• Molecule 2: C3-A



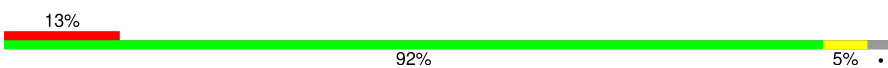
• Molecule 2: C3-A

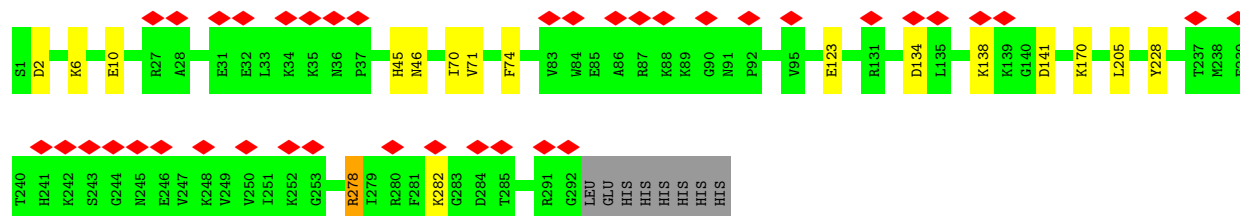


• Molecule 2: C3-A



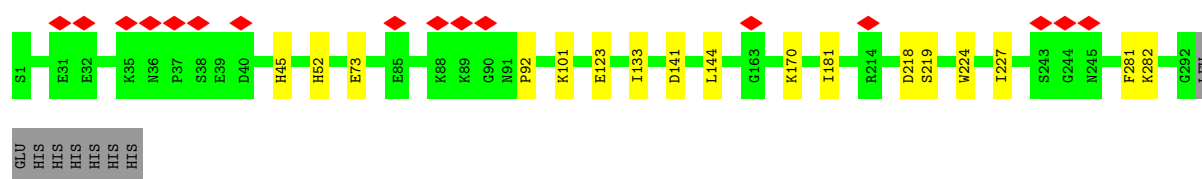
- Molecule 2: C3-A

Chain DL: 



- Molecule 2: C3-A

Chain DN: 



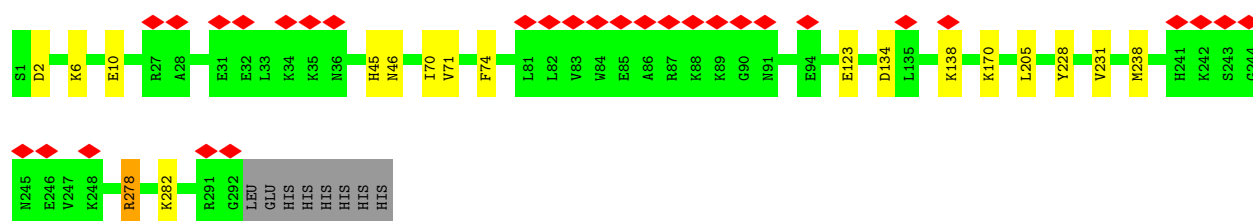
- Molecule 2: C3-A

Chain DP: 



- Molecule 2: C3-A

Chain DR: 



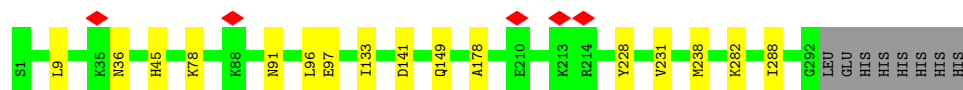
- Molecule 2: C3-A

Chain DT: 

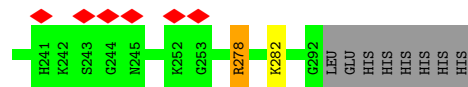
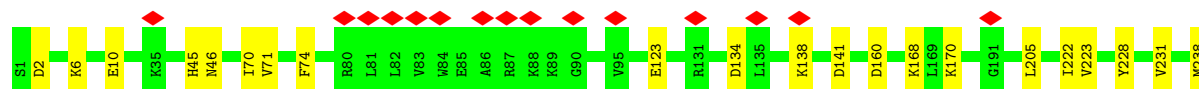
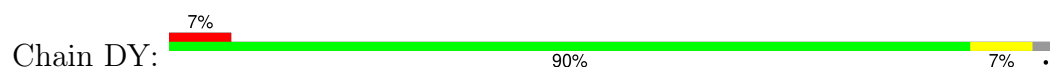


- Molecule 2: C3-A

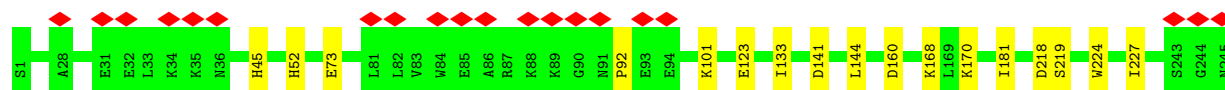
Chain DW: 



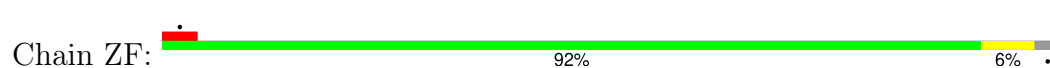
• Molecule 2: C3-A



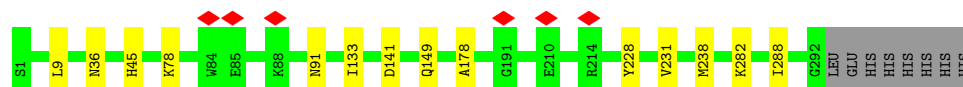
• Molecule 2: C3-A



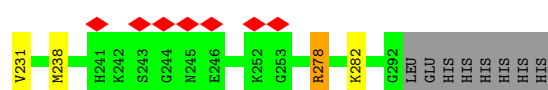
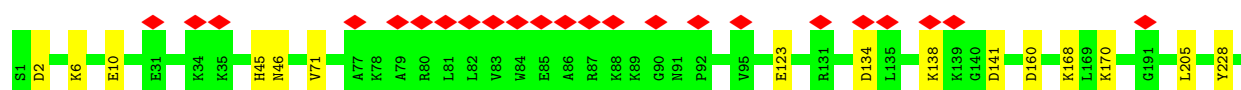
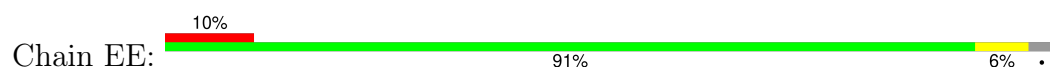
• Molecule 2: C3-A



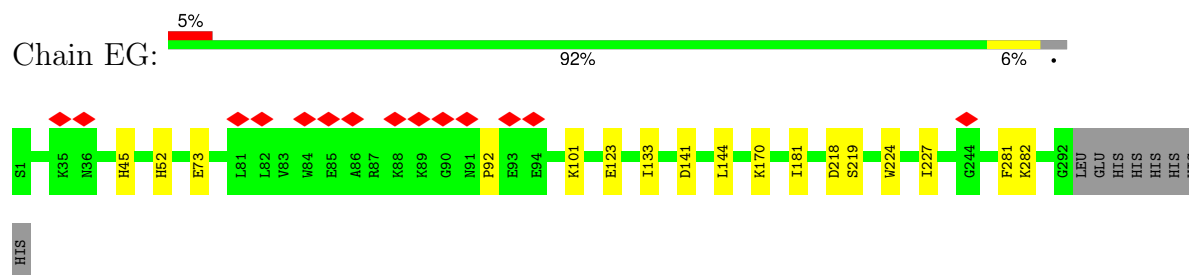
• Molecule 2: C3-A



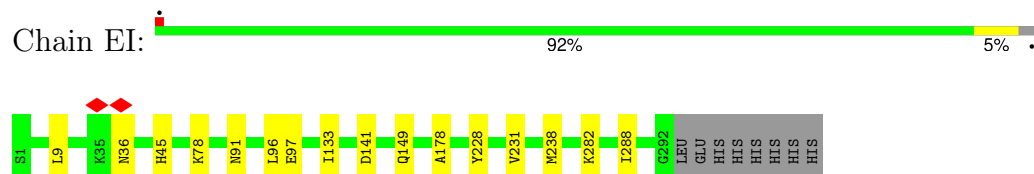
• Molecule 2: C3-A



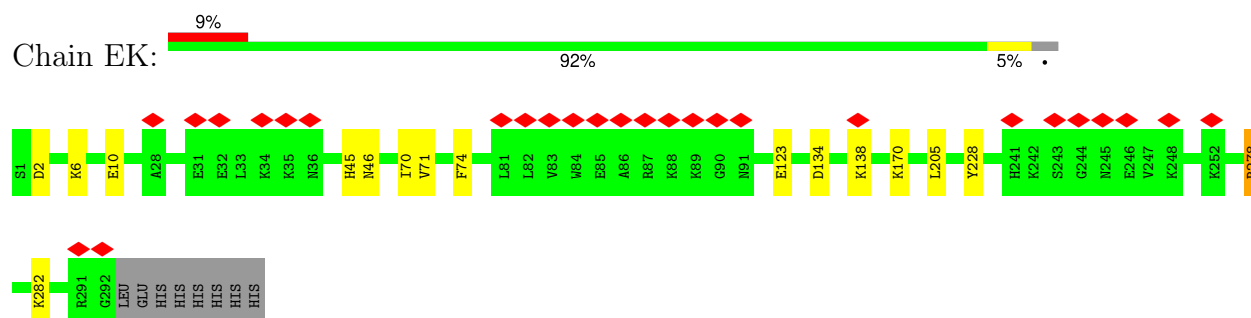
- Molecule 2: C3-A



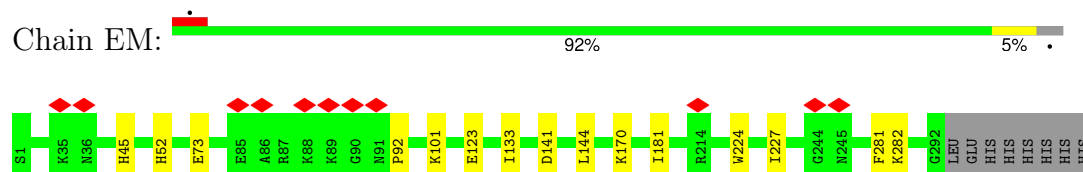
- Molecule 2: C3-A



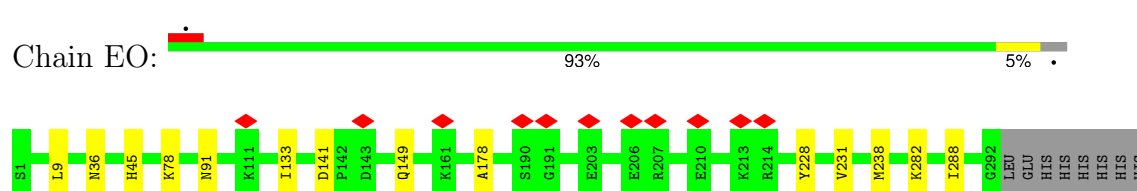
- Molecule 2: C3-A



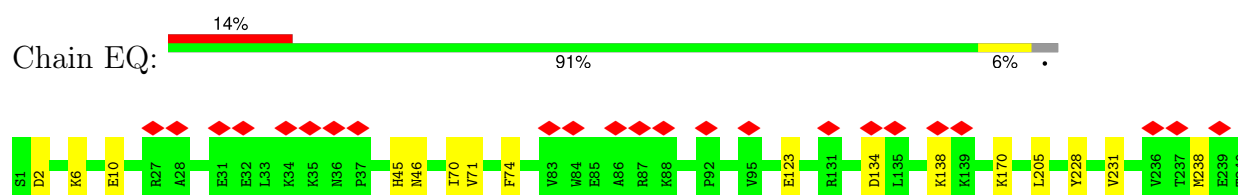
- Molecule 2: C3-A

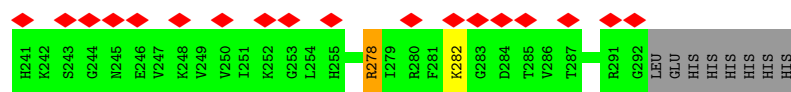


- Molecule 2: C3-A

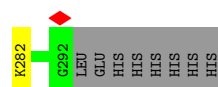
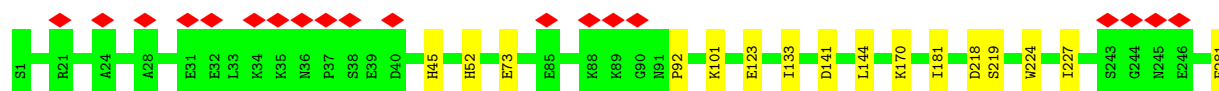
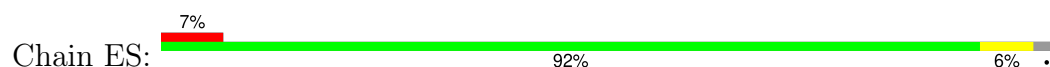


- Molecule 2: C3-A





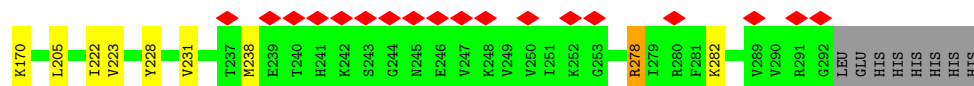
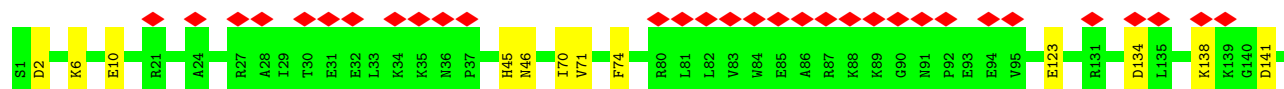
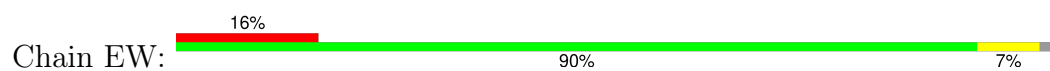
• Molecule 2: C3-A



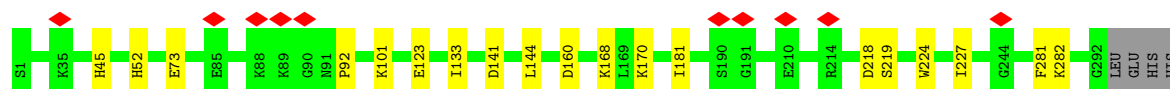
• Molecule 2: C3-A



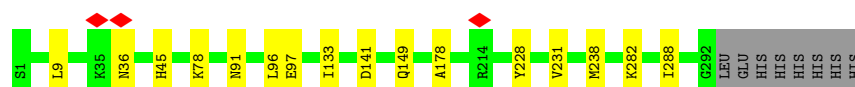
• Molecule 2: C3-A



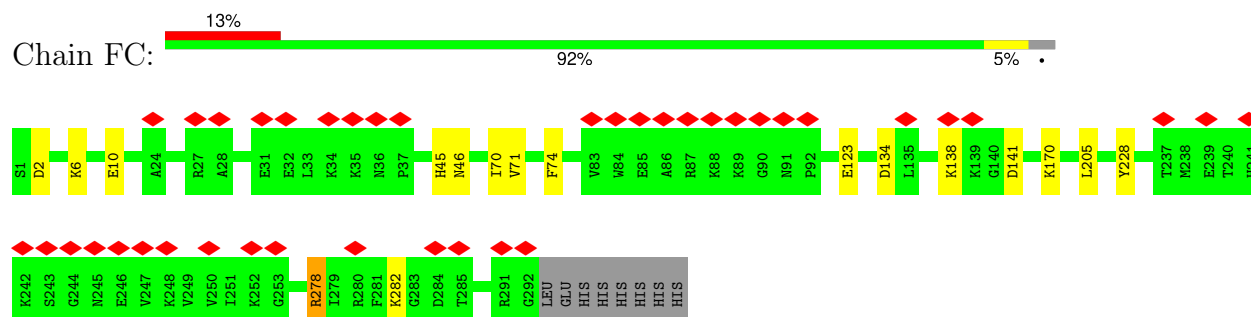
• Molecule 2: C3-A



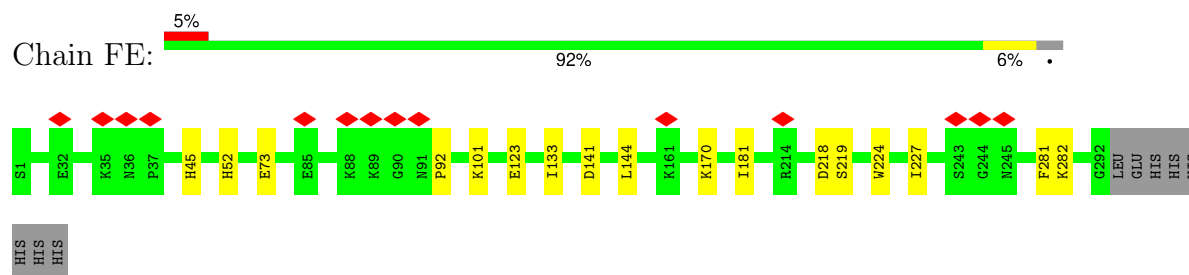
• Molecule 2: C3-A



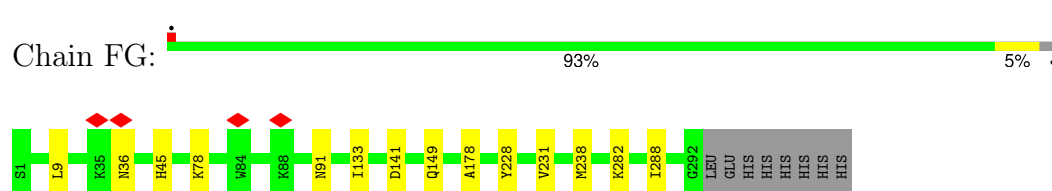
• Molecule 2: C3-A



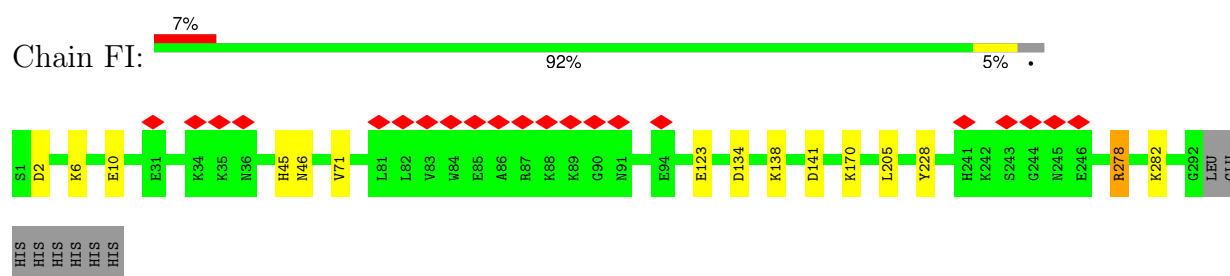
• Molecule 2: C3-A



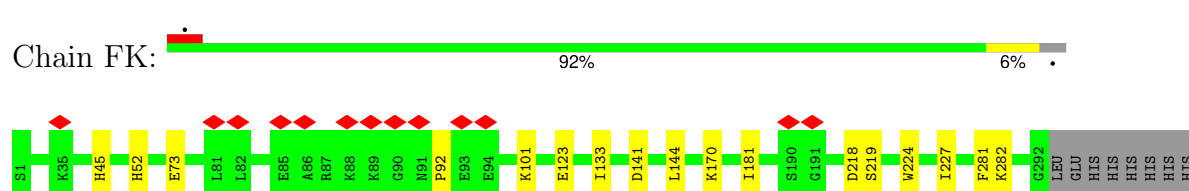
• Molecule 2: C3-A



• Molecule 2: C3-A

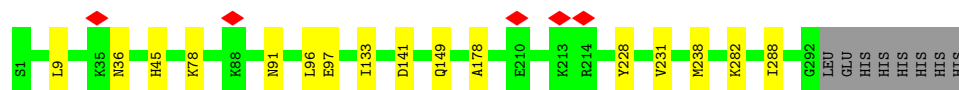


• Molecule 2: C3-A

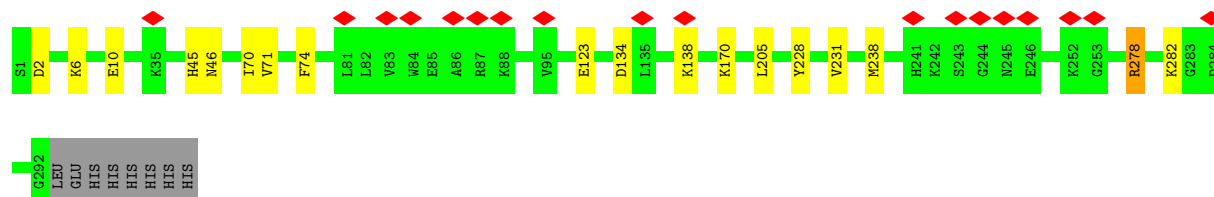


• Molecule 2: C3-A

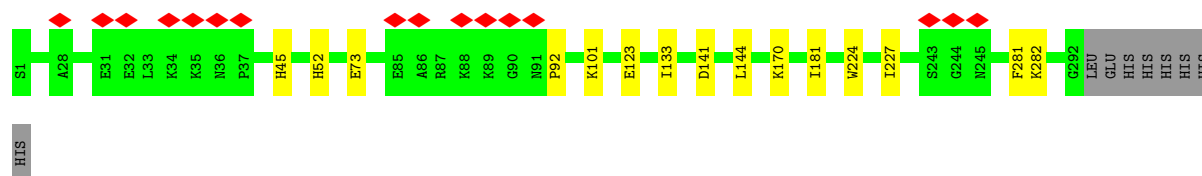




- Molecule 2: C3-A



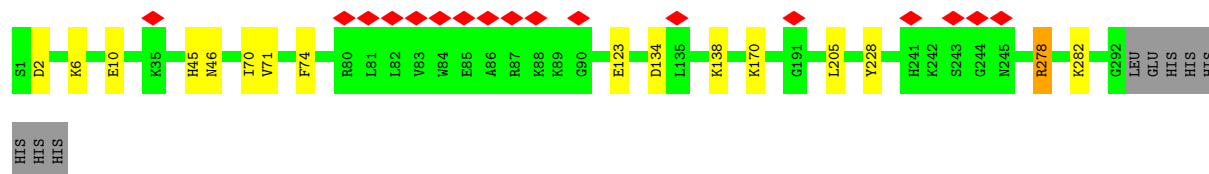
- Molecule 2: C3-A



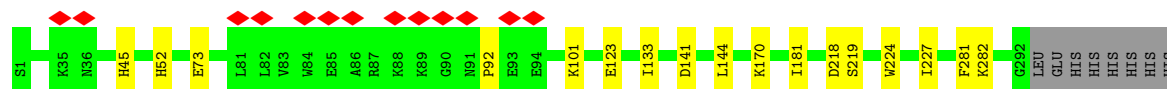
- Molecule 2: C3-A



- Molecule 2: C3-A



- Molecule 2: C3-A



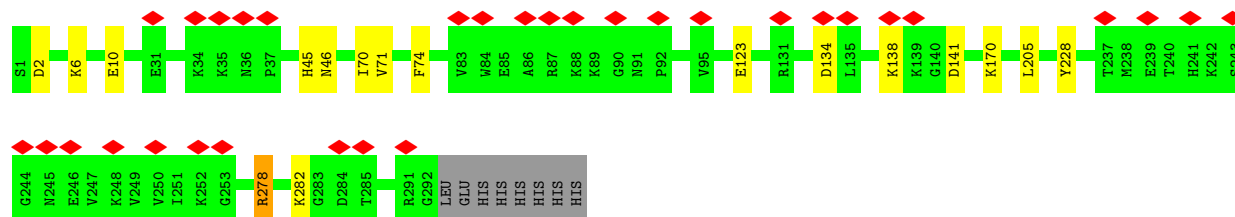
- Molecule 2: C3-A

Chain FY:  92% 5% .



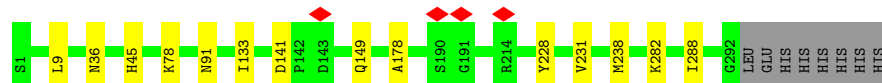
• Molecule 2: C3-A

Chain GA:  11% 92% 5% .



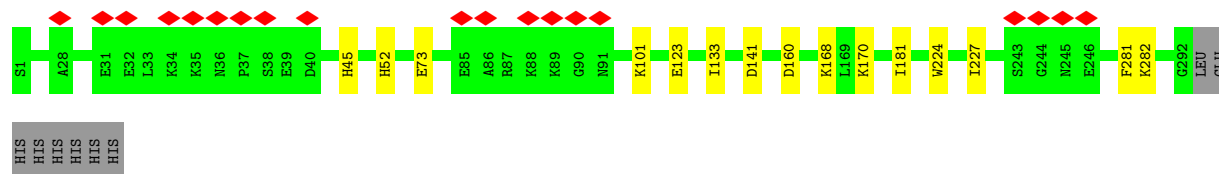
• Molecule 2: C3-A

Chain ZH:  93% 5% .



• Molecule 2: C3-A

Chain GC:  6% 92% 5% .



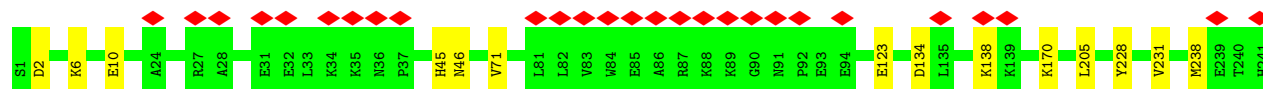
• Molecule 2: C3-A

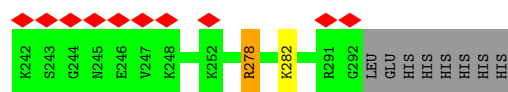
Chain GE:  92% 5% .



• Molecule 2: C3-A

Chain GG:  12% 92% 5% .





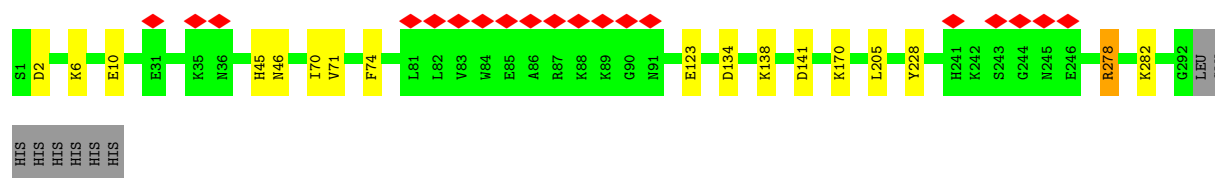
• Molecule 2: C3-A



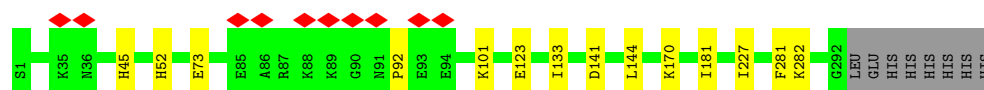
• Molecule 2: C3-A



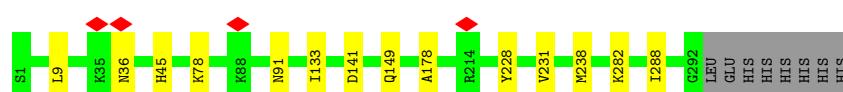
• Molecule 2: C3-A



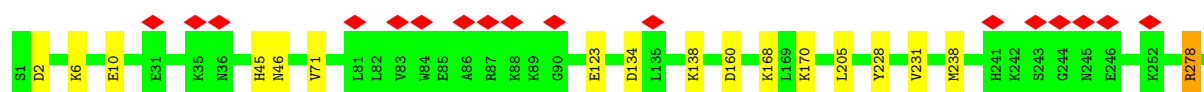
• Molecule 2: C3-A

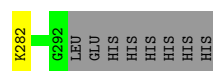


• Molecule 2: C3-A



• Molecule 2: C3-A





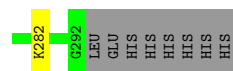
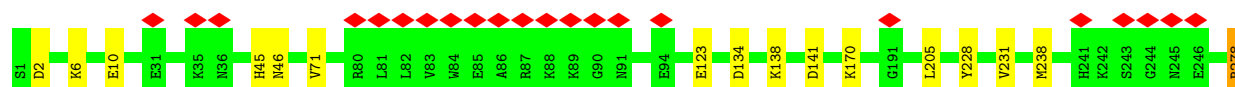
- Molecule 2: C3-A



- Molecule 2: C3-A



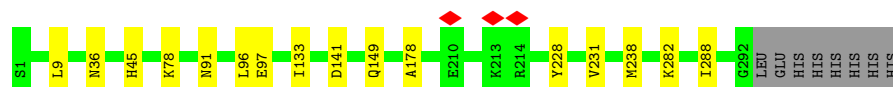
- Molecule 2: C3-A



- Molecule 2: C3-A

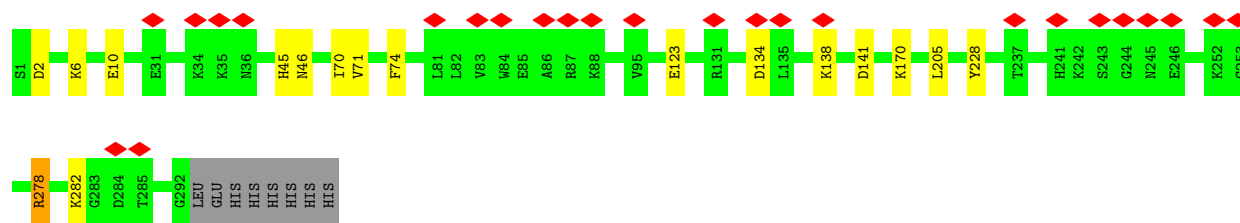


- Molecule 2: C3-A

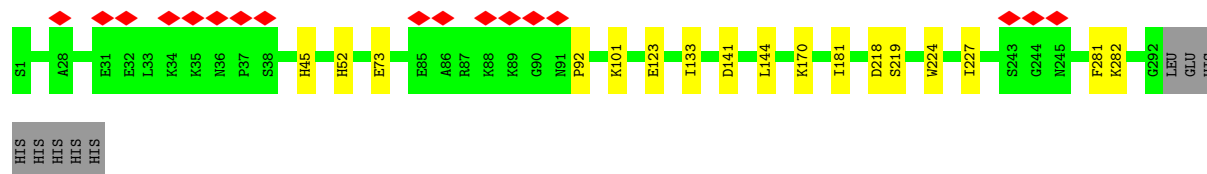


- Molecule 2: C3-A





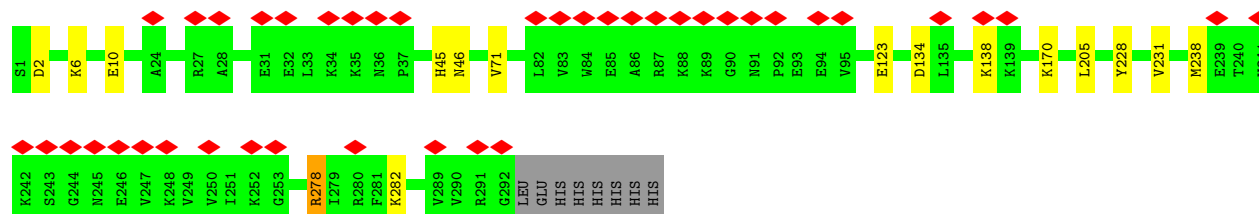
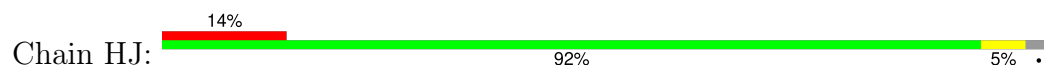
- Molecule 2: C3-A



- Molecule 2: C3-A



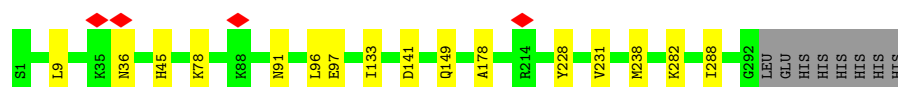
- Molecule 2: C3-A



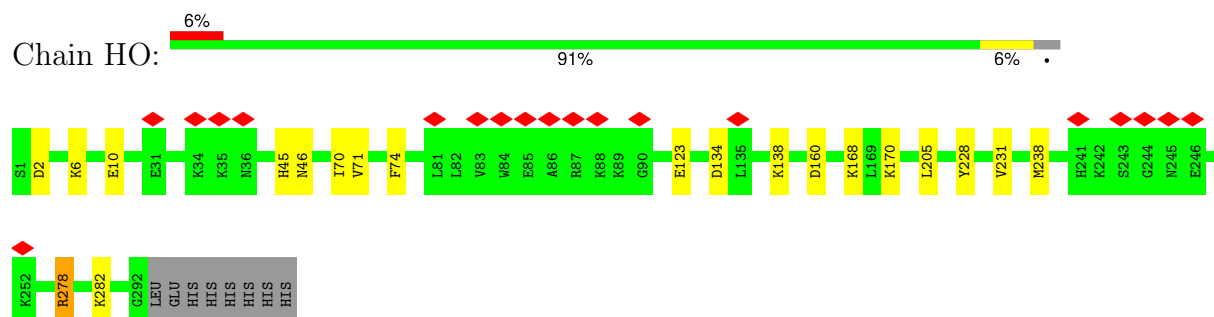
- Molecule 2: C3-A



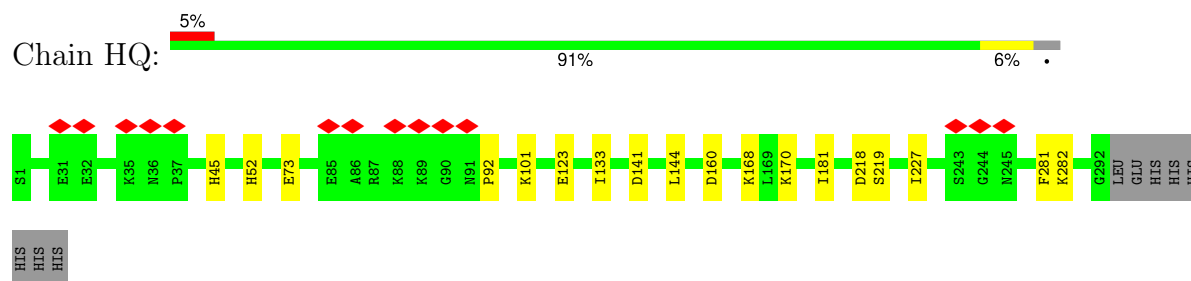
- Molecule 2: C3-A



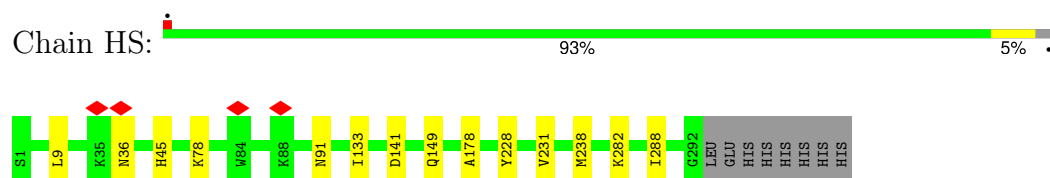
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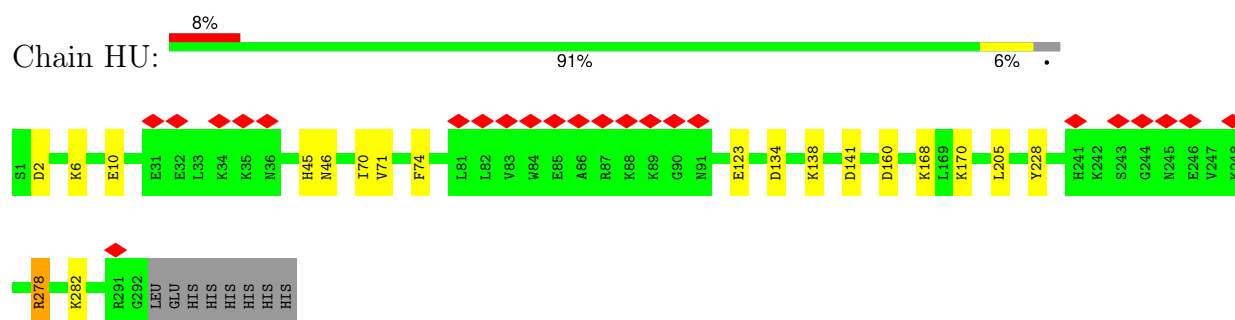
- Molecule 2: C3-A



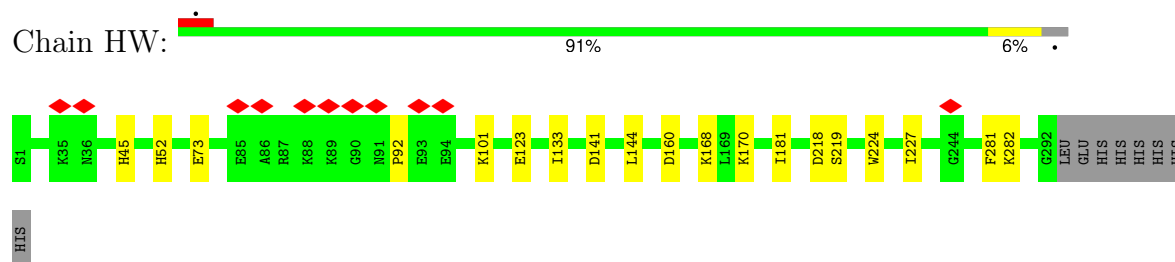
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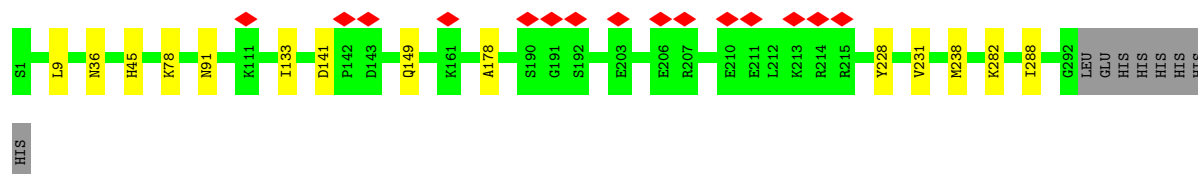
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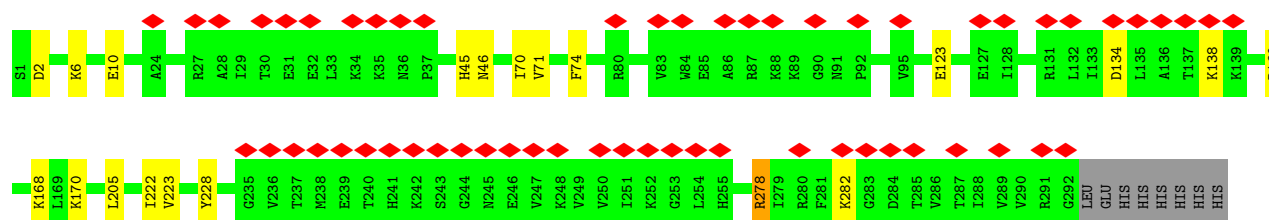
- Molecule 2: C3-A



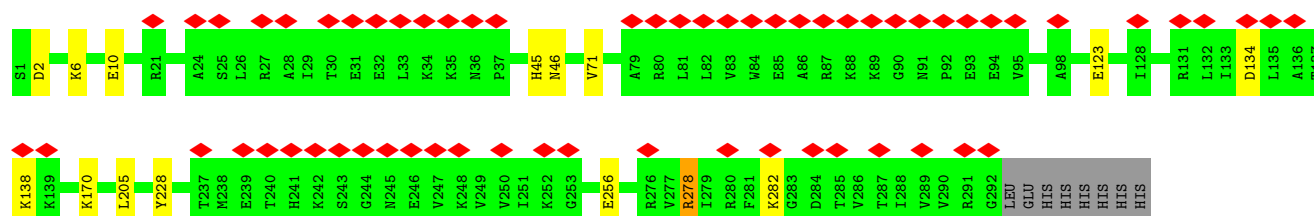
- Molecule 2: C3-A



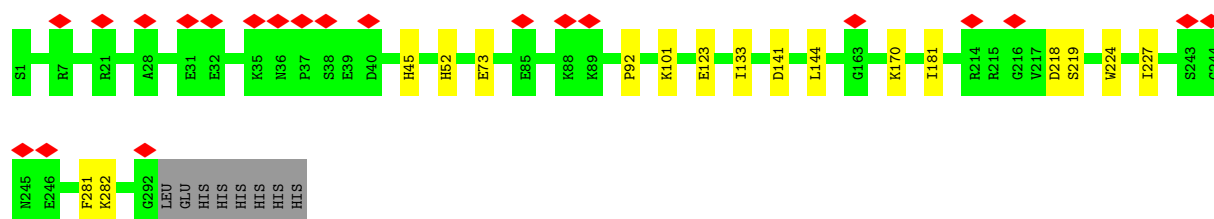
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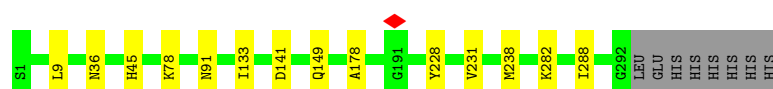
- Molecule 2: C3-A



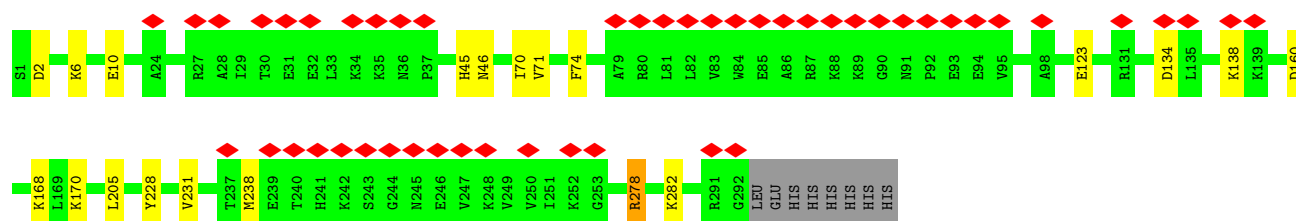
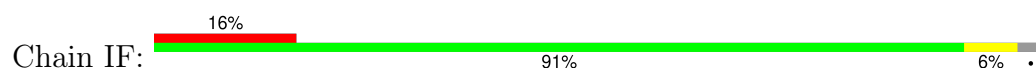
- Molecule 2: C3-A



- Molecule 2: C3-A



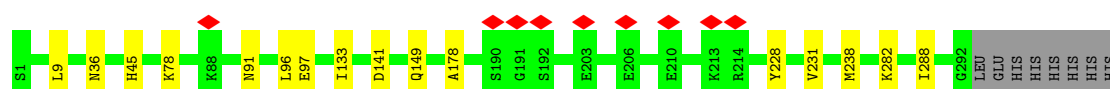
- Molecule 2: C3-A



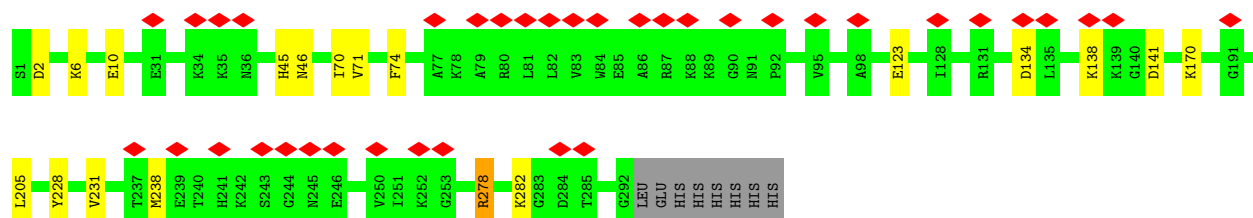
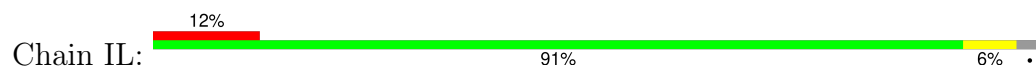
- Molecule 2: C3-A



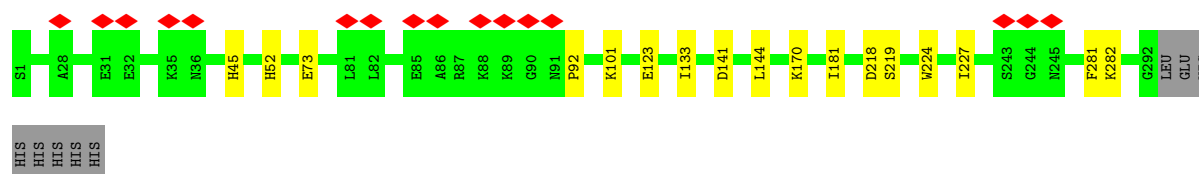
- Molecule 2: C3-A



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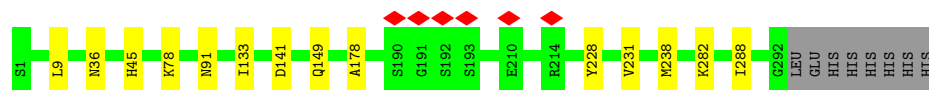


- Molecule 2: C3-A

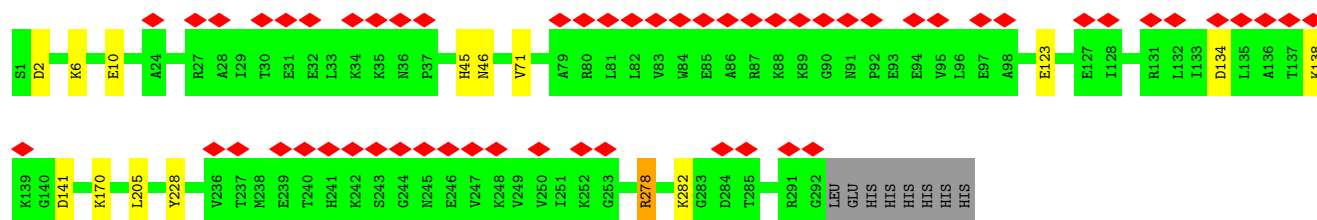


- Molecule 2: C3-A

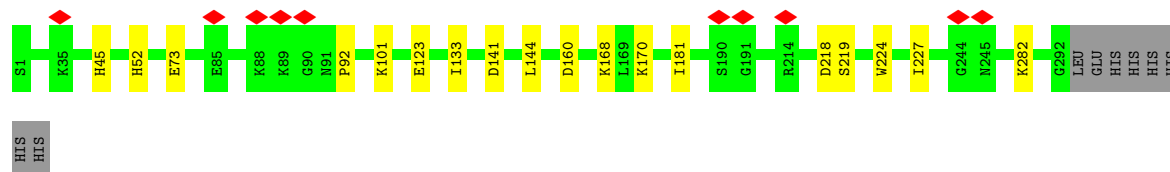




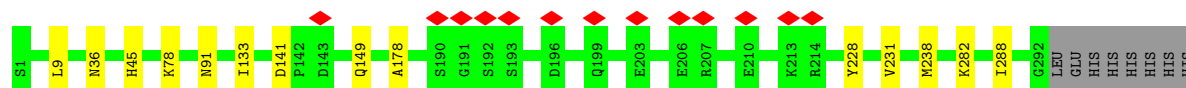
- Molecule 2: C3-A



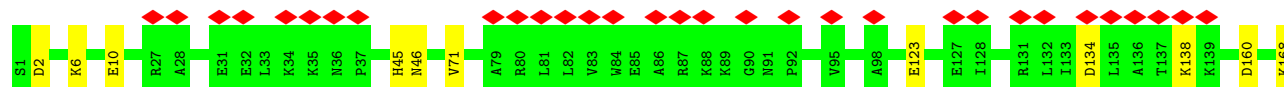
- Molecule 2: C3-A



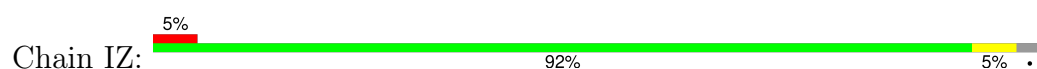
- Molecule 2: C3-A



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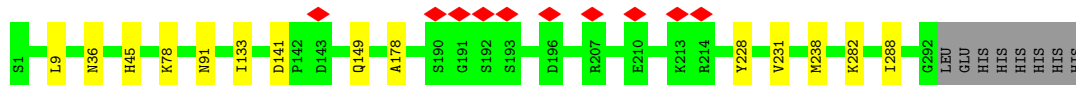
- Molecule 2: C3-A



HIS
HIS
HIS

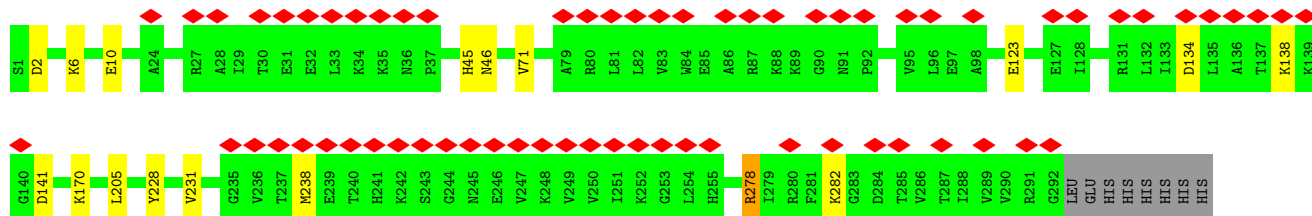
• Molecule 2: C3-A

Chain JB:  93% 5%



• Molecule 2: C3-A

Chain JD:  22% 92% 5%



• Molecule 2: C3-A

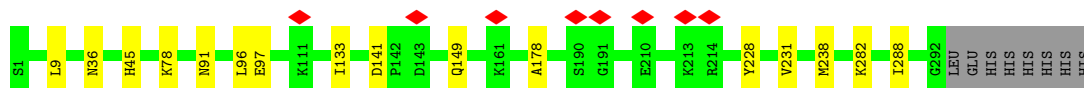
Chain JF:  92% 6%




HIS
HIS
HIS
HIS
HIS

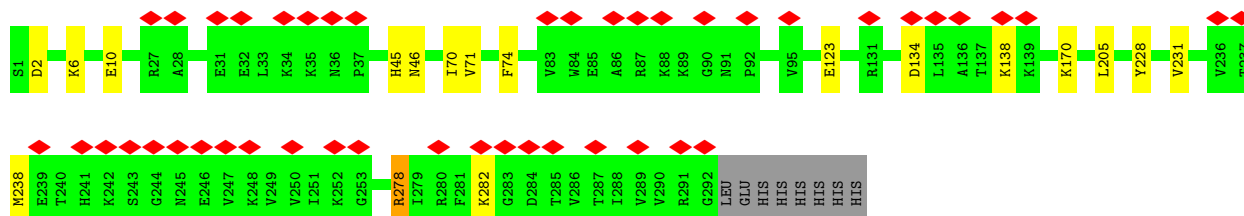
• Molecule 2: C3-A

Chain JH:  92% 5%

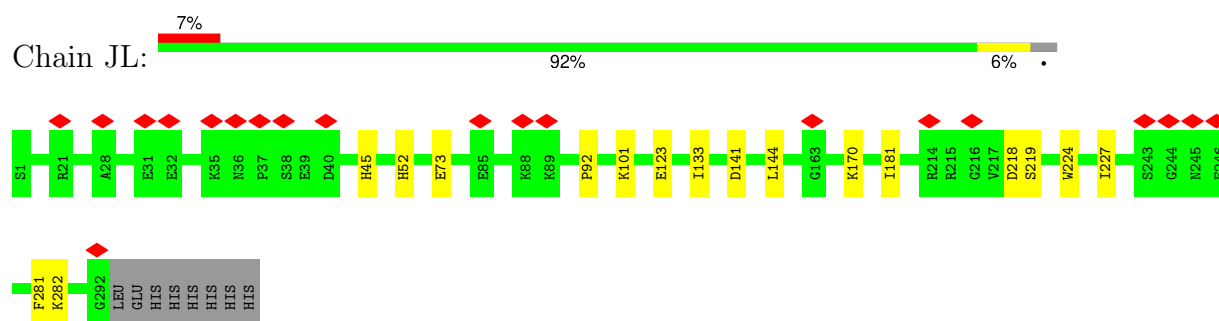


• Molecule 2: C3-A

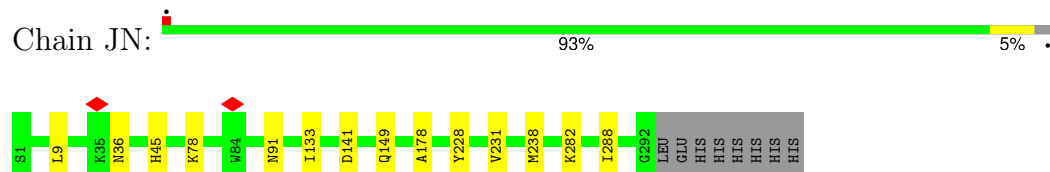
Chain JJ:  15% 91% 6%



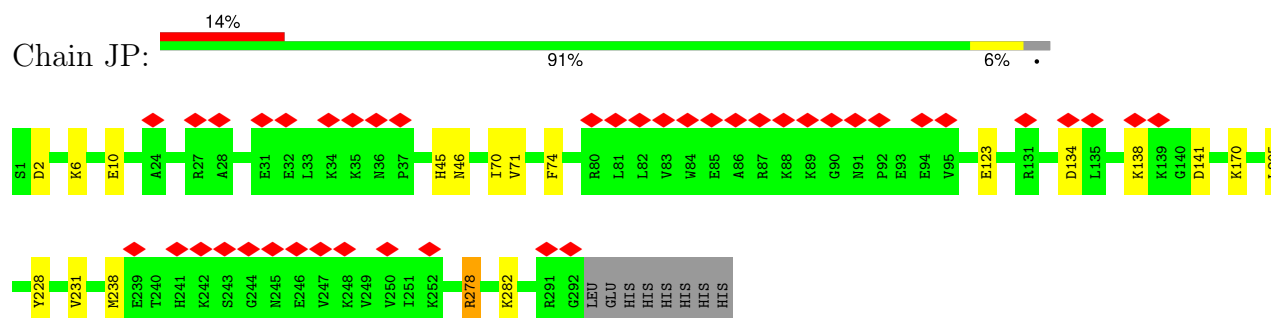
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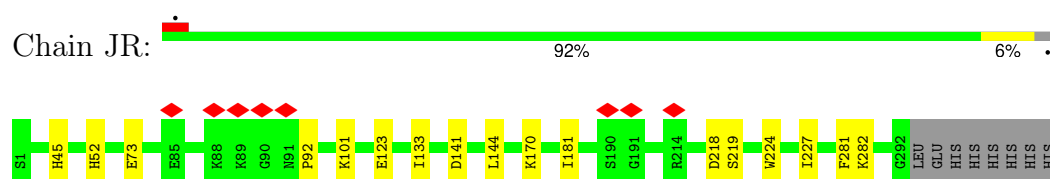
- Molecule 2: C3-A



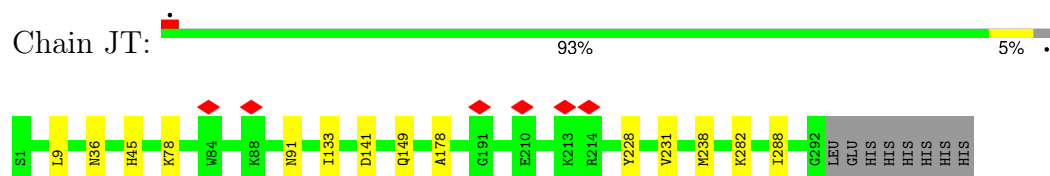
- Molecule 2: C3-A



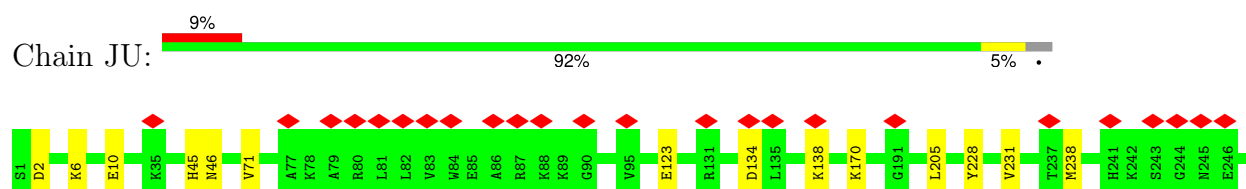
- Molecule 2: C3-A

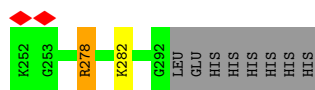


- Molecule 2: C3-A

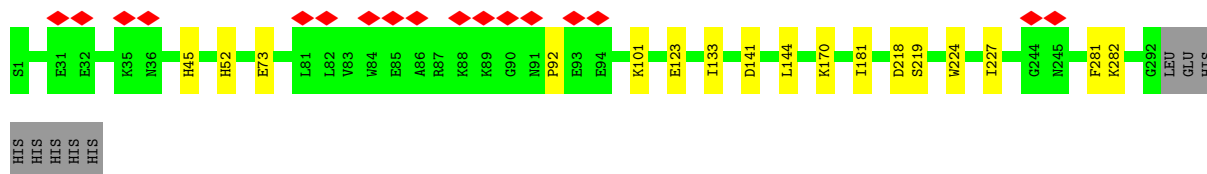


- Molecule 2: C3-A

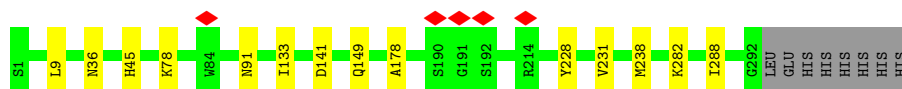




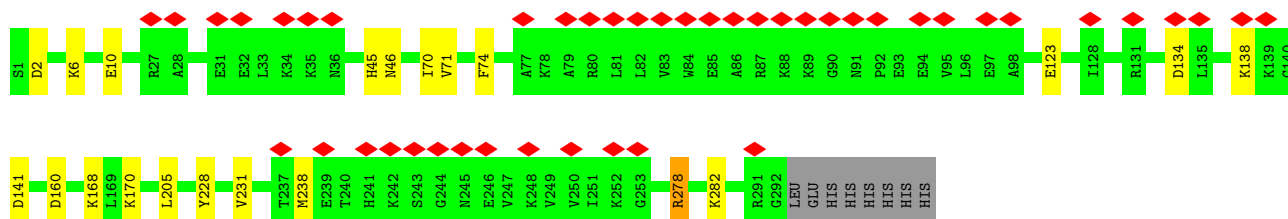
- Molecule 2: C3-A



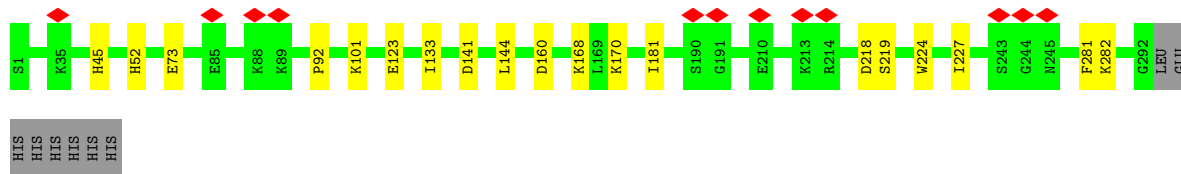
- Molecule 2: C3-A



- Molecule 2: C3-A



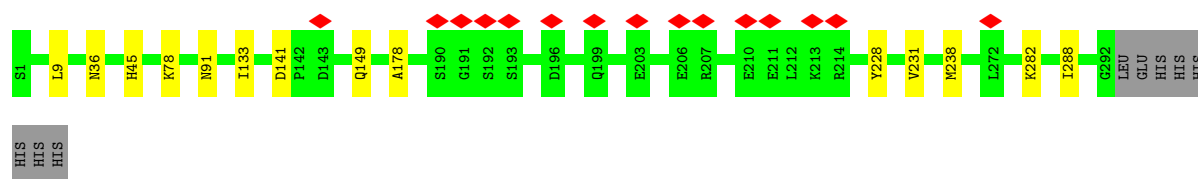
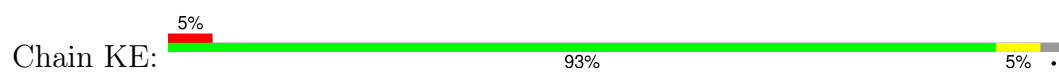
- Molecule 2: C3-A



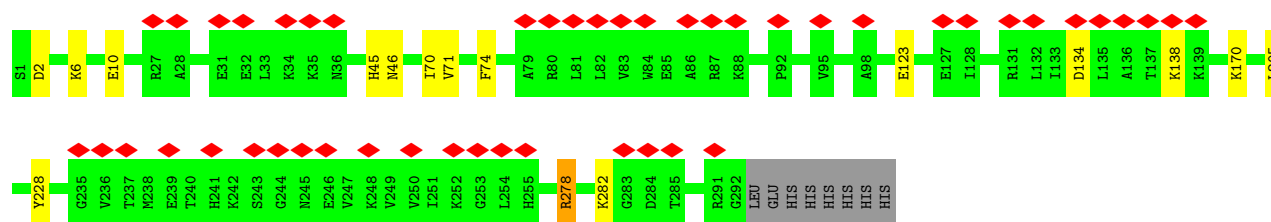
- Molecule 2: C3-A



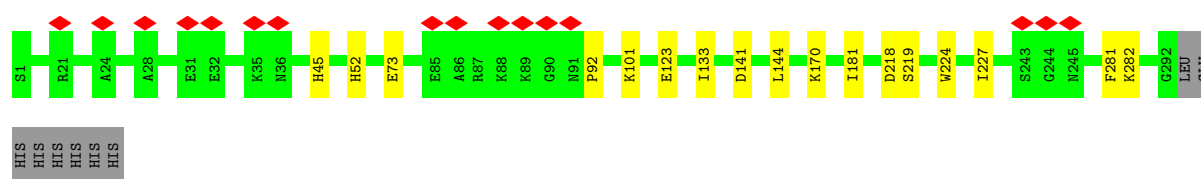
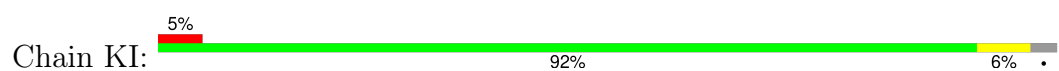
- Molecule 2: C3-A



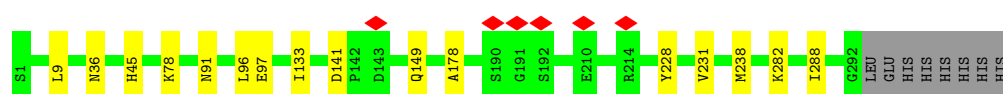
- Molecule 2: C3-A



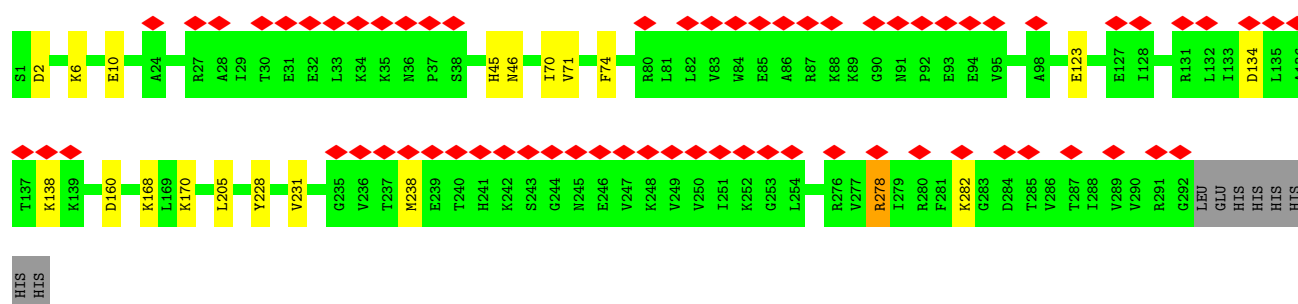
- Molecule 2: C3-A



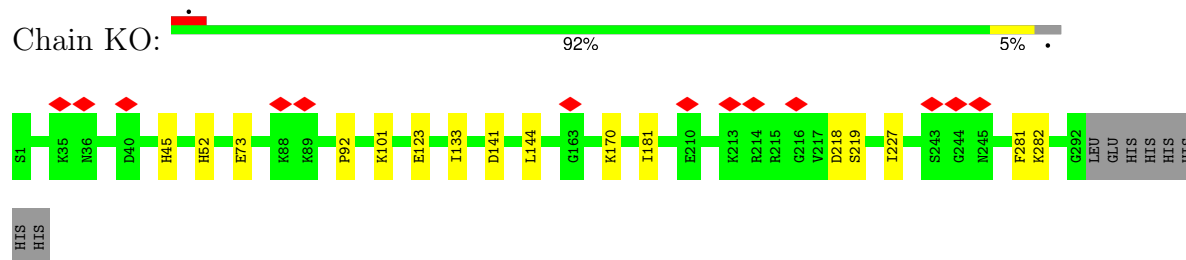
- Molecule 2: C3-A



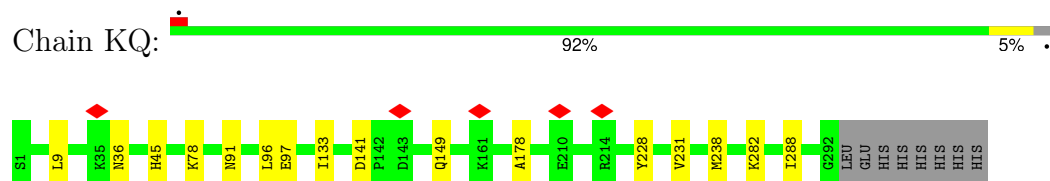
- Molecule 2: C3-A



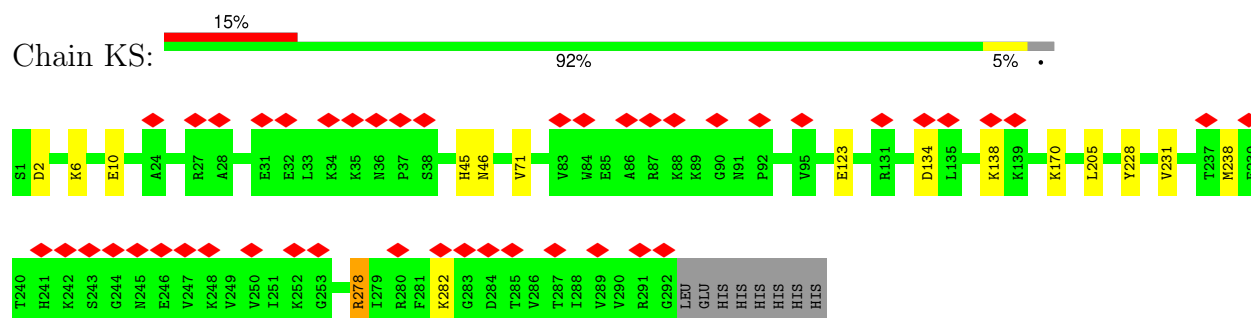
• Molecule 2: C3-A



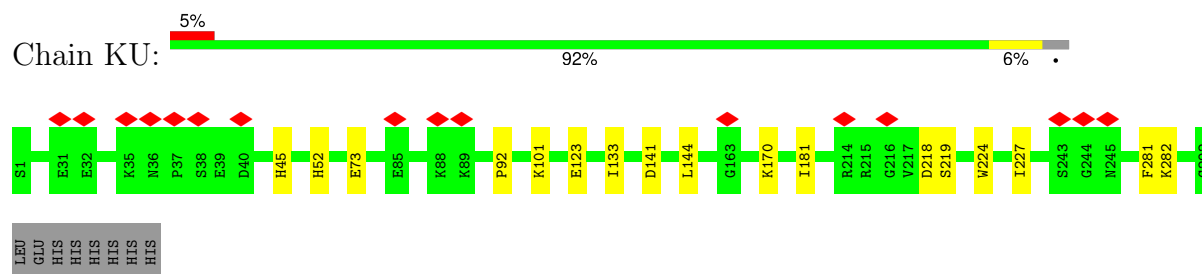
• Molecule 2: C3-A



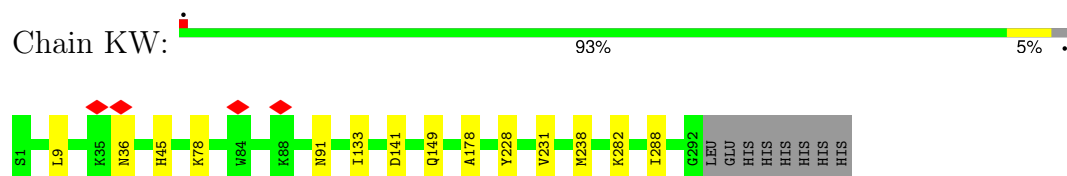
• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A



• Molecule 2: C3-A





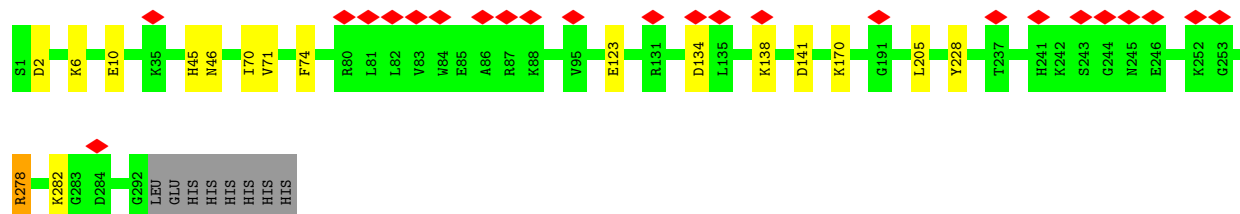
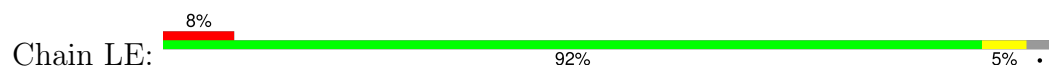
• Molecule 2: C3-A



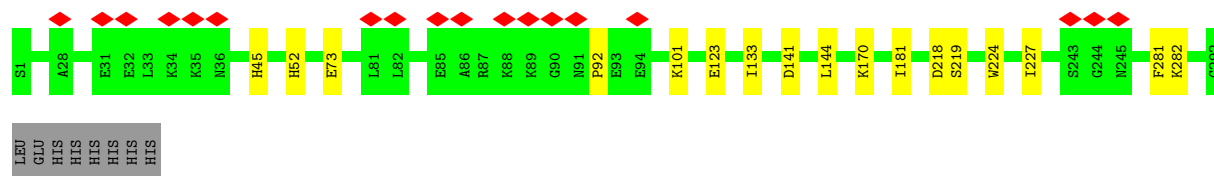
• Molecule 2: C3-A



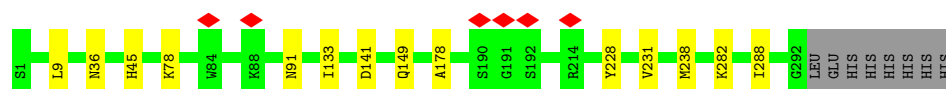
• Molecule 2: C3-A



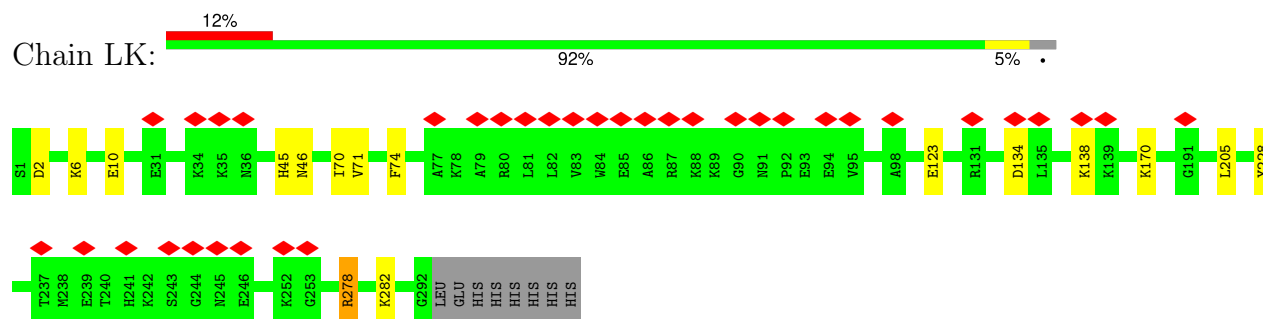
• Molecule 2: C3-A



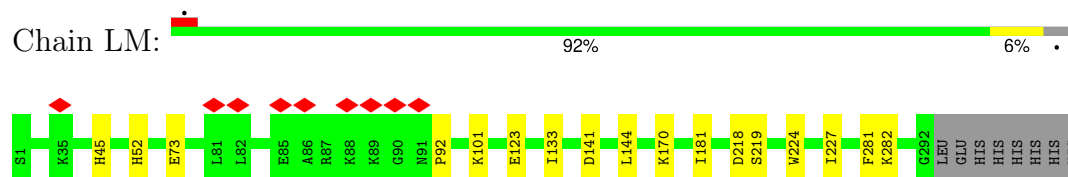
• Molecule 2: C3-A



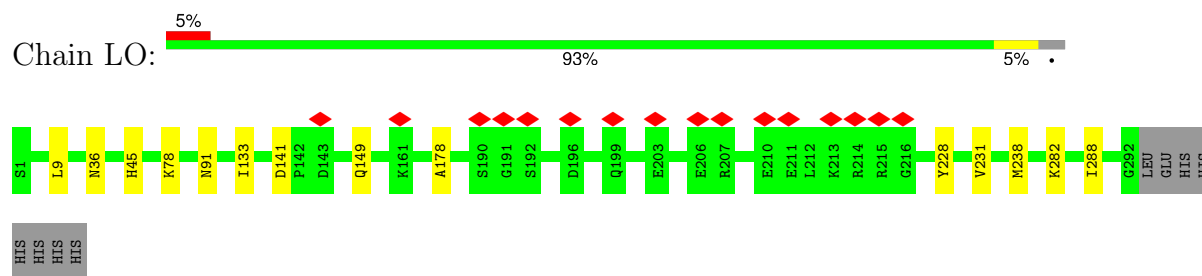
• Molecule 2: C3-A



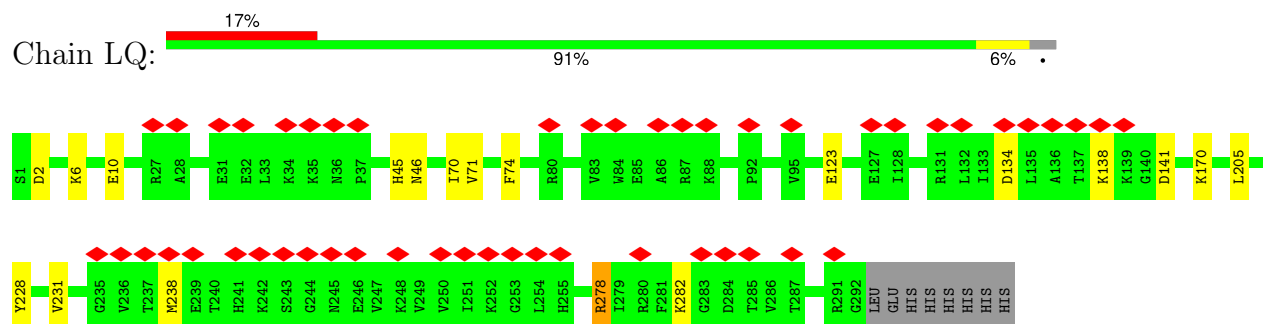
• Molecule 2: C3-A



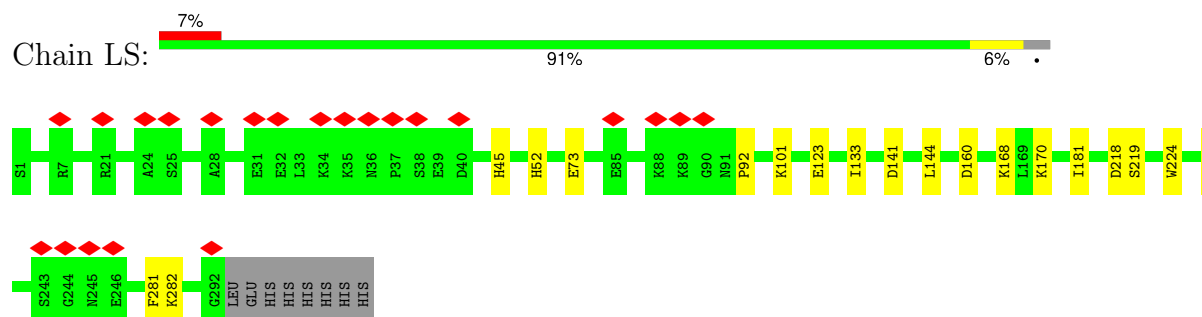
• Molecule 2: C3-A



• Molecule 2: C3-A



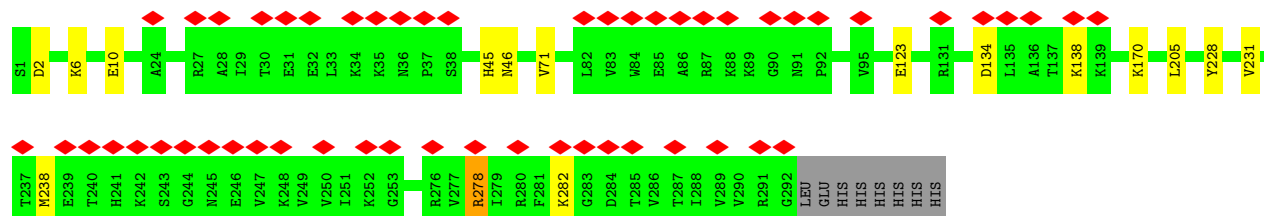
• Molecule 2: C3-A



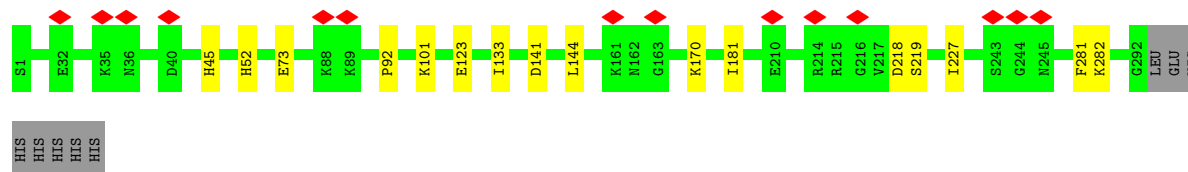
• Molecule 2: C3-A

Chain ZN:  93% 5% .

• Molecule 2: C3-A

Chain ZP:  18% 92% 5% .

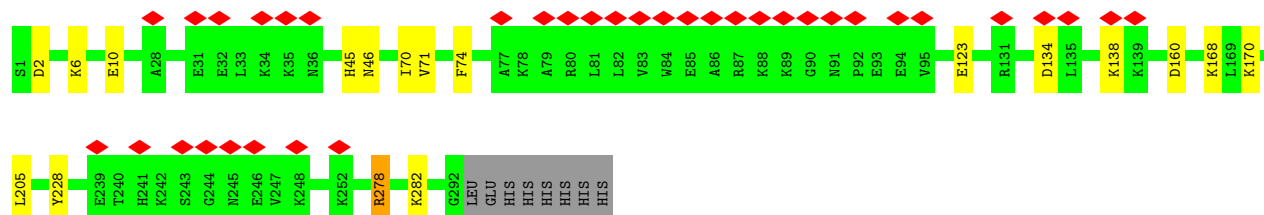
• Molecule 2: C3-A

Chain ZR:  5% 92% 5% .

• Molecule 2: C3-A

Chain ZT:  93% 5% .

• Molecule 2: C3-A

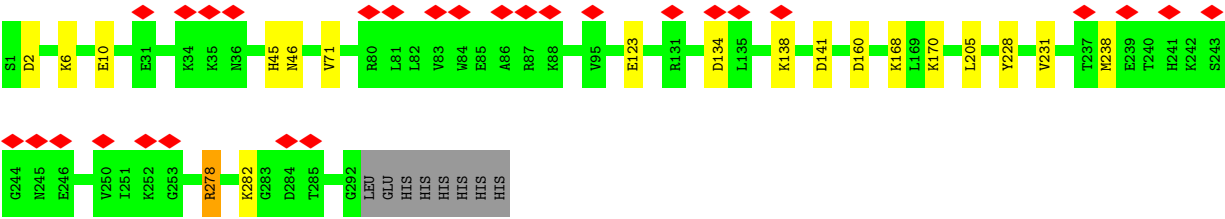
Chain ZV:  12% 91% 6% .

• Molecule 2: C3-A

Chain ZX:  91% 6% .



• Molecule 2: C3-A



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of subtomograms used | 462 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS GLACIOS | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 110 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 22000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 4095.000 | Depositor |
| Minimum map value | 1.000 | Depositor |
| Average map value | 1211.762 | Depositor |
| Map value standard deviation | 264.152 | Depositor |
| Recommended contour level | 1854 | Depositor |
| Map size (\AA) | 868.8, 868.8, 868.8 | wwPDB |
| Map dimensions | 240, 240, 240 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 3.62, 3.62, 3.62 | 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 | AA | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | AC | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | AE | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | AG | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | AI | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | AK | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | AM | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | AP | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | AR | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | AS | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | AU | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | AW | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | AY | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | BA | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | BC | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | BE | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | BG | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | BI | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | BK | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | BM | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | BO | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | BQ | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | BS | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | BU | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | BW | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | BY | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | CA | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | CC | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | CE | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | CG | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | CI | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | CK | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | CM | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | CO | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | CQ | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | CS | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | CU | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | CW | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | CY | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | DA | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | DC | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | DE | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | DG | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | DI | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | DK | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | DM | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | DO | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | DQ | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | DS | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | DU | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | DX | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | DZ | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | EB | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | ED | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | EF | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | EH | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | EJ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | EL | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | EN | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | EP | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | ER | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | ET | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | EV | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | EX | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | EZ | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | FB | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | FD | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | FF | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | FH | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | FJ | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | FL | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | FN | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | FP | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | FR | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | FT | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | FV | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | FX | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | FZ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | GB | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | GD | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | GF | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | GH | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | GJ | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | GL | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | GN | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | GP | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | GR | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | GT | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | GV | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | GX | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | GZ | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | HB | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | HD | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | HG | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | HI | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | HL | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | HN | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | HP | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | HR | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | HT | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | HV | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | HX | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | HZ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | IC | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | IE | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | IH | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | II | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | IK | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | IM | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | IO | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | IQ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | IS | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | IU | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | IW | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | IY | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | JA | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | JC | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | JE | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | JG | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | JI | 1.05 | 0/816 | 1.47 | 11/1106 (1.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | JK | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | JM | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | JO | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | JQ | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | JS | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | JV | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | JX | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | JZ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | KB | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | KD | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | KF | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | KH | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | KJ | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | KL | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | KN | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | KP | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | KR | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | KT | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | KV | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | KX | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | KZ | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | LB | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | LD | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | LF | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | LH | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | LJ | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | LL | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | LN | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | LP | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | LR | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | WA | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | WB | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | WC | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | WD | 1.05 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | YA | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | YC | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | YE | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | YG | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | YI | 1.11 | 0/816 | 1.37 | 11/1106 (1.0%) |
| 1 | YK | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | YM | 1.05 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | YO | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | YQ | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | YS | 1.05 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | YU | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | YW | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | YY | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | ZA | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | ZC | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | ZE | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | ZG | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | ZI | 1.06 | 0/816 | 1.46 | 11/1106 (1.0%) |
| 1 | ZK | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | ZM | 1.05 | 1/816 (0.1%) | 1.39 | 9/1106 (0.8%) |
| 1 | ZO | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | ZQ | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | ZS | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 1 | ZU | 1.06 | 0/816 | 1.47 | 11/1106 (1.0%) |
| 1 | ZW | 1.11 | 0/816 | 1.38 | 11/1106 (1.0%) |
| 1 | ZY | 1.05 | 1/816 (0.1%) | 1.39 | 11/1106 (1.0%) |
| 2 | AB | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | AD | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | AF | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | AH | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | AJ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | AL | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | AN | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | AO | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | AQ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | AT | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | AV | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | AX | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | AZ | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | BB | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | BD | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | BF | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | BH | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | BJ | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | BL | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | BN | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | BP | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | BR | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | BT | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | BV | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | BX | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | BZ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | CB | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | CD | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | CF | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | CH | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | CJ | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | CL | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | CN | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | CP | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | CR | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | CT | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | CV | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | CX | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | CZ | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | DB | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | DD | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | DF | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | DH | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | DJ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | DL | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | DN | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | DP | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | DR | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | DT | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | DW | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | DY | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | EA | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | EC | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | EE | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | EG | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | EI | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | EK | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | EM | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | EO | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | EQ | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ES | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | EU | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | EW | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | EY | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | FA | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | FC | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | FE | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | FG | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | FI | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | FK | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | FM | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | FO | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | FQ | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | FS | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | FU | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | FW | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | FY | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | GA | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | GC | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | GE | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | GG | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | GI | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | GK | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | GM | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | GO | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | GQ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | GS | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | GU | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | GW | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | GY | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | HA | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | HC | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | HE | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | HF | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | HH | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | HJ | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | HK | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | HM | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | HO | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | HQ | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | HS | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | HU | 0.98 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | HW | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | HY | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | IA | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | IB | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | ID | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | IF | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | IG | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | IJ | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | IL | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | IN | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | IP | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | IR | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | IT | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | IV | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | IX | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | IZ | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | JB | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | JD | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | JF | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | JH | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | JJ | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | JL | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | JN | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | JP | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | JR | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | JT | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | JU | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | JW | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | JY | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | KA | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | KC | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | KE | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | KG | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | KI | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | KK | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | KM | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | KO | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | KQ | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | KS | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | KU | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | KW | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | KY | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | LA | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | LC | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | LE | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | LG | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | LI | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | LK | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | LM | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | LO | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | LQ | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | LS | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | YB | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | YD | 1.00 | 2/2283 (0.1%) | 1.08 | 3/3073 (0.1%) |
| 2 | YF | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | YH | 0.99 | 2/2283 (0.1%) | 1.07 | 4/3073 (0.1%) |
| 2 | YJ | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | YL | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | YN | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | YP | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | YR | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | YT | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | YV | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | YX | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | YZ | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ZB | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | ZD | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ZF | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | ZH | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | ZJ | 0.98 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ZL | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | ZN | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | ZP | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ZR | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | ZT | 0.94 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| 2 | ZV | 0.99 | 2/2283 (0.1%) | 1.07 | 2/3073 (0.1%) |
| 2 | ZX | 1.00 | 2/2283 (0.1%) | 1.07 | 3/3073 (0.1%) |
| 2 | ZZ | 0.95 | 0/2283 | 1.09 | 9/3073 (0.3%) |
| All | All | 1.00 | 300/557820 (0.1%) | 1.18 | 2832/752220 (0.4%) |

All (300) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | CW | 1 | PRO | N-CD | -8.01 | 1.36 | 1.47 |
| 1 | EH | 1 | PRO | N-CD | -8.01 | 1.36 | 1.47 |
| 1 | AC | 1 | PRO | N-CD | -7.98 | 1.36 | 1.47 |
| 1 | HR | 1 | PRO | N-CD | -7.98 | 1.36 | 1.47 |
| 1 | BA | 1 | PRO | N-CD | -7.98 | 1.36 | 1.47 |
| 1 | HG | 1 | PRO | N-CD | -7.98 | 1.36 | 1.47 |
| 1 | YK | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | JS | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | KJ | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | LH | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | ZG | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | KD | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | ZY | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | BG | 1 | PRO | N-CD | -7.97 | 1.36 | 1.47 |
| 1 | DO | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | FL | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | CE | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | EB | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | IU | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | KP | 1 | PRO | N-CD | -7.96 | 1.36 | 1.47 |
| 1 | ZA | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | AI | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | DC | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | GJ | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | JX | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | LN | 1 | PRO | N-CD | -7.95 | 1.36 | 1.47 |
| 1 | BY | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | ET | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | JA | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | KV | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | BS | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | DU | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | EZ | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | ZS | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | CK | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | EN | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | FX | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | II | 1 | PRO | N-CD | -7.94 | 1.36 | 1.47 |
| 1 | DI | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | FF | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | YE | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | YQ | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | GD | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | HX | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | JG | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | JM | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | YW | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | HL | 1 | PRO | N-CD | -7.93 | 1.36 | 1.47 |
| 1 | AU | 1 | PRO | N-CD | -7.92 | 1.36 | 1.47 |
| 1 | HB | 1 | PRO | N-CD | -7.92 | 1.36 | 1.47 |
| 1 | AR | 1 | PRO | N-CD | -7.91 | 1.36 | 1.47 |
| 1 | GV | 1 | PRO | N-CD | -7.91 | 1.36 | 1.47 |
| 1 | FR | 1 | PRO | N-CD | -7.91 | 1.36 | 1.47 |
| 1 | IC | 1 | PRO | N-CD | -7.91 | 1.36 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | IO | 1 | PRO | N-CD | -7.90 | 1.36 | 1.47 |
| 1 | LB | 1 | PRO | N-CD | -7.90 | 1.36 | 1.47 |
| 1 | BM | 1 | PRO | N-CD | -7.89 | 1.36 | 1.47 |
| 1 | CQ | 1 | PRO | N-CD | -7.89 | 1.36 | 1.47 |
| 1 | GP | 1 | PRO | N-CD | -7.89 | 1.36 | 1.47 |
| 1 | ZM | 1 | PRO | N-CD | -7.89 | 1.36 | 1.47 |
| 2 | AH | 45 | HIS | CB-CG | -6.75 | 1.40 | 1.50 |
| 2 | HW | 45 | HIS | CB-CG | -6.75 | 1.40 | 1.50 |
| 2 | YP | 45 | HIS | CB-CG | -6.75 | 1.40 | 1.50 |
| 2 | JW | 45 | HIS | CB-CG | -6.75 | 1.40 | 1.50 |
| 2 | GI | 45 | HIS | CB-CG | -6.74 | 1.40 | 1.50 |
| 2 | IB | 45 | HIS | CB-CG | -6.74 | 1.40 | 1.50 |
| 2 | ZL | 45 | HIS | CB-CG | -6.73 | 1.40 | 1.50 |
| 2 | KI | 45 | HIS | CB-CG | -6.73 | 1.40 | 1.50 |
| 2 | YD | 45 | HIS | CB-CG | -6.73 | 1.40 | 1.50 |
| 2 | BL | 45 | HIS | CB-CG | -6.73 | 1.40 | 1.50 |
| 2 | CJ | 45 | HIS | CB-CG | -6.72 | 1.40 | 1.50 |
| 2 | EG | 45 | HIS | CB-CG | -6.72 | 1.40 | 1.50 |
| 2 | IT | 45 | HIS | CB-CG | -6.72 | 1.40 | 1.50 |
| 2 | LG | 45 | HIS | CB-CG | -6.72 | 1.40 | 1.50 |
| 2 | CD | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | CP | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | ES | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | EY | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | AN | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | AZ | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | ZF | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | HF | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | BF | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | DN | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | EA | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | FE | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | FK | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | FW | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | HK | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | IG | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | DH | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | DT | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | FQ | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | GO | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | IZ | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | KU | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | KC | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | LS | 45 | HIS | CB-CG | -6.71 | 1.40 | 1.50 |
| 2 | BX | 45 | HIS | CB-CG | -6.70 | 1.40 | 1.50 |
| 2 | ZX | 45 | HIS | CB-CG | -6.70 | 1.40 | 1.50 |
| 2 | DB | 45 | HIS | CB-CG | -6.70 | 1.40 | 1.50 |
| 2 | EM | 45 | HIS | CB-CG | -6.70 | 1.40 | 1.50 |
| 2 | BR | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | JF | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | LA | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | ZR | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | CV | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | GU | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | GC | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | IN | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | KO | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | LM | 45 | HIS | CB-CG | -6.69 | 1.40 | 1.50 |
| 2 | YV | 45 | HIS | CB-CG | -6.68 | 1.40 | 1.50 |
| 2 | JL | 45 | HIS | CB-CG | -6.68 | 1.40 | 1.50 |
| 2 | AT | 45 | HIS | CB-CG | -6.68 | 1.40 | 1.50 |
| 2 | HA | 45 | HIS | CB-CG | -6.68 | 1.40 | 1.50 |
| 2 | YJ | 45 | HIS | CB-CG | -6.66 | 1.40 | 1.50 |
| 2 | JR | 45 | HIS | CB-CG | -6.66 | 1.40 | 1.50 |
| 2 | AB | 45 | HIS | CB-CG | -6.65 | 1.40 | 1.50 |
| 2 | HQ | 45 | HIS | CB-CG | -6.65 | 1.40 | 1.50 |
| 2 | DL | 205 | LEU | CB-CG | 5.45 | 1.64 | 1.53 |
| 2 | FI | 205 | LEU | CB-CG | 5.45 | 1.64 | 1.53 |
| 2 | KA | 205 | LEU | CB-CG | 5.45 | 1.64 | 1.53 |
| 2 | LQ | 205 | LEU | CB-CG | 5.45 | 1.64 | 1.53 |
| 2 | GA | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | IL | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | YT | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | JJ | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | IX | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | KS | 205 | LEU | CB-CG | 5.44 | 1.64 | 1.53 |
| 2 | AX | 205 | LEU | CB-CG | 5.43 | 1.64 | 1.53 |
| 2 | CH | 205 | LEU | CB-CG | 5.43 | 1.64 | 1.53 |
| 2 | EE | 205 | LEU | CB-CG | 5.43 | 1.64 | 1.53 |
| 2 | HE | 205 | LEU | CB-CG | 5.43 | 1.64 | 1.53 |
| 2 | JD | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | KY | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | AF | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | HU | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | AL | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | ZD | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | AO | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | CB | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | EW | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | GY | 205 | LEU | CB-CG | 5.42 | 1.64 | 1.53 |
| 2 | CT | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | CZ | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | DY | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | EK | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | FC | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | GS | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | GG | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | IA | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | BV | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | DF | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | GM | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | ZV | 205 | LEU | CB-CG | 5.41 | 1.64 | 1.53 |
| 2 | BD | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | BJ | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | HJ | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | YB | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | YH | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | YZ | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | CN | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | EQ | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | HO | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | IR | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | JP | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | LE | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | FU | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | IF | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | DR | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | FO | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | KM | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | LK | 205 | LEU | CB-CG | 5.40 | 1.64 | 1.53 |
| 2 | YN | 205 | LEU | CB-CG | 5.39 | 1.64 | 1.53 |
| 2 | JU | 205 | LEU | CB-CG | 5.39 | 1.64 | 1.53 |
| 2 | ZJ | 205 | LEU | CB-CG | 5.38 | 1.64 | 1.53 |
| 2 | KG | 205 | LEU | CB-CG | 5.38 | 1.64 | 1.53 |
| 2 | BP | 205 | LEU | CB-CG | 5.37 | 1.64 | 1.53 |
| 2 | ZP | 205 | LEU | CB-CG | 5.37 | 1.64 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | DT | 52 | HIS | CB-CG | -5.23 | 1.42 | 1.50 |
| 2 | FQ | 52 | HIS | CB-CG | -5.23 | 1.42 | 1.50 |
| 2 | IZ | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | KU | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | FW | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | IG | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | GI | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | IB | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | YD | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | BL | 52 | HIS | CB-CG | -5.21 | 1.42 | 1.50 |
| 2 | CJ | 52 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | CT | 45 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | EG | 52 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | GS | 45 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | KO | 52 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | LM | 52 | HIS | CB-CG | -5.20 | 1.42 | 1.50 |
| 2 | CZ | 45 | HIS | CB-CG | -5.19 | 1.42 | 1.50 |
| 2 | EK | 45 | HIS | CB-CG | -5.19 | 1.42 | 1.50 |
| 2 | CV | 52 | HIS | CB-CG | -5.19 | 1.42 | 1.50 |
| 2 | GU | 52 | HIS | CB-CG | -5.19 | 1.42 | 1.50 |
| 2 | GC | 52 | HIS | CB-CG | -5.18 | 1.42 | 1.50 |
| 2 | IN | 52 | HIS | CB-CG | -5.18 | 1.42 | 1.50 |
| 2 | BX | 52 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | IT | 52 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | IX | 45 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | KS | 45 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | LG | 52 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | ZX | 52 | HIS | CB-CG | -5.18 | 1.43 | 1.50 |
| 2 | YT | 45 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | JJ | 45 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | DB | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | EM | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | BR | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | ZR | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | YH | 45 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | YJ | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | JP | 45 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | JR | 52 | HIS | CB-CG | -5.17 | 1.43 | 1.50 |
| 2 | ZL | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | KI | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | AZ | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | DY | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | FC | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | GA | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | HF | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | IL | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | FU | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | IF | 45 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | KC | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | LS | 52 | HIS | CB-CG | -5.16 | 1.43 | 1.50 |
| 2 | AN | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | ZF | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | DR | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | EA | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | FE | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | FO | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | DH | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | GO | 52 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | BV | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | CH | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | EE | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | ZV | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | AX | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | HE | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | KM | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | LK | 45 | HIS | CB-CG | -5.15 | 1.43 | 1.50 |
| 2 | AL | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | ZD | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | CD | 52 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | EY | 52 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | ZJ | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | IR | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | JD | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | KG | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | KY | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | LE | 45 | HIS | CB-CG | -5.14 | 1.43 | 1.50 |
| 2 | JF | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | LA | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | AH | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | BF | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | BJ | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | HK | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | HW | 52 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | YB | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | CN | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | EQ | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | BD | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | HJ | 45 | HIS | CB-CG | -5.13 | 1.43 | 1.50 |
| 2 | YZ | 45 | HIS | CB-CG | -5.12 | 1.43 | 1.50 |
| 2 | CP | 52 | HIS | CB-CG | -5.12 | 1.43 | 1.50 |
| 2 | ES | 52 | HIS | CB-CG | -5.12 | 1.43 | 1.50 |
| 2 | HO | 45 | HIS | CB-CG | -5.12 | 1.43 | 1.50 |
| 2 | DL | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | FI | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | BP | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | KA | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | LQ | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | ZP | 45 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | YP | 52 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | JW | 52 | HIS | CB-CG | -5.11 | 1.43 | 1.50 |
| 2 | AT | 52 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | GG | 45 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | HA | 52 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | IA | 45 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | DF | 45 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | GM | 45 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | AB | 52 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | HQ | 52 | HIS | CB-CG | -5.10 | 1.43 | 1.50 |
| 2 | YV | 52 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | JL | 52 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | YN | 45 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | JU | 45 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | CB | 45 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | EW | 45 | HIS | CB-CG | -5.09 | 1.43 | 1.50 |
| 2 | AF | 45 | HIS | CB-CG | -5.08 | 1.43 | 1.50 |
| 2 | DN | 52 | HIS | CB-CG | -5.08 | 1.43 | 1.50 |
| 2 | FK | 52 | HIS | CB-CG | -5.08 | 1.43 | 1.50 |
| 2 | HU | 45 | HIS | CB-CG | -5.08 | 1.43 | 1.50 |
| 2 | AO | 45 | HIS | CB-CG | -5.06 | 1.43 | 1.50 |
| 2 | GY | 45 | HIS | CB-CG | -5.06 | 1.43 | 1.50 |

All (2832) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | CY | 48 | GLY | CA-C-N | 9.89 | 129.95 | 119.76 |
| 1 | CY | 48 | GLY | C-N-CA | 9.89 | 129.95 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | EJ | 48 | GLY | CA-C-N | 9.89 | 129.95 | 119.76 |
| 1 | EJ | 48 | GLY | C-N-CA | 9.89 | 129.95 | 119.76 |
| 1 | BO | 48 | GLY | CA-C-N | 9.87 | 129.92 | 119.76 |
| 1 | BO | 48 | GLY | C-N-CA | 9.87 | 129.92 | 119.76 |
| 1 | ZO | 48 | GLY | CA-C-N | 9.87 | 129.92 | 119.76 |
| 1 | ZO | 48 | GLY | C-N-CA | 9.87 | 129.92 | 119.76 |
| 1 | IQ | 48 | GLY | CA-C-N | 9.86 | 129.92 | 119.76 |
| 1 | IQ | 48 | GLY | C-N-CA | 9.86 | 129.92 | 119.76 |
| 1 | LD | 48 | GLY | CA-C-N | 9.86 | 129.92 | 119.76 |
| 1 | LD | 48 | GLY | C-N-CA | 9.86 | 129.92 | 119.76 |
| 1 | CA | 48 | GLY | CA-C-N | 9.86 | 129.91 | 119.76 |
| 1 | CA | 48 | GLY | C-N-CA | 9.86 | 129.91 | 119.76 |
| 1 | EV | 48 | GLY | CA-C-N | 9.86 | 129.91 | 119.76 |
| 1 | EV | 48 | GLY | C-N-CA | 9.86 | 129.91 | 119.76 |
| 1 | AE | 48 | GLY | CA-C-N | 9.86 | 129.91 | 119.76 |
| 1 | AE | 48 | GLY | C-N-CA | 9.86 | 129.91 | 119.76 |
| 1 | HT | 48 | GLY | CA-C-N | 9.86 | 129.91 | 119.76 |
| 1 | HT | 48 | GLY | C-N-CA | 9.86 | 129.91 | 119.76 |
| 1 | AP | 48 | GLY | CA-C-N | 9.85 | 129.91 | 119.76 |
| 1 | AP | 48 | GLY | C-N-CA | 9.85 | 129.91 | 119.76 |
| 1 | GX | 48 | GLY | CA-C-N | 9.85 | 129.91 | 119.76 |
| 1 | GX | 48 | GLY | C-N-CA | 9.85 | 129.91 | 119.76 |
| 1 | JZ | 48 | GLY | CA-C-N | 9.84 | 129.89 | 119.76 |
| 1 | JZ | 48 | GLY | C-N-CA | 9.84 | 129.89 | 119.76 |
| 1 | LP | 48 | GLY | CA-C-N | 9.84 | 129.89 | 119.76 |
| 1 | LP | 48 | GLY | C-N-CA | 9.84 | 129.89 | 119.76 |
| 1 | YM | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | YM | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | YY | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | YY | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | HN | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | HN | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | WD | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | WD | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | KL | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | KL | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | LJ | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | LJ | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | BI | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | BI | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | YA | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | YA | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | AK | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | AK | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | ZC | 48 | GLY | CA-C-N | 9.83 | 129.88 | 119.76 |
| 1 | ZC | 48 | GLY | C-N-CA | 9.83 | 129.88 | 119.76 |
| 1 | AW | 48 | GLY | CA-C-N | 9.82 | 129.88 | 119.76 |
| 1 | AW | 48 | GLY | C-N-CA | 9.82 | 129.88 | 119.76 |
| 1 | HD | 48 | GLY | CA-C-N | 9.82 | 129.88 | 119.76 |
| 1 | HD | 48 | GLY | C-N-CA | 9.82 | 129.88 | 119.76 |
| 1 | YG | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | YG | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | JO | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | JO | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | CM | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | CM | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | DK | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | DK | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | EP | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | EP | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | FH | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | FH | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | FT | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | FT | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | IE | 48 | GLY | CA-C-N | 9.82 | 129.87 | 119.76 |
| 1 | IE | 48 | GLY | C-N-CA | 9.82 | 129.87 | 119.76 |
| 1 | DE | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | DE | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | GL | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | GL | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | IW | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | IW | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | KR | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | KR | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | GF | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | GF | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | HZ | 48 | GLY | CA-C-N | 9.81 | 129.86 | 119.76 |
| 1 | HZ | 48 | GLY | C-N-CA | 9.81 | 129.86 | 119.76 |
| 1 | JC | 48 | GLY | CA-C-N | 9.80 | 129.86 | 119.76 |
| 1 | JC | 48 | GLY | C-N-CA | 9.80 | 129.86 | 119.76 |
| 1 | KX | 48 | GLY | CA-C-N | 9.80 | 129.86 | 119.76 |
| 1 | KX | 48 | GLY | C-N-CA | 9.80 | 129.86 | 119.76 |
| 1 | DX | 48 | GLY | CA-C-N | 9.80 | 129.86 | 119.76 |
| 1 | DX | 48 | GLY | C-N-CA | 9.80 | 129.86 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | FB | 48 | GLY | CA-C-N | 9.80 | 129.86 | 119.76 |
| 1 | FB | 48 | GLY | C-N-CA | 9.80 | 129.86 | 119.76 |
| 1 | BU | 48 | GLY | CA-C-N | 9.80 | 129.85 | 119.76 |
| 1 | BU | 48 | GLY | C-N-CA | 9.80 | 129.85 | 119.76 |
| 1 | ZU | 48 | GLY | CA-C-N | 9.80 | 129.85 | 119.76 |
| 1 | ZU | 48 | GLY | C-N-CA | 9.80 | 129.85 | 119.76 |
| 1 | CG | 48 | GLY | CA-C-N | 9.80 | 129.85 | 119.76 |
| 1 | CG | 48 | GLY | C-N-CA | 9.80 | 129.85 | 119.76 |
| 1 | ED | 48 | GLY | CA-C-N | 9.80 | 129.85 | 119.76 |
| 1 | ED | 48 | GLY | C-N-CA | 9.80 | 129.85 | 119.76 |
| 1 | BC | 48 | GLY | CA-C-N | 9.79 | 129.85 | 119.76 |
| 1 | BC | 48 | GLY | C-N-CA | 9.79 | 129.85 | 119.76 |
| 1 | HI | 48 | GLY | CA-C-N | 9.79 | 129.85 | 119.76 |
| 1 | HI | 48 | GLY | C-N-CA | 9.79 | 129.85 | 119.76 |
| 1 | DQ | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | DQ | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | FN | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | FN | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | FZ | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | FZ | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | IK | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | IK | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | YS | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | YS | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | JI | 48 | GLY | CA-C-N | 9.79 | 129.84 | 119.76 |
| 1 | JI | 48 | GLY | C-N-CA | 9.79 | 129.84 | 119.76 |
| 1 | CS | 48 | GLY | CA-C-N | 9.77 | 129.82 | 119.76 |
| 1 | CS | 48 | GLY | C-N-CA | 9.77 | 129.82 | 119.76 |
| 1 | GR | 48 | GLY | CA-C-N | 9.77 | 129.82 | 119.76 |
| 1 | GR | 48 | GLY | C-N-CA | 9.77 | 129.82 | 119.76 |
| 1 | ZI | 48 | GLY | CA-C-N | 9.76 | 129.81 | 119.76 |
| 1 | ZI | 48 | GLY | C-N-CA | 9.76 | 129.81 | 119.76 |
| 1 | KF | 48 | GLY | CA-C-N | 9.76 | 129.81 | 119.76 |
| 1 | KF | 48 | GLY | C-N-CA | 9.76 | 129.81 | 119.76 |
| 1 | YM | 46 | ARG | CA-C-N | 9.28 | 129.52 | 119.87 |
| 1 | YM | 46 | ARG | C-N-CA | 9.28 | 129.52 | 119.87 |
| 1 | WD | 46 | ARG | CA-C-N | 9.28 | 129.52 | 119.87 |
| 1 | WD | 46 | ARG | C-N-CA | 9.28 | 129.52 | 119.87 |
| 1 | BO | 46 | ARG | CA-C-N | 9.27 | 129.50 | 119.87 |
| 1 | BO | 46 | ARG | C-N-CA | 9.27 | 129.50 | 119.87 |
| 1 | BU | 46 | ARG | CA-C-N | 9.27 | 129.51 | 119.87 |
| 1 | BU | 46 | ARG | C-N-CA | 9.27 | 129.51 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | ZO | 46 | ARG | CA-C-N | 9.27 | 129.50 | 119.87 |
| 1 | ZO | 46 | ARG | C-N-CA | 9.27 | 129.50 | 119.87 |
| 1 | ZU | 46 | ARG | CA-C-N | 9.27 | 129.51 | 119.87 |
| 1 | ZU | 46 | ARG | C-N-CA | 9.27 | 129.51 | 119.87 |
| 1 | FZ | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | FZ | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | IK | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | IK | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | IW | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | IW | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | KR | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | KR | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | CG | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | CG | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | ED | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | ED | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | AW | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | AW | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | DE | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | DE | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | DX | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | DX | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | FB | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | FB | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | GL | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | GL | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | HD | 46 | ARG | CA-C-N | 9.26 | 129.50 | 119.87 |
| 1 | HD | 46 | ARG | C-N-CA | 9.26 | 129.50 | 119.87 |
| 1 | JC | 46 | ARG | CA-C-N | 9.25 | 129.49 | 119.87 |
| 1 | JC | 46 | ARG | C-N-CA | 9.25 | 129.49 | 119.87 |
| 1 | KX | 46 | ARG | CA-C-N | 9.25 | 129.49 | 119.87 |
| 1 | KX | 46 | ARG | C-N-CA | 9.25 | 129.49 | 119.87 |
| 1 | AE | 46 | ARG | CA-C-N | 9.25 | 129.49 | 119.87 |
| 1 | AE | 46 | ARG | C-N-CA | 9.25 | 129.49 | 119.87 |
| 1 | HT | 46 | ARG | CA-C-N | 9.25 | 129.49 | 119.87 |
| 1 | HT | 46 | ARG | C-N-CA | 9.25 | 129.49 | 119.87 |
| 1 | JZ | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | JZ | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | LP | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | LP | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | BC | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | BC | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | HI | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | HI | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | FT | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | FT | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | IE | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | IE | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | YS | 46 | ARG | CA-C-N | 9.24 | 129.47 | 119.87 |
| 1 | YS | 46 | ARG | C-N-CA | 9.24 | 129.47 | 119.87 |
| 1 | AK | 46 | ARG | CA-C-N | 9.24 | 129.47 | 119.87 |
| 1 | AK | 46 | ARG | C-N-CA | 9.24 | 129.47 | 119.87 |
| 1 | ZC | 46 | ARG | CA-C-N | 9.24 | 129.47 | 119.87 |
| 1 | ZC | 46 | ARG | C-N-CA | 9.24 | 129.47 | 119.87 |
| 1 | BI | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | BI | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | JI | 46 | ARG | CA-C-N | 9.24 | 129.47 | 119.87 |
| 1 | JI | 46 | ARG | C-N-CA | 9.24 | 129.47 | 119.87 |
| 1 | YA | 46 | ARG | CA-C-N | 9.24 | 129.48 | 119.87 |
| 1 | YA | 46 | ARG | C-N-CA | 9.24 | 129.48 | 119.87 |
| 1 | CS | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | CS | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | GR | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | GR | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | YY | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | YY | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | AP | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | AP | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | CM | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | CM | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | EP | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | EP | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | GX | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | GX | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | HN | 46 | ARG | CA-C-N | 9.23 | 129.47 | 119.87 |
| 1 | HN | 46 | ARG | C-N-CA | 9.23 | 129.47 | 119.87 |
| 1 | DK | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | DK | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |
| 1 | FH | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | FH | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |
| 1 | IQ | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | IQ | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |
| 1 | LD | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | LD | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | CA | 46 | ARG | CA-C-N | 9.22 | 129.45 | 119.87 |
| 1 | CA | 46 | ARG | C-N-CA | 9.22 | 129.45 | 119.87 |
| 1 | EV | 46 | ARG | CA-C-N | 9.22 | 129.45 | 119.87 |
| 1 | EV | 46 | ARG | C-N-CA | 9.22 | 129.45 | 119.87 |
| 1 | ZI | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | ZI | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |
| 1 | KF | 46 | ARG | CA-C-N | 9.22 | 129.46 | 119.87 |
| 1 | KF | 46 | ARG | C-N-CA | 9.22 | 129.46 | 119.87 |
| 1 | GF | 46 | ARG | CA-C-N | 9.21 | 129.45 | 119.87 |
| 1 | GF | 46 | ARG | C-N-CA | 9.21 | 129.45 | 119.87 |
| 1 | HZ | 46 | ARG | CA-C-N | 9.21 | 129.45 | 119.87 |
| 1 | HZ | 46 | ARG | C-N-CA | 9.21 | 129.45 | 119.87 |
| 1 | YG | 46 | ARG | CA-C-N | 9.21 | 129.44 | 119.87 |
| 1 | YG | 46 | ARG | C-N-CA | 9.21 | 129.44 | 119.87 |
| 1 | JO | 46 | ARG | CA-C-N | 9.21 | 129.44 | 119.87 |
| 1 | JO | 46 | ARG | C-N-CA | 9.21 | 129.44 | 119.87 |
| 1 | KL | 46 | ARG | CA-C-N | 9.21 | 129.44 | 119.87 |
| 1 | KL | 46 | ARG | C-N-CA | 9.21 | 129.44 | 119.87 |
| 1 | LJ | 46 | ARG | CA-C-N | 9.21 | 129.44 | 119.87 |
| 1 | LJ | 46 | ARG | C-N-CA | 9.21 | 129.44 | 119.87 |
| 1 | CY | 46 | ARG | CA-C-N | 9.20 | 129.44 | 119.87 |
| 1 | CY | 46 | ARG | C-N-CA | 9.20 | 129.44 | 119.87 |
| 1 | EJ | 46 | ARG | CA-C-N | 9.20 | 129.44 | 119.87 |
| 1 | EJ | 46 | ARG | C-N-CA | 9.20 | 129.44 | 119.87 |
| 1 | DQ | 46 | ARG | CA-C-N | 9.20 | 129.43 | 119.87 |
| 1 | DQ | 46 | ARG | C-N-CA | 9.20 | 129.43 | 119.87 |
| 1 | FN | 46 | ARG | CA-C-N | 9.20 | 129.43 | 119.87 |
| 1 | FN | 46 | ARG | C-N-CA | 9.20 | 129.43 | 119.87 |
| 1 | AE | 29 | ALA | CA-C-N | 6.79 | 126.49 | 119.56 |
| 1 | AE | 29 | ALA | C-N-CA | 6.79 | 126.49 | 119.56 |
| 1 | HT | 29 | ALA | CA-C-N | 6.79 | 126.49 | 119.56 |
| 1 | HT | 29 | ALA | C-N-CA | 6.79 | 126.49 | 119.56 |
| 1 | CA | 29 | ALA | CA-C-N | 6.79 | 126.48 | 119.56 |
| 1 | CA | 29 | ALA | C-N-CA | 6.79 | 126.48 | 119.56 |
| 1 | EV | 29 | ALA | CA-C-N | 6.79 | 126.48 | 119.56 |
| 1 | EV | 29 | ALA | C-N-CA | 6.79 | 126.48 | 119.56 |
| 1 | IW | 29 | ALA | CA-C-N | 6.78 | 126.48 | 119.56 |
| 1 | IW | 29 | ALA | C-N-CA | 6.78 | 126.48 | 119.56 |
| 1 | KR | 29 | ALA | CA-C-N | 6.78 | 126.48 | 119.56 |
| 1 | KR | 29 | ALA | C-N-CA | 6.78 | 126.48 | 119.56 |
| 1 | BI | 29 | ALA | CA-C-N | 6.78 | 126.48 | 119.56 |
| 1 | BI | 29 | ALA | C-N-CA | 6.78 | 126.48 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | YA | 29 | ALA | CA-C-N | 6.78 | 126.48 | 119.56 |
| 1 | YA | 29 | ALA | C-N-CA | 6.78 | 126.48 | 119.56 |
| 1 | AP | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | AP | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | BO | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | BO | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | CY | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | CY | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | EJ | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | EJ | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | GX | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | GX | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | ZO | 29 | ALA | CA-C-N | 6.78 | 126.47 | 119.56 |
| 1 | ZO | 29 | ALA | C-N-CA | 6.78 | 126.47 | 119.56 |
| 1 | DX | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | DX | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | FB | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | FB | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | YM | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | YM | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | WD | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | WD | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | FT | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | FT | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | IE | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | IE | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | IQ | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | IQ | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | LD | 29 | ALA | CA-C-N | 6.77 | 126.47 | 119.56 |
| 1 | LD | 29 | ALA | C-N-CA | 6.77 | 126.47 | 119.56 |
| 1 | FZ | 29 | ALA | CA-C-N | 6.77 | 126.46 | 119.56 |
| 1 | FZ | 29 | ALA | C-N-CA | 6.77 | 126.46 | 119.56 |
| 1 | IK | 29 | ALA | CA-C-N | 6.77 | 126.46 | 119.56 |
| 1 | IK | 29 | ALA | C-N-CA | 6.77 | 126.46 | 119.56 |
| 1 | KL | 29 | ALA | CA-C-N | 6.76 | 126.46 | 119.56 |
| 1 | KL | 29 | ALA | C-N-CA | 6.76 | 126.46 | 119.56 |
| 1 | LJ | 29 | ALA | CA-C-N | 6.76 | 126.46 | 119.56 |
| 1 | LJ | 29 | ALA | C-N-CA | 6.76 | 126.46 | 119.56 |
| 1 | AK | 29 | ALA | CA-C-N | 6.76 | 126.45 | 119.56 |
| 1 | AK | 29 | ALA | C-N-CA | 6.76 | 126.45 | 119.56 |
| 1 | ZC | 29 | ALA | CA-C-N | 6.76 | 126.45 | 119.56 |
| 1 | ZC | 29 | ALA | C-N-CA | 6.76 | 126.45 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | GF | 29 | ALA | CA-C-N | 6.76 | 126.45 | 119.56 |
| 1 | GF | 29 | ALA | C-N-CA | 6.76 | 126.45 | 119.56 |
| 1 | HZ | 29 | ALA | CA-C-N | 6.76 | 126.45 | 119.56 |
| 1 | HZ | 29 | ALA | C-N-CA | 6.76 | 126.45 | 119.56 |
| 1 | YS | 29 | ALA | CA-C-N | 6.75 | 126.45 | 119.56 |
| 1 | YS | 29 | ALA | C-N-CA | 6.75 | 126.45 | 119.56 |
| 1 | CK | 29 | ALA | CA-C-N | 6.75 | 126.45 | 119.56 |
| 1 | CK | 29 | ALA | C-N-CA | 6.75 | 126.45 | 119.56 |
| 1 | EN | 29 | ALA | CA-C-N | 6.75 | 126.45 | 119.56 |
| 1 | EN | 29 | ALA | C-N-CA | 6.75 | 126.45 | 119.56 |
| 1 | JI | 29 | ALA | CA-C-N | 6.75 | 126.45 | 119.56 |
| 1 | JI | 29 | ALA | C-N-CA | 6.75 | 126.45 | 119.56 |
| 1 | BU | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | BU | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | ZU | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | ZU | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | AW | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | AW | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | DQ | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | DQ | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | FN | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | FN | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | HD | 29 | ALA | CA-C-N | 6.75 | 126.44 | 119.56 |
| 1 | HD | 29 | ALA | C-N-CA | 6.75 | 126.44 | 119.56 |
| 1 | YY | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | YY | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | DE | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | DE | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | GL | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | GL | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | HN | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | HN | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | YE | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | YE | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | CG | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | CG | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | ED | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | ED | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | JM | 29 | ALA | CA-C-N | 6.74 | 126.44 | 119.56 |
| 1 | JM | 29 | ALA | C-N-CA | 6.74 | 126.44 | 119.56 |
| 1 | YG | 29 | ALA | CA-C-N | 6.74 | 126.43 | 119.56 |
| 1 | YG | 29 | ALA | C-N-CA | 6.74 | 126.43 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | JO | 29 | ALA | CA-C-N | 6.74 | 126.43 | 119.56 |
| 1 | JO | 29 | ALA | C-N-CA | 6.74 | 126.43 | 119.56 |
| 1 | BC | 29 | ALA | CA-C-N | 6.73 | 126.43 | 119.56 |
| 1 | BC | 29 | ALA | C-N-CA | 6.73 | 126.43 | 119.56 |
| 1 | HI | 29 | ALA | CA-C-N | 6.73 | 126.43 | 119.56 |
| 1 | HI | 29 | ALA | C-N-CA | 6.73 | 126.43 | 119.56 |
| 1 | ZI | 29 | ALA | CA-C-N | 6.73 | 126.42 | 119.56 |
| 1 | ZI | 29 | ALA | C-N-CA | 6.73 | 126.42 | 119.56 |
| 1 | KF | 29 | ALA | CA-C-N | 6.73 | 126.42 | 119.56 |
| 1 | KF | 29 | ALA | C-N-CA | 6.73 | 126.42 | 119.56 |
| 1 | DK | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | DK | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | FH | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | FH | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | IS | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | IS | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | JC | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | JC | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | KX | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | KX | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | LF | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | LF | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | CQ | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | CQ | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | GD | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | GD | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | GP | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | GP | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | HX | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | HX | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | JZ | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | JZ | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | LP | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | LP | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | ZK | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | ZK | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | KH | 29 | ALA | CA-C-N | 6.72 | 126.42 | 119.56 |
| 1 | KH | 29 | ALA | C-N-CA | 6.72 | 126.42 | 119.56 |
| 1 | BA | 29 | ALA | CA-C-N | 6.72 | 126.41 | 119.56 |
| 1 | BA | 29 | ALA | C-N-CA | 6.72 | 126.41 | 119.56 |
| 1 | HG | 29 | ALA | CA-C-N | 6.72 | 126.41 | 119.56 |
| 1 | HG | 29 | ALA | C-N-CA | 6.72 | 126.41 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | ZY | 29 | ALA | CA-C-N | 6.71 | 126.41 | 119.56 |
| 1 | ZY | 29 | ALA | C-N-CA | 6.71 | 126.41 | 119.56 |
| 1 | BG | 29 | ALA | CA-C-N | 6.71 | 126.41 | 119.56 |
| 1 | BG | 29 | ALA | C-N-CA | 6.71 | 126.41 | 119.56 |
| 1 | YW | 29 | ALA | CA-C-N | 6.71 | 126.41 | 119.56 |
| 1 | YW | 29 | ALA | C-N-CA | 6.71 | 126.41 | 119.56 |
| 1 | HL | 29 | ALA | CA-C-N | 6.71 | 126.41 | 119.56 |
| 1 | HL | 29 | ALA | C-N-CA | 6.71 | 126.41 | 119.56 |
| 1 | CS | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | CS | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | GH | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | GH | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | GR | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | GR | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | WC | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | WC | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | AR | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | AR | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | GV | 29 | ALA | CA-C-N | 6.71 | 126.40 | 119.56 |
| 1 | GV | 29 | ALA | C-N-CA | 6.71 | 126.40 | 119.56 |
| 1 | IU | 29 | ALA | CA-C-N | 6.70 | 126.40 | 119.56 |
| 1 | IU | 29 | ALA | C-N-CA | 6.70 | 126.40 | 119.56 |
| 1 | KP | 29 | ALA | CA-C-N | 6.70 | 126.40 | 119.56 |
| 1 | KP | 29 | ALA | C-N-CA | 6.70 | 126.40 | 119.56 |
| 1 | YK | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | YK | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | DC | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | DC | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | GJ | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | GJ | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | JS | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | JS | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | KB | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | KB | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | LR | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | LR | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | DO | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | DO | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | FL | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | FL | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | CE | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | CE | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | EB | 29 | ALA | CA-C-N | 6.70 | 126.39 | 119.56 |
| 1 | EB | 29 | ALA | C-N-CA | 6.70 | 126.39 | 119.56 |
| 1 | DM | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | DM | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | DZ | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | DZ | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | ZG | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | ZG | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | FD | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | FD | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | FJ | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | FJ | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | KD | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | KD | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | IO | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | IO | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | LB | 29 | ALA | CA-C-N | 6.69 | 126.39 | 119.56 |
| 1 | LB | 29 | ALA | C-N-CA | 6.69 | 126.39 | 119.56 |
| 1 | ZA | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | ZA | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | AI | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | AI | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | CM | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | CM | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | DI | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | DI | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | EP | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | EP | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | FF | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | FF | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | CO | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | CO | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | DG | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | DG | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | ER | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | ER | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | GN | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | GN | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | JA | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | JA | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | KV | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | KV | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | DU | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | DU | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | EZ | 29 | ALA | CA-C-N | 6.69 | 126.38 | 119.56 |
| 1 | EZ | 29 | ALA | C-N-CA | 6.69 | 126.38 | 119.56 |
| 1 | CU | 29 | ALA | CA-C-N | 6.68 | 126.38 | 119.56 |
| 1 | CU | 29 | ALA | C-N-CA | 6.68 | 126.38 | 119.56 |
| 1 | GT | 29 | ALA | CA-C-N | 6.68 | 126.38 | 119.56 |
| 1 | GT | 29 | ALA | C-N-CA | 6.68 | 126.38 | 119.56 |
| 1 | CI | 29 | ALA | CA-C-N | 6.68 | 126.38 | 119.56 |
| 1 | CI | 29 | ALA | C-N-CA | 6.68 | 126.38 | 119.56 |
| 1 | EF | 29 | ALA | CA-C-N | 6.68 | 126.38 | 119.56 |
| 1 | EF | 29 | ALA | C-N-CA | 6.68 | 126.38 | 119.56 |
| 1 | JE | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | JE | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | KZ | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | KZ | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | YC | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | YC | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | AY | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | AY | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | BK | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | BK | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | WB | 29 | ALA | CA-C-N | 6.68 | 126.37 | 119.56 |
| 1 | WB | 29 | ALA | C-N-CA | 6.68 | 126.37 | 119.56 |
| 1 | DS | 29 | ALA | CA-C-N | 6.67 | 126.37 | 119.56 |
| 1 | DS | 29 | ALA | C-N-CA | 6.67 | 126.37 | 119.56 |
| 1 | FP | 29 | ALA | CA-C-N | 6.67 | 126.37 | 119.56 |
| 1 | FP | 29 | ALA | C-N-CA | 6.67 | 126.37 | 119.56 |
| 1 | AM | 29 | ALA | CA-C-N | 6.67 | 126.37 | 119.56 |
| 1 | AM | 29 | ALA | C-N-CA | 6.67 | 126.37 | 119.56 |
| 1 | ZE | 29 | ALA | CA-C-N | 6.67 | 126.37 | 119.56 |
| 1 | ZE | 29 | ALA | C-N-CA | 6.67 | 126.37 | 119.56 |
| 1 | AC | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | AC | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | AU | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | AU | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | FV | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | FV | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | HB | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | HB | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | HR | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | HR | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | IH | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | IH | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | KJ | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | KJ | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | LH | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | LH | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | AG | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | AG | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | CC | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | CC | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | EX | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | EX | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | HV | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | HV | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | IY | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | IY | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | KN | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | KN | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | KT | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | KT | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | LL | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | LL | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | BY | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | BY | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | ET | 29 | ALA | CA-C-N | 6.67 | 126.36 | 119.56 |
| 1 | ET | 29 | ALA | C-N-CA | 6.67 | 126.36 | 119.56 |
| 1 | BE | 29 | ALA | CA-C-N | 6.66 | 126.36 | 119.56 |
| 1 | BE | 29 | ALA | C-N-CA | 6.66 | 126.36 | 119.56 |
| 1 | WA | 29 | ALA | CA-C-N | 6.66 | 126.36 | 119.56 |
| 1 | WA | 29 | ALA | C-N-CA | 6.66 | 126.36 | 119.56 |
| 1 | JX | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | JX | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | LN | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | LN | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | YQ | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | YQ | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | JG | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | JG | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | YU | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | YU | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | CW | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | CW | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | EH | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | EH | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | FX | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | FX | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | II | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | II | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | JK | 29 | ALA | CA-C-N | 6.66 | 126.35 | 119.56 |
| 1 | JK | 29 | ALA | C-N-CA | 6.66 | 126.35 | 119.56 |
| 1 | DA | 29 | ALA | CA-C-N | 6.65 | 126.35 | 119.56 |
| 1 | DA | 29 | ALA | C-N-CA | 6.65 | 126.35 | 119.56 |
| 1 | EL | 29 | ALA | CA-C-N | 6.65 | 126.35 | 119.56 |
| 1 | EL | 29 | ALA | C-N-CA | 6.65 | 126.35 | 119.56 |
| 1 | YO | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | YO | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | GB | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | GB | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | IM | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | IM | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | JV | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | JV | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | BW | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | BW | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | ZW | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | ZW | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | AA | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | AA | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | BM | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | BM | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | HP | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | HP | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | ZM | 29 | ALA | CA-C-N | 6.65 | 126.34 | 119.56 |
| 1 | ZM | 29 | ALA | C-N-CA | 6.65 | 126.34 | 119.56 |
| 1 | BS | 29 | ALA | CA-C-N | 6.64 | 126.33 | 119.56 |
| 1 | BS | 29 | ALA | C-N-CA | 6.64 | 126.33 | 119.56 |
| 1 | ZS | 29 | ALA | CA-C-N | 6.64 | 126.33 | 119.56 |
| 1 | ZS | 29 | ALA | C-N-CA | 6.64 | 126.33 | 119.56 |
| 1 | YI | 29 | ALA | CA-C-N | 6.64 | 126.33 | 119.56 |
| 1 | YI | 29 | ALA | C-N-CA | 6.64 | 126.33 | 119.56 |
| 1 | JQ | 29 | ALA | CA-C-N | 6.64 | 126.33 | 119.56 |
| 1 | JQ | 29 | ALA | C-N-CA | 6.64 | 126.33 | 119.56 |
| 1 | AS | 29 | ALA | CA-C-N | 6.63 | 126.33 | 119.56 |
| 1 | AS | 29 | ALA | C-N-CA | 6.63 | 126.33 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | BQ | 29 | ALA | CA-C-N | 6.63 | 126.33 | 119.56 |
| 1 | BQ | 29 | ALA | C-N-CA | 6.63 | 126.33 | 119.56 |
| 1 | GZ | 29 | ALA | CA-C-N | 6.63 | 126.33 | 119.56 |
| 1 | GZ | 29 | ALA | C-N-CA | 6.63 | 126.33 | 119.56 |
| 1 | ZQ | 29 | ALA | CA-C-N | 6.63 | 126.33 | 119.56 |
| 1 | ZQ | 29 | ALA | C-N-CA | 6.63 | 126.33 | 119.56 |
| 1 | FR | 29 | ALA | CA-C-N | 6.61 | 126.31 | 119.56 |
| 1 | FR | 29 | ALA | C-N-CA | 6.61 | 126.31 | 119.56 |
| 1 | IC | 29 | ALA | CA-C-N | 6.61 | 126.31 | 119.56 |
| 1 | IC | 29 | ALA | C-N-CA | 6.61 | 126.31 | 119.56 |
| 1 | ZK | 48 | GLY | CA-C-N | 6.27 | 126.03 | 119.76 |
| 1 | ZK | 48 | GLY | C-N-CA | 6.27 | 126.03 | 119.76 |
| 1 | KH | 48 | GLY | CA-C-N | 6.27 | 126.03 | 119.76 |
| 1 | KH | 48 | GLY | C-N-CA | 6.27 | 126.03 | 119.76 |
| 1 | BQ | 48 | GLY | CA-C-N | 6.27 | 126.03 | 119.76 |
| 1 | BQ | 48 | GLY | C-N-CA | 6.27 | 126.03 | 119.76 |
| 1 | ZQ | 48 | GLY | CA-C-N | 6.27 | 126.03 | 119.76 |
| 1 | ZQ | 48 | GLY | C-N-CA | 6.27 | 126.03 | 119.76 |
| 1 | AY | 48 | GLY | CA-C-N | 6.25 | 126.02 | 119.76 |
| 1 | AY | 48 | GLY | C-N-CA | 6.25 | 126.02 | 119.76 |
| 1 | WB | 48 | GLY | CA-C-N | 6.25 | 126.02 | 119.76 |
| 1 | WB | 48 | GLY | C-N-CA | 6.25 | 126.02 | 119.76 |
| 1 | CU | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | CU | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | GT | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | GT | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | AS | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | AS | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | GH | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | GH | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | GZ | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | GZ | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | WC | 48 | GLY | CA-C-N | 6.25 | 126.01 | 119.76 |
| 1 | WC | 48 | GLY | C-N-CA | 6.25 | 126.01 | 119.76 |
| 1 | YU | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | YU | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | CO | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | CO | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | ER | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | ER | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | JK | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | JK | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | CI | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | CI | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | EF | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | EF | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | IS | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | IS | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | LF | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | LF | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | YI | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | YI | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | JQ | 48 | GLY | CA-C-N | 6.24 | 126.00 | 119.76 |
| 1 | JQ | 48 | GLY | C-N-CA | 6.24 | 126.00 | 119.76 |
| 1 | AM | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | AM | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | ZE | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | ZE | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | FV | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | FV | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | IH | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | IH | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | DM | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | DM | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | FJ | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | FJ | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | BE | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | BE | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | DA | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | DA | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | EL | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | EL | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | WA | 48 | GLY | CA-C-N | 6.23 | 125.99 | 119.76 |
| 1 | WA | 48 | GLY | C-N-CA | 6.23 | 125.99 | 119.76 |
| 1 | IY | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | IY | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | KT | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | KT | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | CC | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | CC | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | EX | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | EX | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | YC | 46 | ARG | CA-C-N | 6.22 | 125.84 | 119.56 |
| 1 | YC | 46 | ARG | C-N-CA | 6.22 | 125.84 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | YC | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | YC | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | YO | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | YO | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | BK | 46 | ARG | CA-C-N | 6.22 | 125.84 | 119.56 |
| 1 | BK | 46 | ARG | C-N-CA | 6.22 | 125.84 | 119.56 |
| 1 | BK | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | BK | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | DZ | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | DZ | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | FD | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | FD | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | JV | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | JV | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | KN | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | KN | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | LL | 48 | GLY | CA-C-N | 6.22 | 125.98 | 119.76 |
| 1 | LL | 48 | GLY | C-N-CA | 6.22 | 125.98 | 119.76 |
| 1 | DG | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | DG | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | DS | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | DS | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | FP | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | FP | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | GN | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | GN | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | KB | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | KB | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | LR | 48 | GLY | CA-C-N | 6.21 | 125.97 | 119.76 |
| 1 | LR | 48 | GLY | C-N-CA | 6.21 | 125.97 | 119.76 |
| 1 | AA | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | AA | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |
| 1 | CC | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | CC | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | EX | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | EX | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | HP | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | HP | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |
| 1 | JE | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | JE | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |
| 1 | KZ | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | KZ | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | BW | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | BW | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |
| 1 | ZW | 48 | GLY | CA-C-N | 6.20 | 125.96 | 119.76 |
| 1 | ZW | 48 | GLY | C-N-CA | 6.20 | 125.96 | 119.76 |
| 1 | YO | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | YO | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | AG | 48 | GLY | CA-C-N | 6.20 | 125.95 | 119.76 |
| 1 | AG | 48 | GLY | C-N-CA | 6.20 | 125.95 | 119.76 |
| 1 | HV | 48 | GLY | CA-C-N | 6.20 | 125.95 | 119.76 |
| 1 | HV | 48 | GLY | C-N-CA | 6.20 | 125.95 | 119.76 |
| 1 | ZK | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | ZK | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | JV | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | JV | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | KH | 46 | ARG | CA-C-N | 6.20 | 125.82 | 119.56 |
| 1 | KH | 46 | ARG | C-N-CA | 6.20 | 125.82 | 119.56 |
| 1 | AG | 46 | ARG | CA-C-N | 6.19 | 125.82 | 119.56 |
| 1 | AG | 46 | ARG | C-N-CA | 6.19 | 125.82 | 119.56 |
| 1 | HV | 46 | ARG | CA-C-N | 6.19 | 125.82 | 119.56 |
| 1 | HV | 46 | ARG | C-N-CA | 6.19 | 125.82 | 119.56 |
| 1 | YU | 46 | ARG | CA-C-N | 6.18 | 125.81 | 119.56 |
| 1 | YU | 46 | ARG | C-N-CA | 6.18 | 125.81 | 119.56 |
| 1 | JK | 46 | ARG | CA-C-N | 6.18 | 125.81 | 119.56 |
| 1 | JK | 46 | ARG | C-N-CA | 6.18 | 125.81 | 119.56 |
| 1 | IS | 46 | ARG | CA-C-N | 6.18 | 125.80 | 119.56 |
| 1 | IS | 46 | ARG | C-N-CA | 6.18 | 125.80 | 119.56 |
| 1 | LF | 46 | ARG | CA-C-N | 6.18 | 125.80 | 119.56 |
| 1 | LF | 46 | ARG | C-N-CA | 6.18 | 125.80 | 119.56 |
| 1 | BW | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | BW | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | ZW | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | ZW | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | CO | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | CO | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | CU | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | CU | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | ER | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | ER | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | GT | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | GT | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | AM | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | AM | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | BQ | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | BQ | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | ZE | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | ZE | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | ZQ | 46 | ARG | CA-C-N | 6.17 | 125.79 | 119.56 |
| 1 | ZQ | 46 | ARG | C-N-CA | 6.17 | 125.79 | 119.56 |
| 1 | AS | 46 | ARG | CA-C-N | 6.16 | 125.79 | 119.56 |
| 1 | AS | 46 | ARG | C-N-CA | 6.16 | 125.79 | 119.56 |
| 1 | GZ | 46 | ARG | CA-C-N | 6.16 | 125.79 | 119.56 |
| 1 | GZ | 46 | ARG | C-N-CA | 6.16 | 125.79 | 119.56 |
| 1 | IY | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | IY | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | KT | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | KT | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | GB | 48 | GLY | CA-C-N | 6.16 | 125.92 | 119.76 |
| 1 | GB | 48 | GLY | C-N-CA | 6.16 | 125.92 | 119.76 |
| 1 | IM | 48 | GLY | CA-C-N | 6.16 | 125.92 | 119.76 |
| 1 | IM | 48 | GLY | C-N-CA | 6.16 | 125.92 | 119.76 |
| 1 | AA | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | AA | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | HP | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | HP | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | BE | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | BE | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | DM | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | DM | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | FJ | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | FJ | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | WA | 46 | ARG | CA-C-N | 6.16 | 125.78 | 119.56 |
| 1 | WA | 46 | ARG | C-N-CA | 6.16 | 125.78 | 119.56 |
| 1 | GB | 46 | ARG | CA-C-N | 6.15 | 125.78 | 119.56 |
| 1 | GB | 46 | ARG | C-N-CA | 6.15 | 125.78 | 119.56 |
| 1 | IM | 46 | ARG | CA-C-N | 6.15 | 125.78 | 119.56 |
| 1 | IM | 46 | ARG | C-N-CA | 6.15 | 125.78 | 119.56 |
| 1 | CC | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | CC | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |
| 1 | EX | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | EX | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |
| 1 | YO | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | YO | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |
| 1 | JV | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | JV | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | BW | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | BW | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |
| 1 | ZW | 33 | ALA | CA-C-N | 6.00 | 125.68 | 119.56 |
| 1 | ZW | 33 | ALA | C-N-CA | 6.00 | 125.68 | 119.56 |
| 1 | AG | 33 | ALA | CA-C-N | 6.00 | 125.67 | 119.56 |
| 1 | AG | 33 | ALA | C-N-CA | 6.00 | 125.67 | 119.56 |
| 1 | HV | 33 | ALA | CA-C-N | 6.00 | 125.67 | 119.56 |
| 1 | HV | 33 | ALA | C-N-CA | 6.00 | 125.67 | 119.56 |
| 1 | DA | 33 | ALA | CA-C-N | 5.99 | 125.67 | 119.56 |
| 1 | DA | 33 | ALA | C-N-CA | 5.99 | 125.67 | 119.56 |
| 1 | EL | 33 | ALA | CA-C-N | 5.99 | 125.67 | 119.56 |
| 1 | EL | 33 | ALA | C-N-CA | 5.99 | 125.67 | 119.56 |
| 1 | DM | 33 | ALA | CA-C-N | 5.99 | 125.67 | 119.56 |
| 1 | DM | 33 | ALA | C-N-CA | 5.99 | 125.67 | 119.56 |
| 1 | FJ | 33 | ALA | CA-C-N | 5.99 | 125.67 | 119.56 |
| 1 | FJ | 33 | ALA | C-N-CA | 5.99 | 125.67 | 119.56 |
| 1 | AA | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | AA | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | HP | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | HP | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | AS | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | AS | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | GZ | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | GZ | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | BQ | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | BQ | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | ZQ | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | ZQ | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | YC | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | YC | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | BK | 33 | ALA | CA-C-N | 5.98 | 125.66 | 119.56 |
| 1 | BK | 33 | ALA | C-N-CA | 5.98 | 125.66 | 119.56 |
| 1 | CO | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | CO | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |
| 1 | ER | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | ER | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |
| 1 | IS | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | IS | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |
| 1 | LF | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | LF | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |
| 1 | GH | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | GH | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | WC | 33 | ALA | CA-C-N | 5.97 | 125.65 | 119.56 |
| 1 | WC | 33 | ALA | C-N-CA | 5.97 | 125.65 | 119.56 |
| 1 | ZK | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | ZK | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | KH | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | KH | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | JE | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | JE | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | KZ | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | KZ | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | BE | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | BE | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | WA | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | WA | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | DS | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | DS | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | FP | 33 | ALA | CA-C-N | 5.96 | 125.64 | 119.56 |
| 1 | FP | 33 | ALA | C-N-CA | 5.96 | 125.64 | 119.56 |
| 1 | AY | 33 | ALA | CA-C-N | 5.96 | 125.63 | 119.56 |
| 1 | AY | 33 | ALA | C-N-CA | 5.96 | 125.63 | 119.56 |
| 1 | WB | 33 | ALA | CA-C-N | 5.96 | 125.63 | 119.56 |
| 1 | WB | 33 | ALA | C-N-CA | 5.96 | 125.63 | 119.56 |
| 1 | AM | 33 | ALA | CA-C-N | 5.95 | 125.63 | 119.56 |
| 1 | AM | 33 | ALA | C-N-CA | 5.95 | 125.63 | 119.56 |
| 1 | ZE | 33 | ALA | CA-C-N | 5.95 | 125.63 | 119.56 |
| 1 | ZE | 33 | ALA | C-N-CA | 5.95 | 125.63 | 119.56 |
| 1 | CI | 33 | ALA | CA-C-N | 5.95 | 125.62 | 119.56 |
| 1 | CI | 33 | ALA | C-N-CA | 5.95 | 125.62 | 119.56 |
| 1 | EF | 33 | ALA | CA-C-N | 5.95 | 125.62 | 119.56 |
| 1 | EF | 33 | ALA | C-N-CA | 5.95 | 125.62 | 119.56 |
| 1 | KN | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | KN | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | LL | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | LL | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | KB | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | KB | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | LR | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | LR | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | DG | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | DG | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | GN | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | GN | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | IY | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | IY | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | KT | 33 | ALA | CA-C-N | 5.94 | 125.62 | 119.56 |
| 1 | KT | 33 | ALA | C-N-CA | 5.94 | 125.62 | 119.56 |
| 1 | DZ | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | DZ | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | FD | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | FD | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | FV | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | FV | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | IH | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | IH | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | CU | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | CU | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | GT | 33 | ALA | CA-C-N | 5.93 | 125.61 | 119.56 |
| 1 | GT | 33 | ALA | C-N-CA | 5.93 | 125.61 | 119.56 |
| 1 | GB | 33 | ALA | CA-C-N | 5.92 | 125.60 | 119.56 |
| 1 | GB | 33 | ALA | C-N-CA | 5.92 | 125.60 | 119.56 |
| 1 | IM | 33 | ALA | CA-C-N | 5.92 | 125.60 | 119.56 |
| 1 | IM | 33 | ALA | C-N-CA | 5.92 | 125.60 | 119.56 |
| 1 | YI | 33 | ALA | CA-C-N | 5.91 | 125.59 | 119.56 |
| 1 | YI | 33 | ALA | C-N-CA | 5.91 | 125.59 | 119.56 |
| 1 | JQ | 33 | ALA | CA-C-N | 5.91 | 125.59 | 119.56 |
| 1 | JQ | 33 | ALA | C-N-CA | 5.91 | 125.59 | 119.56 |
| 1 | YU | 33 | ALA | CA-C-N | 5.91 | 125.58 | 119.56 |
| 1 | YU | 33 | ALA | C-N-CA | 5.91 | 125.58 | 119.56 |
| 1 | JK | 33 | ALA | CA-C-N | 5.91 | 125.58 | 119.56 |
| 1 | JK | 33 | ALA | C-N-CA | 5.91 | 125.58 | 119.56 |
| 1 | YS | 19 | ARG | N-CA-C | -5.83 | 105.01 | 111.36 |
| 1 | JI | 19 | ARG | N-CA-C | -5.83 | 105.01 | 111.36 |
| 1 | YY | 19 | ARG | N-CA-C | -5.83 | 105.01 | 111.36 |
| 1 | HN | 19 | ARG | N-CA-C | -5.83 | 105.01 | 111.36 |
| 1 | BI | 19 | ARG | N-CA-C | -5.82 | 105.01 | 111.36 |
| 1 | YA | 19 | ARG | N-CA-C | -5.82 | 105.01 | 111.36 |
| 1 | JZ | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | LP | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | FT | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | IE | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | JC | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | KX | 19 | ARG | N-CA-C | -5.82 | 105.02 | 111.36 |
| 1 | GF | 19 | ARG | N-CA-C | -5.81 | 105.03 | 111.36 |
| 1 | HZ | 19 | ARG | N-CA-C | -5.81 | 105.03 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | CY | 19 | ARG | N-CA-C | -5.81 | 105.03 | 111.36 |
| 1 | EJ | 19 | ARG | N-CA-C | -5.81 | 105.03 | 111.36 |
| 1 | CM | 19 | ARG | N-CA-C | -5.80 | 105.03 | 111.36 |
| 1 | EP | 19 | ARG | N-CA-C | -5.80 | 105.03 | 111.36 |
| 1 | ZI | 19 | ARG | N-CA-C | -5.80 | 105.03 | 111.36 |
| 1 | KF | 19 | ARG | N-CA-C | -5.80 | 105.03 | 111.36 |
| 1 | AK | 19 | ARG | N-CA-C | -5.80 | 105.04 | 111.36 |
| 1 | ZC | 19 | ARG | N-CA-C | -5.80 | 105.04 | 111.36 |
| 1 | KL | 19 | ARG | N-CA-C | -5.80 | 105.04 | 111.36 |
| 1 | LJ | 19 | ARG | N-CA-C | -5.80 | 105.04 | 111.36 |
| 1 | YG | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | CA | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | CG | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | DK | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | ED | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | EV | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | FH | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | IQ | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | JO | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | LD | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | BC | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | DQ | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | FN | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | HI | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | AP | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | GX | 19 | ARG | N-CA-C | -5.79 | 105.05 | 111.36 |
| 1 | BO | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | ZO | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | AE | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | HT | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | DX | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | FB | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | AW | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | FZ | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | HD | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | IK | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | BU | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | ZU | 19 | ARG | N-CA-C | -5.78 | 105.06 | 111.36 |
| 1 | DE | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | GL | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | YM | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | WD | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | CS | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | GR | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | IW | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | KR | 19 | ARG | N-CA-C | -5.77 | 105.07 | 111.36 |
| 1 | GH | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | GH | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | WC | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | WC | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | AY | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | AY | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | WB | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | WB | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | YI | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | YI | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | JQ | 46 | ARG | CA-C-N | 5.70 | 125.80 | 119.87 |
| 1 | JQ | 46 | ARG | C-N-CA | 5.70 | 125.80 | 119.87 |
| 1 | CI | 46 | ARG | CA-C-N | 5.69 | 125.79 | 119.87 |
| 1 | CI | 46 | ARG | C-N-CA | 5.69 | 125.79 | 119.87 |
| 1 | DZ | 46 | ARG | CA-C-N | 5.69 | 125.78 | 119.87 |
| 1 | DZ | 46 | ARG | C-N-CA | 5.69 | 125.78 | 119.87 |
| 1 | EF | 46 | ARG | CA-C-N | 5.69 | 125.79 | 119.87 |
| 1 | EF | 46 | ARG | C-N-CA | 5.69 | 125.79 | 119.87 |
| 1 | FD | 46 | ARG | CA-C-N | 5.69 | 125.78 | 119.87 |
| 1 | FD | 46 | ARG | C-N-CA | 5.69 | 125.78 | 119.87 |
| 1 | DG | 46 | ARG | CA-C-N | 5.68 | 125.77 | 119.87 |
| 1 | DG | 46 | ARG | C-N-CA | 5.68 | 125.77 | 119.87 |
| 1 | GN | 46 | ARG | CA-C-N | 5.68 | 125.77 | 119.87 |
| 1 | GN | 46 | ARG | C-N-CA | 5.68 | 125.77 | 119.87 |
| 1 | KB | 46 | ARG | CA-C-N | 5.67 | 125.76 | 119.87 |
| 1 | KB | 46 | ARG | C-N-CA | 5.67 | 125.76 | 119.87 |
| 1 | LR | 46 | ARG | CA-C-N | 5.67 | 125.76 | 119.87 |
| 1 | LR | 46 | ARG | C-N-CA | 5.67 | 125.76 | 119.87 |
| 1 | KN | 46 | ARG | CA-C-N | 5.66 | 125.75 | 119.87 |
| 1 | KN | 46 | ARG | C-N-CA | 5.66 | 125.75 | 119.87 |
| 1 | LL | 46 | ARG | CA-C-N | 5.66 | 125.75 | 119.87 |
| 1 | LL | 46 | ARG | C-N-CA | 5.66 | 125.75 | 119.87 |
| 1 | DS | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | DS | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |
| 1 | FP | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | FP | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |
| 1 | DA | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | DA | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | EL | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | EL | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |
| 1 | FV | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | FV | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |
| 1 | IH | 46 | ARG | CA-C-N | 5.65 | 125.75 | 119.87 |
| 1 | IH | 46 | ARG | C-N-CA | 5.65 | 125.75 | 119.87 |
| 1 | JE | 46 | ARG | CA-C-N | 5.65 | 125.74 | 119.87 |
| 1 | JE | 46 | ARG | C-N-CA | 5.65 | 125.74 | 119.87 |
| 1 | KZ | 46 | ARG | CA-C-N | 5.65 | 125.74 | 119.87 |
| 1 | KZ | 46 | ARG | C-N-CA | 5.65 | 125.74 | 119.87 |
| 1 | CQ | 33 | ALA | CA-C-N | 5.61 | 125.29 | 119.56 |
| 1 | CQ | 33 | ALA | C-N-CA | 5.61 | 125.29 | 119.56 |
| 1 | GP | 33 | ALA | CA-C-N | 5.61 | 125.29 | 119.56 |
| 1 | GP | 33 | ALA | C-N-CA | 5.61 | 125.29 | 119.56 |
| 1 | ZG | 33 | ALA | CA-C-N | 5.61 | 125.28 | 119.56 |
| 1 | ZG | 33 | ALA | C-N-CA | 5.61 | 125.28 | 119.56 |
| 1 | KD | 33 | ALA | CA-C-N | 5.61 | 125.28 | 119.56 |
| 1 | KD | 33 | ALA | C-N-CA | 5.61 | 125.28 | 119.56 |
| 1 | GD | 33 | ALA | CA-C-N | 5.58 | 125.26 | 119.56 |
| 1 | GD | 33 | ALA | C-N-CA | 5.58 | 125.26 | 119.56 |
| 1 | HX | 33 | ALA | CA-C-N | 5.58 | 125.26 | 119.56 |
| 1 | HX | 33 | ALA | C-N-CA | 5.58 | 125.26 | 119.56 |
| 1 | YW | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | YW | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | HL | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | HL | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | IO | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | IO | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | LB | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | LB | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | YK | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | YK | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | JS | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | JS | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | AU | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | AU | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | HB | 33 | ALA | CA-C-N | 5.57 | 125.24 | 119.56 |
| 1 | HB | 33 | ALA | C-N-CA | 5.57 | 125.24 | 119.56 |
| 1 | JA | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | JA | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | KV | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | KV | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | CK | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | CK | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | EN | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | EN | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | DO | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | DO | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | DU | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | DU | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | EZ | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | EZ | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | FL | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | FL | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | CW | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | CW | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | EH | 33 | ALA | CA-C-N | 5.56 | 125.23 | 119.56 |
| 1 | EH | 33 | ALA | C-N-CA | 5.56 | 125.23 | 119.56 |
| 1 | AR | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | AR | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 1 | GV | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | GV | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 1 | AC | 60 | VAL | N-CA-C | 5.55 | 116.11 | 108.12 |
| 1 | BS | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | BS | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 2 | DD | 91 | ASN | CA-C-N | 5.55 | 125.64 | 119.87 |
| 2 | DD | 91 | ASN | C-N-CA | 5.55 | 125.64 | 119.87 |
| 1 | DI | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | DI | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 1 | FF | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | FF | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 2 | GK | 91 | ASN | CA-C-N | 5.55 | 125.64 | 119.87 |
| 2 | GK | 91 | ASN | C-N-CA | 5.55 | 125.64 | 119.87 |
| 1 | HR | 60 | VAL | N-CA-C | 5.55 | 116.11 | 108.12 |
| 1 | ZS | 33 | ALA | CA-C-N | 5.55 | 125.22 | 119.56 |
| 1 | ZS | 33 | ALA | C-N-CA | 5.55 | 125.22 | 119.56 |
| 1 | BA | 60 | VAL | N-CA-C | 5.54 | 116.11 | 108.12 |
| 1 | HG | 60 | VAL | N-CA-C | 5.54 | 116.11 | 108.12 |
| 1 | YE | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | YE | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | YE | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | DC | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | DC | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | FX | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | FX | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | GJ | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | GJ | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | II | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | II | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | JM | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | JM | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | JM | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | BA | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | BA | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | HG | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | HG | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | JX | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | LN | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | AC | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | AC | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | HR | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | HR | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | JA | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | KV | 60 | VAL | N-CA-C | 5.54 | 116.10 | 108.12 |
| 1 | ZA | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | ZA | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | AI | 33 | ALA | CA-C-N | 5.54 | 125.21 | 119.56 |
| 1 | AI | 33 | ALA | C-N-CA | 5.54 | 125.21 | 119.56 |
| 1 | DU | 60 | VAL | N-CA-C | 5.54 | 116.09 | 108.12 |
| 1 | EZ | 60 | VAL | N-CA-C | 5.54 | 116.09 | 108.12 |
| 1 | CE | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 1 | DC | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 1 | EB | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 1 | GJ | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 1 | CK | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 1 | EN | 60 | VAL | N-CA-C | 5.53 | 116.09 | 108.12 |
| 2 | YL | 91 | ASN | CA-C-N | 5.53 | 125.62 | 119.87 |
| 2 | YL | 91 | ASN | C-N-CA | 5.53 | 125.62 | 119.87 |
| 1 | DO | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | FL | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 2 | JT | 91 | ASN | CA-C-N | 5.53 | 125.62 | 119.87 |
| 2 | JT | 91 | ASN | C-N-CA | 5.53 | 125.62 | 119.87 |
| 1 | ZA | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | YQ | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | AI | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 2 | DF | 278 | ARG | CA-C-N | -5.53 | 115.90 | 123.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | DF | 278 | ARG | C-N-CA | -5.53 | 115.90 | 123.14 |
| 1 | ZG | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 2 | GM | 278 | ARG | CA-C-N | -5.53 | 115.90 | 123.14 |
| 2 | GM | 278 | ARG | C-N-CA | -5.53 | 115.90 | 123.14 |
| 1 | JG | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | KD | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | ZY | 33 | ALA | CA-C-N | 5.53 | 125.20 | 119.56 |
| 1 | ZY | 33 | ALA | C-N-CA | 5.53 | 125.20 | 119.56 |
| 1 | BG | 33 | ALA | CA-C-N | 5.53 | 125.20 | 119.56 |
| 1 | BG | 33 | ALA | C-N-CA | 5.53 | 125.20 | 119.56 |
| 1 | YW | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 2 | AX | 278 | ARG | CA-C-N | -5.53 | 115.90 | 123.14 |
| 2 | AX | 278 | ARG | C-N-CA | -5.53 | 115.90 | 123.14 |
| 1 | BS | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | CQ | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | FR | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | GP | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 2 | HE | 278 | ARG | CA-C-N | -5.53 | 115.90 | 123.14 |
| 2 | HE | 278 | ARG | C-N-CA | -5.53 | 115.90 | 123.14 |
| 1 | HL | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | IC | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | IU | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | KP | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | ZS | 60 | VAL | N-CA-C | 5.53 | 116.08 | 108.12 |
| 1 | YQ | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | YQ | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | DY | 278 | ARG | CA-C-N | -5.52 | 115.90 | 123.14 |
| 2 | DY | 278 | ARG | C-N-CA | -5.52 | 115.90 | 123.14 |
| 2 | FC | 278 | ARG | CA-C-N | -5.52 | 115.90 | 123.14 |
| 2 | FC | 278 | ARG | C-N-CA | -5.52 | 115.90 | 123.14 |
| 2 | JB | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | JB | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 1 | JG | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | JG | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | KW | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | KW | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 1 | CW | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 1 | EH | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 1 | FR | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | FR | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | FY | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | FY | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | IC | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | IC | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | IJ | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | IJ | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 1 | IO | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 1 | KJ | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | KJ | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | LB | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 1 | LH | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | LH | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | BY | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | BY | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | DP | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | DP | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 1 | ET | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | ET | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | FM | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | FM | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 2 | GE | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | GE | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 2 | HY | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | HY | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 1 | KJ | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 1 | LH | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 2 | AF | 278 | ARG | CA-C-N | -5.52 | 115.91 | 123.14 |
| 2 | AF | 278 | ARG | C-N-CA | -5.52 | 115.91 | 123.14 |
| 2 | CF | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | CF | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 2 | CX | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | CX | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 2 | EC | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | EC | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 2 | EI | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | EI | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 1 | FX | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 2 | HU | 278 | ARG | CA-C-N | -5.52 | 115.91 | 123.14 |
| 2 | HU | 278 | ARG | C-N-CA | -5.52 | 115.91 | 123.14 |
| 1 | II | 60 | VAL | N-CA-C | 5.52 | 116.07 | 108.12 |
| 2 | BD | 278 | ARG | CA-C-N | -5.52 | 115.91 | 123.14 |
| 2 | BD | 278 | ARG | C-N-CA | -5.52 | 115.91 | 123.14 |
| 2 | BN | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | BN | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | BY | 60 | VAL | N-CA-C | 5.52 | 116.06 | 108.12 |
| 2 | BZ | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | BZ | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 1 | ET | 60 | VAL | N-CA-C | 5.52 | 116.06 | 108.12 |
| 2 | EU | 36 | ASN | CA-C-N | 5.52 | 125.42 | 119.85 |
| 2 | EU | 36 | ASN | C-N-CA | 5.52 | 125.42 | 119.85 |
| 2 | HJ | 278 | ARG | CA-C-N | -5.52 | 115.91 | 123.14 |
| 2 | HJ | 278 | ARG | C-N-CA | -5.52 | 115.91 | 123.14 |
| 1 | IU | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | IU | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | JX | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | JX | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | KP | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | KP | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 1 | LN | 33 | ALA | CA-C-N | 5.52 | 125.19 | 119.56 |
| 1 | LN | 33 | ALA | C-N-CA | 5.52 | 125.19 | 119.56 |
| 2 | ZN | 91 | ASN | CA-C-N | 5.52 | 125.61 | 119.87 |
| 2 | ZN | 91 | ASN | C-N-CA | 5.52 | 125.61 | 119.87 |
| 2 | AO | 278 | ARG | CA-C-N | -5.51 | 115.92 | 123.14 |
| 2 | AO | 278 | ARG | C-N-CA | -5.51 | 115.92 | 123.14 |
| 2 | DW | 141 | ASP | CA-C-N | 5.51 | 125.61 | 119.87 |
| 2 | DW | 141 | ASP | C-N-CA | 5.51 | 125.61 | 119.87 |
| 2 | FA | 141 | ASP | CA-C-N | 5.51 | 125.61 | 119.87 |
| 2 | FA | 141 | ASP | C-N-CA | 5.51 | 125.61 | 119.87 |
| 2 | GY | 278 | ARG | CA-C-N | -5.51 | 115.92 | 123.14 |
| 2 | GY | 278 | ARG | C-N-CA | -5.51 | 115.92 | 123.14 |
| 1 | YK | 60 | VAL | N-CA-C | 5.51 | 116.06 | 108.12 |
| 2 | JD | 278 | ARG | CA-C-N | -5.51 | 115.92 | 123.14 |
| 2 | JD | 278 | ARG | C-N-CA | -5.51 | 115.92 | 123.14 |
| 1 | JS | 60 | VAL | N-CA-C | 5.51 | 116.06 | 108.12 |
| 2 | KY | 278 | ARG | CA-C-N | -5.51 | 115.92 | 123.14 |
| 2 | KY | 278 | ARG | C-N-CA | -5.51 | 115.92 | 123.14 |
| 2 | AV | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | AV | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 1 | GD | 60 | VAL | N-CA-C | 5.51 | 116.06 | 108.12 |
| 2 | HC | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | HC | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 1 | HX | 60 | VAL | N-CA-C | 5.51 | 116.06 | 108.12 |
| 1 | ZY | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 1 | BG | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 1 | AR | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 1 | BM | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | DI | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 2 | DP | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | DP | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 1 | FF | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 2 | FM | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | FM | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 1 | GV | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 2 | IP | 141 | ASP | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | IP | 141 | ASP | C-N-CA | 5.51 | 125.60 | 119.87 |
| 1 | ZM | 60 | VAL | N-CA-C | 5.51 | 116.05 | 108.12 |
| 2 | LC | 141 | ASP | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | LC | 141 | ASP | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | AD | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | AD | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | AQ | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | AQ | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | BT | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | BT | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | FS | 36 | ASN | CA-C-N | 5.51 | 125.41 | 119.85 |
| 2 | FS | 36 | ASN | C-N-CA | 5.51 | 125.41 | 119.85 |
| 2 | GW | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | GW | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | HS | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | HS | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | ID | 36 | ASN | CA-C-N | 5.51 | 125.41 | 119.85 |
| 2 | ID | 36 | ASN | C-N-CA | 5.51 | 125.41 | 119.85 |
| 2 | ZT | 91 | ASN | CA-C-N | 5.51 | 125.60 | 119.87 |
| 2 | ZT | 91 | ASN | C-N-CA | 5.51 | 125.60 | 119.87 |
| 2 | CF | 36 | ASN | CA-C-N | 5.50 | 125.41 | 119.85 |
| 2 | CF | 36 | ASN | C-N-CA | 5.50 | 125.41 | 119.85 |
| 2 | EC | 36 | ASN | CA-C-N | 5.50 | 125.41 | 119.85 |
| 2 | EC | 36 | ASN | C-N-CA | 5.50 | 125.41 | 119.85 |
| 2 | YR | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | YR | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | ZB | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | ZB | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | AJ | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | AJ | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | AQ | 36 | ASN | CA-C-N | 5.50 | 125.41 | 119.85 |
| 2 | AQ | 36 | ASN | C-N-CA | 5.50 | 125.41 | 119.85 |
| 2 | GW | 36 | ASN | CA-C-N | 5.50 | 125.41 | 119.85 |
| 2 | GW | 36 | ASN | C-N-CA | 5.50 | 125.41 | 119.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | JH | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | JH | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 1 | AU | 60 | VAL | N-CA-C | 5.50 | 116.04 | 108.12 |
| 1 | CE | 33 | ALA | CA-C-N | 5.50 | 125.17 | 119.56 |
| 1 | CE | 33 | ALA | C-N-CA | 5.50 | 125.17 | 119.56 |
| 1 | EB | 33 | ALA | CA-C-N | 5.50 | 125.17 | 119.56 |
| 1 | EB | 33 | ALA | C-N-CA | 5.50 | 125.17 | 119.56 |
| 1 | HB | 60 | VAL | N-CA-C | 5.50 | 116.04 | 108.12 |
| 2 | DR | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | DR | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | FO | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | FO | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | KK | 141 | ASP | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | KK | 141 | ASP | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | LI | 141 | ASP | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | LI | 141 | ASP | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | ZZ | 36 | ASN | CA-C-N | 5.50 | 125.40 | 119.85 |
| 2 | ZZ | 36 | ASN | C-N-CA | 5.50 | 125.40 | 119.85 |
| 2 | BH | 36 | ASN | CA-C-N | 5.50 | 125.40 | 119.85 |
| 2 | BH | 36 | ASN | C-N-CA | 5.50 | 125.40 | 119.85 |
| 2 | DL | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | DL | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | FI | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | FI | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | YZ | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | YZ | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | ZH | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | ZH | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | HO | 278 | ARG | CA-C-N | -5.50 | 115.94 | 123.14 |
| 2 | HO | 278 | ARG | C-N-CA | -5.50 | 115.94 | 123.14 |
| 2 | KE | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | KE | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | KK | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | KK | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | LI | 91 | ASN | CA-C-N | 5.50 | 125.59 | 119.87 |
| 2 | LI | 91 | ASN | C-N-CA | 5.50 | 125.59 | 119.87 |
| 2 | FS | 91 | ASN | CA-C-N | 5.50 | 125.58 | 119.87 |
| 2 | FS | 91 | ASN | C-N-CA | 5.50 | 125.58 | 119.87 |
| 2 | ID | 91 | ASN | CA-C-N | 5.50 | 125.58 | 119.87 |
| 2 | ID | 91 | ASN | C-N-CA | 5.50 | 125.58 | 119.87 |
| 2 | YT | 278 | ARG | CA-C-N | -5.49 | 115.94 | 123.14 |
| 2 | YT | 278 | ARG | C-N-CA | -5.49 | 115.94 | 123.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | BZ | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | BZ | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | EU | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | EU | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | GA | 278 | ARG | CA-C-N | -5.49 | 115.94 | 123.14 |
| 2 | GA | 278 | ARG | C-N-CA | -5.49 | 115.94 | 123.14 |
| 2 | IL | 278 | ARG | CA-C-N | -5.49 | 115.94 | 123.14 |
| 2 | IL | 278 | ARG | C-N-CA | -5.49 | 115.94 | 123.14 |
| 2 | IV | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | IV | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | JJ | 278 | ARG | CA-C-N | -5.49 | 115.94 | 123.14 |
| 2 | JJ | 278 | ARG | C-N-CA | -5.49 | 115.94 | 123.14 |
| 2 | KQ | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | KQ | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | BN | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | BN | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | CL | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | CL | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | CL | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | CL | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | EO | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | EO | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | EO | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | EO | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | IR | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | IR | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | KA | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | KA | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | LE | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | LE | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | LQ | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | LQ | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | ZN | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | ZN | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | YR | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | YR | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | DW | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | DW | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | FA | 91 | ASN | CA-C-N | 5.49 | 125.58 | 119.87 |
| 2 | FA | 91 | ASN | C-N-CA | 5.49 | 125.58 | 119.87 |
| 2 | JH | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | JH | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | KK | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | KK | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | KM | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | KM | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | LI | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | LI | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | LK | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | LK | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | BP | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | BP | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | ZP | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | ZP | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | GE | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | GE | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | HY | 36 | ASN | CA-C-N | 5.49 | 125.39 | 119.85 |
| 2 | HY | 36 | ASN | C-N-CA | 5.49 | 125.39 | 119.85 |
| 2 | ZJ | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | ZJ | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | KG | 278 | ARG | CA-C-N | -5.49 | 115.95 | 123.14 |
| 2 | KG | 278 | ARG | C-N-CA | -5.49 | 115.95 | 123.14 |
| 2 | AL | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | AL | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | ZD | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | ZD | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | CN | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | CN | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | CX | 91 | ASN | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | CX | 91 | ASN | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | EI | 91 | ASN | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | EI | 91 | ASN | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | EQ | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | EQ | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | FU | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | FU | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | IF | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | IF | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | IV | 36 | ASN | CA-C-N | 5.48 | 125.39 | 119.85 |
| 2 | IV | 36 | ASN | C-N-CA | 5.48 | 125.39 | 119.85 |
| 2 | KQ | 36 | ASN | CA-C-N | 5.48 | 125.39 | 119.85 |
| 2 | KQ | 36 | ASN | C-N-CA | 5.48 | 125.39 | 119.85 |
| 2 | CT | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | CT | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | GS | 278 | ARG | CA-C-N | -5.48 | 115.96 | 123.14 |
| 2 | GS | 278 | ARG | C-N-CA | -5.48 | 115.96 | 123.14 |
| 2 | IP | 36 | ASN | CA-C-N | 5.48 | 125.39 | 119.85 |
| 2 | IP | 36 | ASN | C-N-CA | 5.48 | 125.39 | 119.85 |
| 2 | JY | 91 | ASN | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | JY | 91 | ASN | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | LC | 36 | ASN | CA-C-N | 5.48 | 125.39 | 119.85 |
| 2 | LC | 36 | ASN | C-N-CA | 5.48 | 125.39 | 119.85 |
| 2 | LO | 91 | ASN | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | LO | 91 | ASN | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | CL | 141 | ASP | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | CL | 141 | ASP | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | DJ | 36 | ASN | CA-C-N | 5.48 | 125.38 | 119.85 |
| 2 | DJ | 36 | ASN | C-N-CA | 5.48 | 125.38 | 119.85 |
| 2 | EO | 141 | ASP | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | EO | 141 | ASP | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | FG | 36 | ASN | CA-C-N | 5.48 | 125.38 | 119.85 |
| 2 | FG | 36 | ASN | C-N-CA | 5.48 | 125.38 | 119.85 |
| 2 | BZ | 141 | ASP | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | BZ | 141 | ASP | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | CZ | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | CZ | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | EK | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | EK | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | EU | 141 | ASP | CA-C-N | 5.48 | 125.57 | 119.87 |
| 2 | EU | 141 | ASP | C-N-CA | 5.48 | 125.57 | 119.87 |
| 2 | GG | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | GG | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | IA | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | IA | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | YN | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | YN | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | ZH | 36 | ASN | CA-C-N | 5.48 | 125.38 | 119.85 |
| 2 | ZH | 36 | ASN | C-N-CA | 5.48 | 125.38 | 119.85 |
| 2 | JU | 278 | ARG | CA-C-N | -5.48 | 115.97 | 123.14 |
| 2 | JU | 278 | ARG | C-N-CA | -5.48 | 115.97 | 123.14 |
| 2 | KE | 36 | ASN | CA-C-N | 5.48 | 125.38 | 119.85 |
| 2 | KE | 36 | ASN | C-N-CA | 5.48 | 125.38 | 119.85 |
| 2 | BJ | 278 | ARG | CA-C-N | -5.47 | 115.97 | 123.14 |
| 2 | BJ | 278 | ARG | C-N-CA | -5.47 | 115.97 | 123.14 |
| 1 | BM | 33 | ALA | CA-C-N | 5.47 | 125.14 | 119.56 |
| 1 | BM | 33 | ALA | C-N-CA | 5.47 | 125.14 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | DJ | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | DJ | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | FG | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | FG | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | JB | 36 | ASN | CA-C-N | 5.47 | 125.38 | 119.85 |
| 2 | JB | 36 | ASN | C-N-CA | 5.47 | 125.38 | 119.85 |
| 2 | KW | 36 | ASN | CA-C-N | 5.47 | 125.38 | 119.85 |
| 2 | KW | 36 | ASN | C-N-CA | 5.47 | 125.38 | 119.85 |
| 1 | ZM | 33 | ALA | CA-C-N | 5.47 | 125.14 | 119.56 |
| 1 | ZM | 33 | ALA | C-N-CA | 5.47 | 125.14 | 119.56 |
| 2 | YB | 278 | ARG | CA-C-N | -5.47 | 115.97 | 123.14 |
| 2 | YB | 278 | ARG | C-N-CA | -5.47 | 115.97 | 123.14 |
| 2 | AV | 36 | ASN | CA-C-N | 5.47 | 125.38 | 119.85 |
| 2 | AV | 36 | ASN | C-N-CA | 5.47 | 125.38 | 119.85 |
| 2 | BB | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | BB | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | HC | 36 | ASN | CA-C-N | 5.47 | 125.38 | 119.85 |
| 2 | HC | 36 | ASN | C-N-CA | 5.47 | 125.38 | 119.85 |
| 2 | HH | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | HH | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | YX | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | YX | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | DD | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | DD | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | GK | 141 | ASP | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | GK | 141 | ASP | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | HM | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | HM | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | ZZ | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | ZZ | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | YL | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | YL | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | ZB | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | ZB | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | AJ | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | AJ | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | BH | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | BH | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | CH | 278 | ARG | CA-C-N | -5.47 | 115.97 | 123.14 |
| 2 | CH | 278 | ARG | C-N-CA | -5.47 | 115.97 | 123.14 |
| 2 | EE | 278 | ARG | CA-C-N | -5.47 | 115.97 | 123.14 |
| 2 | EE | 278 | ARG | C-N-CA | -5.47 | 115.97 | 123.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | JT | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | JT | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | CR | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | CR | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | DJ | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | DJ | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | FG | 91 | ASN | CA-C-N | 5.47 | 125.56 | 119.87 |
| 2 | FG | 91 | ASN | C-N-CA | 5.47 | 125.56 | 119.87 |
| 2 | GQ | 36 | ASN | CA-C-N | 5.47 | 125.37 | 119.85 |
| 2 | GQ | 36 | ASN | C-N-CA | 5.47 | 125.37 | 119.85 |
| 2 | YH | 278 | ARG | CA-C-N | -5.47 | 115.98 | 123.14 |
| 2 | YH | 278 | ARG | C-N-CA | -5.47 | 115.98 | 123.14 |
| 2 | IX | 278 | ARG | CA-C-N | -5.47 | 115.98 | 123.14 |
| 2 | IX | 278 | ARG | C-N-CA | -5.47 | 115.98 | 123.14 |
| 2 | JP | 278 | ARG | CA-C-N | -5.47 | 115.98 | 123.14 |
| 2 | JP | 278 | ARG | C-N-CA | -5.47 | 115.98 | 123.14 |
| 2 | KS | 278 | ARG | CA-C-N | -5.47 | 115.98 | 123.14 |
| 2 | KS | 278 | ARG | C-N-CA | -5.47 | 115.98 | 123.14 |
| 2 | ZZ | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | ZZ | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | BH | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | BH | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | DW | 36 | ASN | CA-C-N | 5.46 | 125.37 | 119.85 |
| 2 | DW | 36 | ASN | C-N-CA | 5.46 | 125.37 | 119.85 |
| 2 | FA | 36 | ASN | CA-C-N | 5.46 | 125.37 | 119.85 |
| 2 | FA | 36 | ASN | C-N-CA | 5.46 | 125.37 | 119.85 |
| 2 | ZB | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | ZB | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | AD | 36 | ASN | CA-C-N | 5.46 | 125.37 | 119.85 |
| 2 | AD | 36 | ASN | C-N-CA | 5.46 | 125.37 | 119.85 |
| 2 | AJ | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | AJ | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | CR | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | CR | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | CX | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | CX | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | EI | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | EI | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | GQ | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | GQ | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | HS | 36 | ASN | CA-C-N | 5.46 | 125.37 | 119.85 |
| 2 | HS | 36 | ASN | C-N-CA | 5.46 | 125.37 | 119.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | YX | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | YX | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | BV | 278 | ARG | CA-C-N | -5.46 | 115.98 | 123.14 |
| 2 | BV | 278 | ARG | C-N-CA | -5.46 | 115.98 | 123.14 |
| 2 | HM | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | HM | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | IP | 91 | ASN | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | IP | 91 | ASN | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | LC | 91 | ASN | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | LC | 91 | ASN | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | ZV | 278 | ARG | CA-C-N | -5.46 | 115.98 | 123.14 |
| 2 | ZV | 278 | ARG | C-N-CA | -5.46 | 115.98 | 123.14 |
| 2 | YR | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | YR | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | YX | 36 | ASN | CA-C-N | 5.46 | 125.36 | 119.85 |
| 2 | YX | 36 | ASN | C-N-CA | 5.46 | 125.36 | 119.85 |
| 2 | CR | 91 | ASN | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | CR | 91 | ASN | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | GQ | 91 | ASN | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | GQ | 91 | ASN | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | HM | 36 | ASN | CA-C-N | 5.46 | 125.36 | 119.85 |
| 2 | HM | 36 | ASN | C-N-CA | 5.46 | 125.36 | 119.85 |
| 2 | JH | 141 | ASP | CA-C-N | 5.46 | 125.55 | 119.87 |
| 2 | JH | 141 | ASP | C-N-CA | 5.46 | 125.55 | 119.87 |
| 2 | IV | 141 | ASP | CA-C-N | 5.46 | 125.54 | 119.87 |
| 2 | IV | 141 | ASP | C-N-CA | 5.46 | 125.54 | 119.87 |
| 2 | KQ | 141 | ASP | CA-C-N | 5.46 | 125.54 | 119.87 |
| 2 | KQ | 141 | ASP | C-N-CA | 5.46 | 125.54 | 119.87 |
| 2 | YF | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | YF | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | JN | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | JN | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | CB | 278 | ARG | CA-C-N | -5.45 | 116.00 | 123.14 |
| 2 | CB | 278 | ARG | C-N-CA | -5.45 | 116.00 | 123.14 |
| 2 | EW | 278 | ARG | CA-C-N | -5.45 | 116.00 | 123.14 |
| 2 | EW | 278 | ARG | C-N-CA | -5.45 | 116.00 | 123.14 |
| 2 | GE | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | GE | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | HY | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | HY | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | JB | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | JB | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | KW | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | KW | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | CF | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | CF | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | EC | 141 | ASP | CA-C-N | 5.45 | 125.54 | 119.87 |
| 2 | EC | 141 | ASP | C-N-CA | 5.45 | 125.54 | 119.87 |
| 2 | YF | 36 | ASN | CA-C-N | 5.45 | 125.35 | 119.85 |
| 2 | YF | 36 | ASN | C-N-CA | 5.45 | 125.35 | 119.85 |
| 2 | JN | 36 | ASN | CA-C-N | 5.45 | 125.35 | 119.85 |
| 2 | JN | 36 | ASN | C-N-CA | 5.45 | 125.35 | 119.85 |
| 2 | AQ | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | AQ | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | BN | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | BN | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | BT | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | BT | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | GW | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | GW | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | JY | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | JY | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | LO | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | LO | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | ZN | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | ZN | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | ZT | 141 | ASP | CA-C-N | 5.45 | 125.53 | 119.87 |
| 2 | ZT | 141 | ASP | C-N-CA | 5.45 | 125.53 | 119.87 |
| 2 | BB | 36 | ASN | CA-C-N | 5.44 | 125.35 | 119.85 |
| 2 | BB | 36 | ASN | C-N-CA | 5.44 | 125.35 | 119.85 |
| 2 | HH | 36 | ASN | CA-C-N | 5.44 | 125.35 | 119.85 |
| 2 | HH | 36 | ASN | C-N-CA | 5.44 | 125.35 | 119.85 |
| 2 | YF | 91 | ASN | CA-C-N | 5.44 | 125.53 | 119.87 |
| 2 | YF | 91 | ASN | C-N-CA | 5.44 | 125.53 | 119.87 |
| 2 | DP | 141 | ASP | CA-C-N | 5.44 | 125.53 | 119.87 |
| 2 | DP | 141 | ASP | C-N-CA | 5.44 | 125.53 | 119.87 |
| 2 | FM | 141 | ASP | CA-C-N | 5.44 | 125.53 | 119.87 |
| 2 | FM | 141 | ASP | C-N-CA | 5.44 | 125.53 | 119.87 |
| 2 | JN | 91 | ASN | CA-C-N | 5.44 | 125.53 | 119.87 |
| 2 | JN | 91 | ASN | C-N-CA | 5.44 | 125.53 | 119.87 |
| 2 | BT | 36 | ASN | CA-C-N | 5.44 | 125.34 | 119.85 |
| 2 | BT | 36 | ASN | C-N-CA | 5.44 | 125.34 | 119.85 |
| 2 | ZT | 36 | ASN | CA-C-N | 5.44 | 125.34 | 119.85 |
| 2 | ZT | 36 | ASN | C-N-CA | 5.44 | 125.34 | 119.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | FY | 141 | ASP | CA-C-N | 5.44 | 125.52 | 119.87 |
| 2 | FY | 141 | ASP | C-N-CA | 5.44 | 125.52 | 119.87 |
| 2 | IJ | 141 | ASP | CA-C-N | 5.44 | 125.52 | 119.87 |
| 2 | IJ | 141 | ASP | C-N-CA | 5.44 | 125.52 | 119.87 |
| 2 | YL | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | YL | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | ZH | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | ZH | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | JT | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | JT | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | KE | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | KE | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | DD | 36 | ASN | CA-C-N | 5.43 | 125.34 | 119.85 |
| 2 | DD | 36 | ASN | C-N-CA | 5.43 | 125.34 | 119.85 |
| 2 | GK | 36 | ASN | CA-C-N | 5.43 | 125.34 | 119.85 |
| 2 | GK | 36 | ASN | C-N-CA | 5.43 | 125.34 | 119.85 |
| 2 | FS | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | FS | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | ID | 141 | ASP | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | ID | 141 | ASP | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | JY | 36 | ASN | CA-C-N | 5.43 | 125.33 | 119.85 |
| 2 | JY | 36 | ASN | C-N-CA | 5.43 | 125.33 | 119.85 |
| 2 | LO | 36 | ASN | CA-C-N | 5.43 | 125.33 | 119.85 |
| 2 | LO | 36 | ASN | C-N-CA | 5.43 | 125.33 | 119.85 |
| 2 | BB | 91 | ASN | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | BB | 91 | ASN | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | FY | 36 | ASN | CA-C-N | 5.43 | 125.33 | 119.85 |
| 2 | FY | 36 | ASN | C-N-CA | 5.43 | 125.33 | 119.85 |
| 2 | HH | 91 | ASN | CA-C-N | 5.43 | 125.52 | 119.87 |
| 2 | HH | 91 | ASN | C-N-CA | 5.43 | 125.52 | 119.87 |
| 2 | IJ | 36 | ASN | CA-C-N | 5.43 | 125.33 | 119.85 |
| 2 | IJ | 36 | ASN | C-N-CA | 5.43 | 125.33 | 119.85 |
| 2 | AV | 141 | ASP | CA-C-N | 5.42 | 125.51 | 119.87 |
| 2 | AV | 141 | ASP | C-N-CA | 5.42 | 125.51 | 119.87 |
| 2 | HC | 141 | ASP | CA-C-N | 5.42 | 125.51 | 119.87 |
| 2 | HC | 141 | ASP | C-N-CA | 5.42 | 125.51 | 119.87 |
| 2 | DN | 227 | ILE | CB-CA-C | -5.42 | 105.04 | 111.97 |
| 2 | FK | 227 | ILE | CB-CA-C | -5.42 | 105.04 | 111.97 |
| 2 | AD | 141 | ASP | CA-C-N | 5.41 | 125.50 | 119.87 |
| 2 | AD | 141 | ASP | C-N-CA | 5.41 | 125.50 | 119.87 |
| 2 | HS | 141 | ASP | CA-C-N | 5.41 | 125.50 | 119.87 |
| 2 | HS | 141 | ASP | C-N-CA | 5.41 | 125.50 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | ZL | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | KI | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | BX | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | IT | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | LG | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | ZX | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | GC | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | IN | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | GI | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | IB | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | IZ | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | KU | 227 | ILE | CB-CA-C | -5.39 | 105.07 | 111.97 |
| 2 | YV | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | BR | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | DH | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | GO | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | JL | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | ZR | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | CV | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | GU | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | AN | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | ZF | 227 | ILE | CB-CA-C | -5.38 | 105.08 | 111.97 |
| 2 | YJ | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | AZ | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | HF | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | JR | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | FW | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | IG | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | YP | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | JW | 227 | ILE | CB-CA-C | -5.38 | 105.09 | 111.97 |
| 2 | CJ | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | EG | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | AT | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | DB | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | EM | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | HA | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | KC | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | LS | 227 | ILE | CB-CA-C | -5.37 | 105.09 | 111.97 |
| 2 | AB | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | HQ | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | KO | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | LM | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | YD | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | BL | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | CP | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | ES | 227 | ILE | CB-CA-C | -5.37 | 105.10 | 111.97 |
| 2 | BF | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | CD | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | EY | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | HK | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | EA | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | FE | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | DT | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | FQ | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | JF | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | LA | 227 | ILE | CB-CA-C | -5.36 | 105.11 | 111.97 |
| 2 | AH | 227 | ILE | CB-CA-C | -5.34 | 105.13 | 111.97 |
| 2 | HW | 227 | ILE | CB-CA-C | -5.34 | 105.13 | 111.97 |
| 1 | CS | 36 | VAL | N-CA-C | -5.33 | 105.18 | 110.62 |
| 1 | GR | 36 | VAL | N-CA-C | -5.33 | 105.18 | 110.62 |
| 1 | IQ | 36 | VAL | N-CA-C | -5.33 | 105.19 | 110.62 |
| 1 | LD | 36 | VAL | N-CA-C | -5.33 | 105.19 | 110.62 |
| 1 | JZ | 36 | VAL | N-CA-C | -5.31 | 105.20 | 110.62 |
| 1 | LP | 36 | VAL | N-CA-C | -5.31 | 105.20 | 110.62 |
| 1 | CM | 36 | VAL | N-CA-C | -5.31 | 105.20 | 110.62 |
| 1 | EP | 36 | VAL | N-CA-C | -5.31 | 105.20 | 110.62 |
| 1 | AW | 36 | VAL | N-CA-C | -5.30 | 105.21 | 110.62 |
| 1 | CY | 35 | VAL | N-CA-C | -5.30 | 105.22 | 111.00 |
| 1 | DX | 36 | VAL | N-CA-C | -5.30 | 105.21 | 110.62 |
| 1 | EJ | 35 | VAL | N-CA-C | -5.30 | 105.22 | 111.00 |
| 1 | FB | 36 | VAL | N-CA-C | -5.30 | 105.21 | 110.62 |
| 1 | HD | 36 | VAL | N-CA-C | -5.30 | 105.21 | 110.62 |
| 1 | FT | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | IE | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | YS | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | CA | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | EV | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | JI | 36 | VAL | N-CA-C | -5.30 | 105.22 | 110.62 |
| 1 | ZI | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | KF | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | BA | 1 | PRO | CA-C-N | 5.29 | 128.99 | 121.42 |
| 1 | BA | 1 | PRO | C-N-CA | 5.29 | 128.99 | 121.42 |
| 1 | HG | 1 | PRO | CA-C-N | 5.29 | 128.99 | 121.42 |
| 1 | HG | 1 | PRO | C-N-CA | 5.29 | 128.99 | 121.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | DO | 1 | PRO | CA-C-N | 5.29 | 128.99 | 121.42 |
| 1 | DO | 1 | PRO | C-N-CA | 5.29 | 128.99 | 121.42 |
| 1 | FL | 1 | PRO | CA-C-N | 5.29 | 128.99 | 121.42 |
| 1 | FL | 1 | PRO | C-N-CA | 5.29 | 128.99 | 121.42 |
| 1 | IW | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | JC | 35 | VAL | N-CA-C | -5.29 | 105.23 | 111.00 |
| 1 | KR | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | KX | 35 | VAL | N-CA-C | -5.29 | 105.23 | 111.00 |
| 1 | CG | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | DE | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | ED | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | GL | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | DQ | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | FN | 36 | VAL | N-CA-C | -5.29 | 105.22 | 110.62 |
| 1 | YW | 1 | PRO | CA-C-N | 5.29 | 128.98 | 121.42 |
| 1 | YW | 1 | PRO | C-N-CA | 5.29 | 128.98 | 121.42 |
| 1 | AK | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | ZC | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | CM | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | DE | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | EP | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | GL | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | HL | 1 | PRO | CA-C-N | 5.29 | 128.98 | 121.42 |
| 1 | HL | 1 | PRO | C-N-CA | 5.29 | 128.98 | 121.42 |
| 1 | CY | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | EJ | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | FZ | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | IK | 36 | VAL | N-CA-C | -5.29 | 105.23 | 110.62 |
| 1 | KL | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | LJ | 35 | VAL | N-CA-C | -5.29 | 105.24 | 111.00 |
| 1 | ZY | 1 | PRO | CA-C-N | 5.28 | 128.98 | 121.42 |
| 1 | ZY | 1 | PRO | C-N-CA | 5.28 | 128.98 | 121.42 |
| 1 | YY | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | AP | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | BG | 1 | PRO | CA-C-N | 5.28 | 128.98 | 121.42 |
| 1 | BG | 1 | PRO | C-N-CA | 5.28 | 128.98 | 121.42 |
| 1 | GX | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | HN | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | YS | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | JI | 35 | VAL | N-CA-C | -5.28 | 105.24 | 111.00 |
| 1 | YG | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | BC | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | DK | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |
| 1 | FH | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |
| 1 | HI | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |
| 1 | JO | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | JZ | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | LP | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | BI | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | JC | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |
| 1 | KX | 36 | VAL | N-CA-C | -5.28 | 105.24 | 110.62 |
| 1 | YA | 35 | VAL | N-CA-C | -5.28 | 105.25 | 111.00 |
| 1 | ZG | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | ZG | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | IO | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | IO | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | KD | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | KD | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | LB | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | LB | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | AR | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | AR | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | DQ | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | FN | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | GD | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | GD | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | GV | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | GV | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | HX | 1 | PRO | CA-C-N | 5.27 | 128.96 | 121.42 |
| 1 | HX | 1 | PRO | C-N-CA | 5.27 | 128.96 | 121.42 |
| 1 | YM | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | AP | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | BU | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | DU | 32 | LEU | N-CA-C | -5.27 | 106.98 | 113.41 |
| 1 | EZ | 32 | LEU | N-CA-C | -5.27 | 106.98 | 113.41 |
| 1 | FT | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | FZ | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | GX | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | IE | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | IK | 35 | VAL | N-CA-C | -5.27 | 105.25 | 111.00 |
| 1 | WD | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | ZU | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | YE | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | YE | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | YG | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | BC | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | CK | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | CK | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | DC | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | DC | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | EN | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | EN | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | GJ | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | GJ | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | HI | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | JM | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | JM | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | JO | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | CE | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | CE | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | EB | 1 | PRO | CA-C-N | 5.27 | 128.95 | 121.42 |
| 1 | EB | 1 | PRO | C-N-CA | 5.27 | 128.95 | 121.42 |
| 1 | ZI | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | KF | 35 | VAL | N-CA-C | -5.27 | 105.26 | 111.00 |
| 1 | KL | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | LJ | 36 | VAL | N-CA-C | -5.27 | 105.25 | 110.62 |
| 1 | ZA | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | ZA | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | AI | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | AI | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | CW | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | CW | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | DM | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |
| 1 | EH | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | EH | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | FJ | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |
| 1 | YQ | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | YQ | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | BS | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | BS | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | BY | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | BY | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | CS | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |
| 1 | ET | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | ET | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | GR | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | JG | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | JG | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | KB | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |
| 1 | LR | 35 | VAL | N-CA-C | -5.26 | 105.26 | 111.00 |
| 1 | ZS | 1 | PRO | CA-C-N | 5.26 | 128.95 | 121.42 |
| 1 | ZS | 1 | PRO | C-N-CA | 5.26 | 128.95 | 121.42 |
| 1 | ZY | 32 | LEU | N-CA-C | -5.26 | 106.99 | 113.41 |
| 1 | YY | 36 | VAL | N-CA-C | -5.26 | 105.25 | 110.62 |
| 1 | BG | 32 | LEU | N-CA-C | -5.26 | 106.99 | 113.41 |
| 1 | HN | 36 | VAL | N-CA-C | -5.26 | 105.25 | 110.62 |
| 1 | IU | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | IU | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | KJ | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | KJ | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | KP | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | KP | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | LH | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | LH | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | KJ | 32 | LEU | N-CA-C | -5.26 | 106.99 | 113.41 |
| 1 | LH | 32 | LEU | N-CA-C | -5.26 | 106.99 | 113.41 |
| 1 | AC | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | AC | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | AU | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | AU | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | BO | 36 | VAL | N-CA-C | -5.26 | 105.26 | 110.62 |
| 1 | CQ | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | CQ | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | ZG | 32 | LEU | N-CA-C | -5.26 | 107.00 | 113.41 |
| 1 | GP | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | GP | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | HB | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | HB | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | HR | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | HR | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | KD | 32 | LEU | N-CA-C | -5.26 | 107.00 | 113.41 |
| 1 | ZO | 36 | VAL | N-CA-C | -5.26 | 105.26 | 110.62 |
| 1 | YK | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |
| 1 | YK | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | AK | 35 | VAL | N-CA-C | -5.26 | 105.27 | 111.00 |
| 1 | ZC | 35 | VAL | N-CA-C | -5.26 | 105.27 | 111.00 |
| 1 | IW | 35 | VAL | N-CA-C | -5.26 | 105.27 | 111.00 |
| 1 | JS | 1 | PRO | CA-C-N | 5.26 | 128.94 | 121.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | JS | 1 | PRO | C-N-CA | 5.26 | 128.94 | 121.42 |
| 1 | KR | 35 | VAL | N-CA-C | -5.26 | 105.27 | 111.00 |
| 1 | BO | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | DK | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | DU | 1 | PRO | CA-C-N | 5.25 | 128.94 | 121.42 |
| 1 | DU | 1 | PRO | C-N-CA | 5.25 | 128.94 | 121.42 |
| 1 | EZ | 1 | PRO | CA-C-N | 5.25 | 128.94 | 121.42 |
| 1 | EZ | 1 | PRO | C-N-CA | 5.25 | 128.94 | 121.42 |
| 1 | FH | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | ZO | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | YW | 32 | LEU | N-CA-C | -5.25 | 107.00 | 113.41 |
| 1 | DG | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | GF | 36 | VAL | N-CA-C | -5.25 | 105.26 | 110.62 |
| 1 | GN | 35 | VAL | N-CA-C | -5.25 | 105.27 | 111.00 |
| 1 | HL | 32 | LEU | N-CA-C | -5.25 | 107.00 | 113.41 |
| 1 | HZ | 36 | VAL | N-CA-C | -5.25 | 105.26 | 110.62 |
| 1 | DX | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | FB | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | DS | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | FP | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | FX | 32 | LEU | N-CA-C | -5.25 | 107.00 | 113.41 |
| 1 | II | 32 | LEU | N-CA-C | -5.25 | 107.00 | 113.41 |
| 1 | IY | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | KT | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | AE | 36 | VAL | N-CA-C | -5.25 | 105.27 | 110.62 |
| 1 | AR | 32 | LEU | N-CA-C | -5.25 | 107.01 | 113.41 |
| 1 | BU | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | GV | 32 | LEU | N-CA-C | -5.25 | 107.01 | 113.41 |
| 1 | HT | 36 | VAL | N-CA-C | -5.25 | 105.27 | 110.62 |
| 1 | JA | 1 | PRO | CA-C-N | 5.25 | 128.92 | 121.42 |
| 1 | JA | 1 | PRO | C-N-CA | 5.25 | 128.92 | 121.42 |
| 1 | JX | 1 | PRO | CA-C-N | 5.25 | 128.92 | 121.42 |
| 1 | JX | 1 | PRO | C-N-CA | 5.25 | 128.92 | 121.42 |
| 1 | KV | 1 | PRO | CA-C-N | 5.25 | 128.92 | 121.42 |
| 1 | KV | 1 | PRO | C-N-CA | 5.25 | 128.92 | 121.42 |
| 1 | LN | 1 | PRO | CA-C-N | 5.25 | 128.92 | 121.42 |
| 1 | LN | 1 | PRO | C-N-CA | 5.25 | 128.92 | 121.42 |
| 1 | ZU | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | FV | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | IH | 35 | VAL | N-CA-C | -5.25 | 105.28 | 111.00 |
| 1 | JX | 32 | LEU | N-CA-C | -5.25 | 107.01 | 113.41 |
| 1 | LN | 32 | LEU | N-CA-C | -5.25 | 107.01 | 113.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | BY | 32 | LEU | N-CA-C | -5.24 | 107.01 | 113.41 |
| 1 | ET | 32 | LEU | N-CA-C | -5.24 | 107.01 | 113.41 |
| 1 | FX | 1 | PRO | CA-C-N | 5.24 | 128.92 | 121.42 |
| 1 | FX | 1 | PRO | C-N-CA | 5.24 | 128.92 | 121.42 |
| 1 | GB | 35 | VAL | N-CA-C | -5.24 | 105.28 | 111.00 |
| 1 | II | 1 | PRO | CA-C-N | 5.24 | 128.92 | 121.42 |
| 1 | II | 1 | PRO | C-N-CA | 5.24 | 128.92 | 121.42 |
| 1 | IM | 35 | VAL | N-CA-C | -5.24 | 105.28 | 111.00 |
| 1 | DI | 1 | PRO | CA-C-N | 5.24 | 128.92 | 121.42 |
| 1 | DI | 1 | PRO | C-N-CA | 5.24 | 128.92 | 121.42 |
| 1 | FF | 1 | PRO | CA-C-N | 5.24 | 128.92 | 121.42 |
| 1 | FF | 1 | PRO | C-N-CA | 5.24 | 128.92 | 121.42 |
| 1 | GH | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | WC | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | CG | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | ED | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | IU | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | KP | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | ZA | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | YM | 36 | VAL | N-CA-C | -5.24 | 105.28 | 110.62 |
| 1 | AI | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | BI | 36 | VAL | N-CA-C | -5.24 | 105.28 | 110.62 |
| 1 | DO | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | FL | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | GD | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | HX | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | WD | 36 | VAL | N-CA-C | -5.24 | 105.28 | 110.62 |
| 1 | YA | 36 | VAL | N-CA-C | -5.24 | 105.28 | 110.62 |
| 1 | AE | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | CK | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | DA | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | EL | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | EN | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | HT | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | YK | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | AU | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | GF | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | HB | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | HZ | 35 | VAL | N-CA-C | -5.24 | 105.29 | 111.00 |
| 1 | IO | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | JS | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |
| 1 | LB | 32 | LEU | N-CA-C | -5.24 | 107.02 | 113.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | CE | 32 | LEU | N-CA-C | -5.23 | 107.02 | 113.41 |
| 1 | EB | 32 | LEU | N-CA-C | -5.23 | 107.02 | 113.41 |
| 1 | YC | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | AC | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | BK | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | BM | 1 | PRO | CA-C-N | 5.23 | 128.90 | 121.42 |
| 1 | BM | 1 | PRO | C-N-CA | 5.23 | 128.90 | 121.42 |
| 1 | HR | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | JA | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | KV | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | ZM | 1 | PRO | CA-C-N | 5.23 | 128.90 | 121.42 |
| 1 | ZM | 1 | PRO | C-N-CA | 5.23 | 128.90 | 121.42 |
| 1 | DC | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | GJ | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | ZK | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | KH | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | YI | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | AW | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | HD | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | JQ | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | BA | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | BE | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | BM | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | BQ | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | CO | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | CU | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | DI | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | ER | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | FF | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | GT | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | HG | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | WA | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | ZM | 32 | LEU | N-CA-C | -5.23 | 107.03 | 113.41 |
| 1 | ZQ | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | KN | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | LL | 35 | VAL | N-CA-C | -5.23 | 105.30 | 111.00 |
| 1 | YU | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | AY | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | WB | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | JE | 35 | VAL | N-CA-C | -5.22 | 105.30 | 111.00 |
| 1 | JK | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | JZ | 50 | VAL | CA-C-N | -5.22 | 115.74 | 123.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | JZ | 50 | VAL | C-N-CA | -5.22 | 115.74 | 123.05 |
| 1 | KZ | 35 | VAL | N-CA-C | -5.22 | 105.30 | 111.00 |
| 1 | LP | 50 | VAL | CA-C-N | -5.22 | 115.74 | 123.05 |
| 1 | LP | 50 | VAL | C-N-CA | -5.22 | 115.74 | 123.05 |
| 1 | CA | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | EV | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | YE | 32 | LEU | N-CA-C | -5.22 | 107.04 | 113.41 |
| 1 | CI | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | EF | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | FR | 1 | PRO | CA-C-N | 5.22 | 128.89 | 121.42 |
| 1 | FR | 1 | PRO | C-N-CA | 5.22 | 128.89 | 121.42 |
| 1 | IC | 1 | PRO | CA-C-N | 5.22 | 128.89 | 121.42 |
| 1 | IC | 1 | PRO | C-N-CA | 5.22 | 128.89 | 121.42 |
| 1 | JM | 32 | LEU | N-CA-C | -5.22 | 107.04 | 113.41 |
| 1 | YO | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | AM | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | ZE | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | DZ | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | FD | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | JV | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | YQ | 32 | LEU | N-CA-C | -5.22 | 107.05 | 113.41 |
| 1 | JG | 32 | LEU | N-CA-C | -5.22 | 107.05 | 113.41 |
| 1 | AA | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | BW | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | HP | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | ZW | 35 | VAL | N-CA-C | -5.22 | 105.31 | 111.00 |
| 1 | BS | 32 | LEU | N-CA-C | -5.21 | 107.05 | 113.41 |
| 1 | ZS | 32 | LEU | N-CA-C | -5.21 | 107.05 | 113.41 |
| 1 | IQ | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | LD | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | CC | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | EX | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | AS | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | GZ | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | FR | 32 | LEU | N-CA-C | -5.21 | 107.06 | 113.41 |
| 1 | IC | 32 | LEU | N-CA-C | -5.21 | 107.06 | 113.41 |
| 1 | IS | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | LF | 35 | VAL | N-CA-C | -5.21 | 105.32 | 111.00 |
| 1 | BU | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | BU | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | CY | 50 | VAL | CA-C-N | -5.20 | 115.76 | 123.05 |
| 1 | CY | 50 | VAL | C-N-CA | -5.20 | 115.76 | 123.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | EJ | 50 | VAL | CA-C-N | -5.20 | 115.76 | 123.05 |
| 1 | EJ | 50 | VAL | C-N-CA | -5.20 | 115.76 | 123.05 |
| 1 | FZ | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | FZ | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | IK | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | IK | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | ZU | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | ZU | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | CQ | 32 | LEU | N-CA-C | -5.20 | 107.07 | 113.41 |
| 1 | GP | 32 | LEU | N-CA-C | -5.20 | 107.07 | 113.41 |
| 1 | JC | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | JC | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | KX | 50 | VAL | CA-C-N | -5.20 | 115.77 | 123.05 |
| 1 | KX | 50 | VAL | C-N-CA | -5.20 | 115.77 | 123.05 |
| 1 | KL | 50 | VAL | CA-C-N | -5.19 | 115.78 | 123.05 |
| 1 | KL | 50 | VAL | C-N-CA | -5.19 | 115.78 | 123.05 |
| 1 | LJ | 50 | VAL | CA-C-N | -5.19 | 115.78 | 123.05 |
| 1 | LJ | 50 | VAL | C-N-CA | -5.19 | 115.78 | 123.05 |
| 1 | CG | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | CG | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | ED | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | ED | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | FT | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | FT | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | IE | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | IE | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | IQ | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | IQ | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | LD | 50 | VAL | CA-C-N | -5.19 | 115.79 | 123.05 |
| 1 | LD | 50 | VAL | C-N-CA | -5.19 | 115.79 | 123.05 |
| 1 | CW | 32 | LEU | N-CA-C | -5.19 | 107.08 | 113.41 |
| 1 | EH | 32 | LEU | N-CA-C | -5.19 | 107.08 | 113.41 |
| 1 | CS | 50 | VAL | CA-C-N | -5.18 | 115.79 | 123.05 |
| 1 | CS | 50 | VAL | C-N-CA | -5.18 | 115.79 | 123.05 |
| 1 | DS | 94 | GLU | CA-C-N | -5.18 | 116.20 | 123.10 |
| 1 | DS | 94 | GLU | C-N-CA | -5.18 | 116.20 | 123.10 |
| 1 | FP | 94 | GLU | CA-C-N | -5.18 | 116.20 | 123.10 |
| 1 | FP | 94 | GLU | C-N-CA | -5.18 | 116.20 | 123.10 |
| 1 | GR | 50 | VAL | CA-C-N | -5.18 | 115.79 | 123.05 |
| 1 | GR | 50 | VAL | C-N-CA | -5.18 | 115.79 | 123.05 |
| 1 | YG | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | YG | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | DK | 50 | VAL | CA-C-N | -5.18 | 115.79 | 123.05 |
| 1 | DK | 50 | VAL | C-N-CA | -5.18 | 115.79 | 123.05 |
| 1 | FH | 50 | VAL | CA-C-N | -5.18 | 115.79 | 123.05 |
| 1 | FH | 50 | VAL | C-N-CA | -5.18 | 115.79 | 123.05 |
| 1 | JO | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | JO | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | AW | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | AW | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | ZI | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | ZI | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | HD | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | HD | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | KF | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | KF | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | CM | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | CM | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | DG | 94 | GLU | CA-C-N | -5.18 | 116.21 | 123.10 |
| 1 | DG | 94 | GLU | C-N-CA | -5.18 | 116.21 | 123.10 |
| 1 | EP | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | EP | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | GN | 94 | GLU | CA-C-N | -5.18 | 116.21 | 123.10 |
| 1 | GN | 94 | GLU | C-N-CA | -5.18 | 116.21 | 123.10 |
| 1 | AK | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | AK | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | ZC | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | ZC | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | BI | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | BI | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | DX | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | DX | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | FB | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | FB | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | GF | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | GF | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | HZ | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | HZ | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | YA | 50 | VAL | CA-C-N | -5.18 | 115.80 | 123.05 |
| 1 | YA | 50 | VAL | C-N-CA | -5.18 | 115.80 | 123.05 |
| 1 | BO | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | BO | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | CU | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | CU | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | GT | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | GT | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 1 | ZO | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | ZO | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 2 | BT | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 1 | CA | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | CA | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | EV | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | EV | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 2 | ZT | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 2 | YF | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 1 | YI | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | YI | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 1 | CO | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | CO | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 1 | ER | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | ER | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 2 | JN | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 1 | JQ | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | JQ | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 1 | YY | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | YY | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | HN | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | HN | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | AA | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | AA | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | AP | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | AP | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | DE | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | DE | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 2 | FY | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 1 | GL | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | GL | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | GX | 50 | VAL | CA-C-N | -5.17 | 115.81 | 123.05 |
| 1 | GX | 50 | VAL | C-N-CA | -5.17 | 115.81 | 123.05 |
| 1 | HP | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | HP | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 2 | IJ | 133 | ILE | CB-CA-C | -5.17 | 105.16 | 112.14 |
| 1 | ZK | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | ZK | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |
| 1 | KH | 94 | GLU | CA-C-N | -5.17 | 116.22 | 123.10 |
| 1 | KH | 94 | GLU | C-N-CA | -5.17 | 116.22 | 123.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | AE | 50 | VAL | CA-C-N | -5.17 | 115.82 | 123.05 |
| 1 | AE | 50 | VAL | C-N-CA | -5.17 | 115.82 | 123.05 |
| 1 | AG | 35 | VAL | N-CA-C | -5.17 | 105.37 | 111.00 |
| 2 | BN | 133 | ILE | CB-CA-C | -5.17 | 105.17 | 112.14 |
| 1 | DM | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | DM | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | DQ | 50 | VAL | CA-C-N | -5.17 | 115.82 | 123.05 |
| 1 | DQ | 50 | VAL | C-N-CA | -5.17 | 115.82 | 123.05 |
| 1 | FJ | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | FJ | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | FN | 50 | VAL | CA-C-N | -5.17 | 115.82 | 123.05 |
| 1 | FN | 50 | VAL | C-N-CA | -5.17 | 115.82 | 123.05 |
| 1 | HT | 50 | VAL | CA-C-N | -5.17 | 115.82 | 123.05 |
| 1 | HT | 50 | VAL | C-N-CA | -5.17 | 115.82 | 123.05 |
| 1 | HV | 35 | VAL | N-CA-C | -5.17 | 105.37 | 111.00 |
| 2 | ZN | 133 | ILE | CB-CA-C | -5.17 | 105.17 | 112.14 |
| 1 | YU | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | YU | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | BE | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | BE | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | WA | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | WA | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | JK | 94 | GLU | CA-C-N | -5.17 | 116.23 | 123.10 |
| 1 | JK | 94 | GLU | C-N-CA | -5.17 | 116.23 | 123.10 |
| 1 | YS | 50 | VAL | CA-C-N | -5.16 | 115.82 | 123.05 |
| 1 | YS | 50 | VAL | C-N-CA | -5.16 | 115.82 | 123.05 |
| 1 | AG | 94 | GLU | CA-C-N | -5.16 | 116.23 | 123.10 |
| 1 | AG | 94 | GLU | C-N-CA | -5.16 | 116.23 | 123.10 |
| 2 | CX | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 2 | EI | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 1 | HV | 94 | GLU | CA-C-N | -5.16 | 116.23 | 123.10 |
| 1 | HV | 94 | GLU | C-N-CA | -5.16 | 116.23 | 123.10 |
| 1 | JI | 50 | VAL | CA-C-N | -5.16 | 115.82 | 123.05 |
| 1 | JI | 50 | VAL | C-N-CA | -5.16 | 115.82 | 123.05 |
| 2 | YR | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 1 | AM | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | AM | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | BW | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | BW | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 2 | CR | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 1 | ZE | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | ZE | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | GQ | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 2 | JH | 133 | ILE | CB-CA-C | -5.16 | 105.17 | 112.14 |
| 1 | KB | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | KB | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | LR | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | LR | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | ZW | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | ZW | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | JE | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | JE | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | KZ | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | KZ | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 2 | AQ | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 2 | GW | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 2 | JB | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 2 | KW | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 1 | BQ | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | BQ | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 2 | DW | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 2 | FA | 133 | ILE | CB-CA-C | -5.16 | 105.18 | 112.14 |
| 1 | ZQ | 94 | GLU | CA-C-N | -5.16 | 116.24 | 123.10 |
| 1 | ZQ | 94 | GLU | C-N-CA | -5.16 | 116.24 | 123.10 |
| 1 | YO | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | YO | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | AS | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | AS | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | CI | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | CI | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | EF | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | EF | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | GZ | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | GZ | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | JV | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | JV | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | CC | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | CC | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | DA | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | DA | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | EL | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | EL | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | EX | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | EX | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | IY | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | IY | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 2 | JY | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | KT | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | KT | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 2 | LO | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | BC | 50 | VAL | CA-C-N | -5.15 | 115.84 | 123.05 |
| 1 | BC | 50 | VAL | C-N-CA | -5.15 | 115.84 | 123.05 |
| 1 | HI | 50 | VAL | CA-C-N | -5.15 | 115.84 | 123.05 |
| 1 | HI | 50 | VAL | C-N-CA | -5.15 | 115.84 | 123.05 |
| 2 | DD | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | DZ | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | DZ | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 1 | FD | 94 | GLU | CA-C-N | -5.15 | 116.25 | 123.10 |
| 1 | FD | 94 | GLU | C-N-CA | -5.15 | 116.25 | 123.10 |
| 2 | GK | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | YM | 50 | VAL | CA-C-N | -5.15 | 115.84 | 123.05 |
| 1 | YM | 50 | VAL | C-N-CA | -5.15 | 115.84 | 123.05 |
| 2 | DP | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 2 | FM | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 2 | ZH | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | WD | 50 | VAL | CA-C-N | -5.15 | 115.84 | 123.05 |
| 1 | WD | 50 | VAL | C-N-CA | -5.15 | 115.84 | 123.05 |
| 2 | KE | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 2 | YL | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 2 | JT | 133 | ILE | CB-CA-C | -5.15 | 105.19 | 112.14 |
| 1 | YC | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | YC | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | YX | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 1 | BK | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | BK | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | BZ | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 2 | CL | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 2 | EO | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 2 | EU | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 1 | GB | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | GB | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | HM | 133 | ILE | CB-CA-C | -5.14 | 105.19 | 112.14 |
| 1 | IM | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | IM | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 1 | IW | 50 | VAL | CA-C-N | -5.14 | 115.85 | 123.05 |
| 1 | IW | 50 | VAL | C-N-CA | -5.14 | 115.85 | 123.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | KN | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | KN | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 1 | KR | 50 | VAL | CA-C-N | -5.14 | 115.85 | 123.05 |
| 1 | KR | 50 | VAL | C-N-CA | -5.14 | 115.85 | 123.05 |
| 1 | LL | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | LL | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 1 | AY | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | AY | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | CF | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | EC | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 1 | WB | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | WB | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | KK | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | LI | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | ZB | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | AJ | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | BR | 141 | ASP | CA-C-N | 5.14 | 125.22 | 119.87 |
| 2 | BR | 141 | ASP | C-N-CA | 5.14 | 125.22 | 119.87 |
| 2 | FS | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | ID | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | IP | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | LC | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 2 | ZR | 141 | ASP | CA-C-N | 5.14 | 125.22 | 119.87 |
| 2 | ZR | 141 | ASP | C-N-CA | 5.14 | 125.22 | 119.87 |
| 2 | AD | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 1 | GH | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | GH | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | HS | 133 | ILE | CB-CA-C | -5.14 | 105.20 | 112.14 |
| 1 | WC | 94 | GLU | CA-C-N | -5.14 | 116.26 | 123.10 |
| 1 | WC | 94 | GLU | C-N-CA | -5.14 | 116.26 | 123.10 |
| 2 | DD | 288 | ILE | CA-C-N | -5.14 | 116.44 | 123.12 |
| 2 | DD | 288 | ILE | C-N-CA | -5.14 | 116.44 | 123.12 |
| 2 | GK | 288 | ILE | CA-C-N | -5.14 | 116.44 | 123.12 |
| 2 | GK | 288 | ILE | C-N-CA | -5.14 | 116.44 | 123.12 |
| 2 | AV | 133 | ILE | CB-CA-C | -5.14 | 105.21 | 112.14 |
| 2 | BB | 133 | ILE | CB-CA-C | -5.14 | 105.21 | 112.14 |
| 2 | HC | 133 | ILE | CB-CA-C | -5.14 | 105.21 | 112.14 |
| 2 | HH | 133 | ILE | CB-CA-C | -5.14 | 105.21 | 112.14 |
| 1 | IS | 94 | GLU | CA-C-N | -5.14 | 116.27 | 123.10 |
| 1 | IS | 94 | GLU | C-N-CA | -5.14 | 116.27 | 123.10 |
| 1 | LF | 94 | GLU | CA-C-N | -5.14 | 116.27 | 123.10 |
| 1 | LF | 94 | GLU | C-N-CA | -5.14 | 116.27 | 123.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | BT | 288 | ILE | CA-C-N | -5.13 | 116.44 | 123.12 |
| 2 | BT | 288 | ILE | C-N-CA | -5.13 | 116.44 | 123.12 |
| 1 | FV | 94 | GLU | CA-C-N | -5.13 | 116.27 | 123.10 |
| 1 | FV | 94 | GLU | C-N-CA | -5.13 | 116.27 | 123.10 |
| 1 | IH | 94 | GLU | CA-C-N | -5.13 | 116.27 | 123.10 |
| 1 | IH | 94 | GLU | C-N-CA | -5.13 | 116.27 | 123.10 |
| 2 | ZT | 288 | ILE | CA-C-N | -5.13 | 116.44 | 123.12 |
| 2 | ZT | 288 | ILE | C-N-CA | -5.13 | 116.44 | 123.12 |
| 2 | GE | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | GE | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | HY | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | HY | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | FY | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | FY | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | IJ | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | IJ | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | ZZ | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | ZZ | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | YL | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | YL | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | BH | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | BH | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | DJ | 133 | ILE | CB-CA-C | -5.13 | 105.22 | 112.14 |
| 2 | FG | 133 | ILE | CB-CA-C | -5.13 | 105.22 | 112.14 |
| 2 | JT | 288 | ILE | CA-C-N | -5.13 | 116.45 | 123.12 |
| 2 | JT | 288 | ILE | C-N-CA | -5.13 | 116.45 | 123.12 |
| 2 | IV | 133 | ILE | CB-CA-C | -5.13 | 105.22 | 112.14 |
| 2 | KQ | 133 | ILE | CB-CA-C | -5.13 | 105.22 | 112.14 |
| 2 | YV | 141 | ASP | CA-C-N | 5.12 | 125.20 | 119.87 |
| 2 | YV | 141 | ASP | C-N-CA | 5.12 | 125.20 | 119.87 |
| 2 | DP | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | DP | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | DW | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | DW | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | FA | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | FA | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | FM | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | FM | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | JL | 141 | ASP | CA-C-N | 5.12 | 125.20 | 119.87 |
| 2 | JL | 141 | ASP | C-N-CA | 5.12 | 125.20 | 119.87 |
| 2 | AD | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | AD | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | HS | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | HS | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | JB | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | JB | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | KW | 288 | ILE | CA-C-N | -5.12 | 116.46 | 123.12 |
| 2 | KW | 288 | ILE | C-N-CA | -5.12 | 116.46 | 123.12 |
| 2 | YF | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | YF | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | YR | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | YR | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | DJ | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | DJ | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | FG | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | FG | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | JH | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | JH | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | JN | 288 | ILE | CA-C-N | -5.12 | 116.47 | 123.12 |
| 2 | JN | 288 | ILE | C-N-CA | -5.12 | 116.47 | 123.12 |
| 2 | CV | 141 | ASP | CA-C-N | 5.12 | 125.19 | 119.87 |
| 2 | CV | 141 | ASP | C-N-CA | 5.12 | 125.19 | 119.87 |
| 2 | GU | 141 | ASP | CA-C-N | 5.12 | 125.19 | 119.87 |
| 2 | GU | 141 | ASP | C-N-CA | 5.12 | 125.19 | 119.87 |
| 2 | ZB | 288 | ILE | CA-C-N | -5.11 | 116.47 | 123.12 |
| 2 | ZB | 288 | ILE | C-N-CA | -5.11 | 116.47 | 123.12 |
| 2 | AJ | 288 | ILE | CA-C-N | -5.11 | 116.47 | 123.12 |
| 2 | AJ | 288 | ILE | C-N-CA | -5.11 | 116.47 | 123.12 |
| 2 | IV | 288 | ILE | CA-C-N | -5.11 | 116.47 | 123.12 |
| 2 | IV | 288 | ILE | C-N-CA | -5.11 | 116.47 | 123.12 |
| 2 | KQ | 288 | ILE | CA-C-N | -5.11 | 116.47 | 123.12 |
| 2 | KQ | 288 | ILE | C-N-CA | -5.11 | 116.47 | 123.12 |
| 2 | BF | 141 | ASP | CA-C-N | 5.11 | 125.18 | 119.87 |
| 2 | BF | 141 | ASP | C-N-CA | 5.11 | 125.18 | 119.87 |
| 2 | DN | 141 | ASP | CA-C-N | 5.11 | 125.19 | 119.87 |
| 2 | DN | 141 | ASP | C-N-CA | 5.11 | 125.19 | 119.87 |
| 2 | FK | 141 | ASP | CA-C-N | 5.11 | 125.19 | 119.87 |
| 2 | FK | 141 | ASP | C-N-CA | 5.11 | 125.19 | 119.87 |
| 2 | HK | 141 | ASP | CA-C-N | 5.11 | 125.18 | 119.87 |
| 2 | HK | 141 | ASP | C-N-CA | 5.11 | 125.18 | 119.87 |
| 2 | ZZ | 133 | ILE | CB-CA-C | -5.11 | 105.24 | 112.14 |
| 2 | AV | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | AV | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | BH | 133 | ILE | CB-CA-C | -5.11 | 105.24 | 112.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | HC | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | HC | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | GE | 133 | ILE | CB-CA-C | -5.11 | 105.24 | 112.14 |
| 2 | HY | 133 | ILE | CB-CA-C | -5.11 | 105.24 | 112.14 |
| 2 | IP | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | IP | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | LC | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | LC | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | BB | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | BB | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | FS | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | FS | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | ZH | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | ZH | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | HH | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | HH | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | ID | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | ID | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | KE | 288 | ILE | CA-C-N | -5.11 | 116.48 | 123.12 |
| 2 | KE | 288 | ILE | C-N-CA | -5.11 | 116.48 | 123.12 |
| 2 | YD | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | YD | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | BL | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | BL | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | BN | 288 | ILE | CA-C-N | -5.10 | 116.48 | 123.12 |
| 2 | BN | 288 | ILE | C-N-CA | -5.10 | 116.48 | 123.12 |
| 2 | CX | 288 | ILE | CA-C-N | -5.10 | 116.48 | 123.12 |
| 2 | CX | 288 | ILE | C-N-CA | -5.10 | 116.48 | 123.12 |
| 2 | EI | 288 | ILE | CA-C-N | -5.10 | 116.48 | 123.12 |
| 2 | EI | 288 | ILE | C-N-CA | -5.10 | 116.48 | 123.12 |
| 2 | GI | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | GI | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | IB | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | IB | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | ZN | 288 | ILE | CA-C-N | -5.10 | 116.48 | 123.12 |
| 2 | ZN | 288 | ILE | C-N-CA | -5.10 | 116.48 | 123.12 |
| 2 | AZ | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | AZ | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | BZ | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | BZ | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |
| 2 | CL | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | CL | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | EO | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | EO | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |
| 2 | EU | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | EU | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |
| 2 | HF | 141 | ASP | CA-C-N | 5.10 | 125.18 | 119.87 |
| 2 | HF | 141 | ASP | C-N-CA | 5.10 | 125.18 | 119.87 |
| 2 | DB | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | DB | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | EM | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | EM | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | AH | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | AH | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | BX | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | BX | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | HW | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | HW | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | ZX | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | ZX | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | JY | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | JY | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |
| 2 | ZL | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | ZL | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | KI | 141 | ASP | CA-C-N | 5.10 | 125.17 | 119.87 |
| 2 | KI | 141 | ASP | C-N-CA | 5.10 | 125.17 | 119.87 |
| 2 | LO | 288 | ILE | CA-C-N | -5.10 | 116.49 | 123.12 |
| 2 | LO | 288 | ILE | C-N-CA | -5.10 | 116.49 | 123.12 |
| 2 | CR | 288 | ILE | CA-C-N | -5.10 | 116.50 | 123.12 |
| 2 | CR | 288 | ILE | C-N-CA | -5.10 | 116.50 | 123.12 |
| 2 | GQ | 288 | ILE | CA-C-N | -5.10 | 116.50 | 123.12 |
| 2 | GQ | 288 | ILE | C-N-CA | -5.10 | 116.50 | 123.12 |
| 2 | FW | 141 | ASP | CA-C-N | 5.09 | 125.17 | 119.87 |
| 2 | FW | 141 | ASP | C-N-CA | 5.09 | 125.17 | 119.87 |
| 2 | IG | 141 | ASP | CA-C-N | 5.09 | 125.17 | 119.87 |
| 2 | IG | 141 | ASP | C-N-CA | 5.09 | 125.17 | 119.87 |
| 1 | FR | 19 | ARG | N-CA-C | -5.09 | 105.81 | 111.36 |
| 1 | IC | 19 | ARG | N-CA-C | -5.09 | 105.81 | 111.36 |
| 1 | ZY | 19 | ARG | N-CA-C | -5.09 | 105.81 | 111.36 |
| 1 | BG | 19 | ARG | N-CA-C | -5.09 | 105.81 | 111.36 |
| 2 | CF | 288 | ILE | CA-C-N | -5.09 | 116.50 | 123.12 |
| 2 | CF | 288 | ILE | C-N-CA | -5.09 | 116.50 | 123.12 |
| 2 | EC | 288 | ILE | CA-C-N | -5.09 | 116.50 | 123.12 |
| 2 | EC | 288 | ILE | C-N-CA | -5.09 | 116.50 | 123.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | IT | 141 | ASP | CA-C-N | 5.09 | 125.17 | 119.87 |
| 2 | IT | 141 | ASP | C-N-CA | 5.09 | 125.17 | 119.87 |
| 2 | LG | 141 | ASP | CA-C-N | 5.09 | 125.17 | 119.87 |
| 2 | LG | 141 | ASP | C-N-CA | 5.09 | 125.17 | 119.87 |
| 2 | KK | 288 | ILE | CA-C-N | -5.09 | 116.50 | 123.12 |
| 2 | KK | 288 | ILE | C-N-CA | -5.09 | 116.50 | 123.12 |
| 2 | LI | 288 | ILE | CA-C-N | -5.09 | 116.50 | 123.12 |
| 2 | LI | 288 | ILE | C-N-CA | -5.09 | 116.50 | 123.12 |
| 1 | KJ | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 1 | LH | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 2 | GC | 141 | ASP | CA-C-N | 5.08 | 125.16 | 119.87 |
| 2 | GC | 141 | ASP | C-N-CA | 5.08 | 125.16 | 119.87 |
| 2 | IN | 141 | ASP | CA-C-N | 5.08 | 125.16 | 119.87 |
| 2 | IN | 141 | ASP | C-N-CA | 5.08 | 125.16 | 119.87 |
| 2 | AN | 141 | ASP | CA-C-N | 5.08 | 125.16 | 119.87 |
| 2 | AN | 141 | ASP | C-N-CA | 5.08 | 125.16 | 119.87 |
| 2 | AQ | 288 | ILE | CA-C-N | -5.08 | 116.52 | 123.12 |
| 2 | AQ | 288 | ILE | C-N-CA | -5.08 | 116.52 | 123.12 |
| 1 | AU | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 1 | BS | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 2 | ZF | 141 | ASP | CA-C-N | 5.08 | 125.16 | 119.87 |
| 2 | ZF | 141 | ASP | C-N-CA | 5.08 | 125.16 | 119.87 |
| 2 | GW | 288 | ILE | CA-C-N | -5.08 | 116.52 | 123.12 |
| 2 | GW | 288 | ILE | C-N-CA | -5.08 | 116.52 | 123.12 |
| 1 | HB | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 1 | ZS | 19 | ARG | N-CA-C | -5.08 | 105.82 | 111.36 |
| 2 | AB | 141 | ASP | CA-C-N | 5.08 | 125.15 | 119.87 |
| 2 | AB | 141 | ASP | C-N-CA | 5.08 | 125.15 | 119.87 |
| 1 | DU | 19 | ARG | N-CA-C | -5.08 | 105.83 | 111.36 |
| 1 | EZ | 19 | ARG | N-CA-C | -5.08 | 105.83 | 111.36 |
| 2 | HQ | 141 | ASP | CA-C-N | 5.08 | 125.15 | 119.87 |
| 2 | HQ | 141 | ASP | C-N-CA | 5.08 | 125.15 | 119.87 |
| 2 | CP | 141 | ASP | CA-C-N | 5.08 | 125.15 | 119.87 |
| 2 | CP | 141 | ASP | C-N-CA | 5.08 | 125.15 | 119.87 |
| 2 | ES | 141 | ASP | CA-C-N | 5.08 | 125.15 | 119.87 |
| 2 | ES | 141 | ASP | C-N-CA | 5.08 | 125.15 | 119.87 |
| 2 | YX | 288 | ILE | CA-C-N | -5.07 | 116.52 | 123.12 |
| 2 | YX | 288 | ILE | C-N-CA | -5.07 | 116.52 | 123.12 |
| 2 | HM | 288 | ILE | CA-C-N | -5.07 | 116.52 | 123.12 |
| 2 | HM | 288 | ILE | C-N-CA | -5.07 | 116.52 | 123.12 |
| 1 | IU | 19 | ARG | N-CA-C | -5.07 | 105.83 | 111.36 |
| 1 | KP | 19 | ARG | N-CA-C | -5.07 | 105.83 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | DC | 19 | ARG | N-CA-C | -5.07 | 105.83 | 111.36 |
| 1 | GJ | 19 | ARG | N-CA-C | -5.07 | 105.83 | 111.36 |
| 1 | JX | 19 | ARG | N-CA-C | -5.07 | 105.84 | 111.36 |
| 1 | LN | 19 | ARG | N-CA-C | -5.07 | 105.84 | 111.36 |
| 1 | CK | 19 | ARG | N-CA-C | -5.07 | 105.84 | 111.36 |
| 1 | EN | 19 | ARG | N-CA-C | -5.07 | 105.84 | 111.36 |
| 2 | KC | 141 | ASP | CA-C-N | 5.07 | 125.14 | 119.87 |
| 2 | KC | 141 | ASP | C-N-CA | 5.07 | 125.14 | 119.87 |
| 2 | KO | 141 | ASP | CA-C-N | 5.07 | 125.14 | 119.87 |
| 2 | KO | 141 | ASP | C-N-CA | 5.07 | 125.14 | 119.87 |
| 2 | LM | 141 | ASP | CA-C-N | 5.07 | 125.14 | 119.87 |
| 2 | LM | 141 | ASP | C-N-CA | 5.07 | 125.14 | 119.87 |
| 2 | LS | 141 | ASP | CA-C-N | 5.07 | 125.14 | 119.87 |
| 2 | LS | 141 | ASP | C-N-CA | 5.07 | 125.14 | 119.87 |
| 1 | AR | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | GV | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | YE | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 2 | EA | 141 | ASP | CA-C-N | 5.06 | 125.14 | 119.87 |
| 2 | EA | 141 | ASP | C-N-CA | 5.06 | 125.14 | 119.87 |
| 2 | FE | 141 | ASP | CA-C-N | 5.06 | 125.14 | 119.87 |
| 2 | FE | 141 | ASP | C-N-CA | 5.06 | 125.14 | 119.87 |
| 1 | JM | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | CW | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 2 | DT | 141 | ASP | CA-C-N | 5.06 | 125.13 | 119.87 |
| 2 | DT | 141 | ASP | C-N-CA | 5.06 | 125.13 | 119.87 |
| 1 | EH | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 2 | FQ | 141 | ASP | CA-C-N | 5.06 | 125.13 | 119.87 |
| 2 | FQ | 141 | ASP | C-N-CA | 5.06 | 125.13 | 119.87 |
| 1 | ZA | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | AI | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | BA | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 1 | HG | 19 | ARG | N-CA-C | -5.06 | 105.84 | 111.36 |
| 2 | YJ | 141 | ASP | CA-C-N | 5.06 | 125.13 | 119.87 |
| 2 | YJ | 141 | ASP | C-N-CA | 5.06 | 125.13 | 119.87 |
| 1 | BM | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |
| 1 | IO | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |
| 2 | JR | 141 | ASP | CA-C-N | 5.06 | 125.13 | 119.87 |
| 2 | JR | 141 | ASP | C-N-CA | 5.06 | 125.13 | 119.87 |
| 1 | ZM | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |
| 1 | LB | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |
| 1 | FX | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |
| 1 | II | 19 | ARG | N-CA-C | -5.06 | 105.85 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | YK | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 1 | DO | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 1 | FL | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 1 | JS | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 2 | CJ | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | CJ | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 2 | EG | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | EG | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 1 | ZG | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 2 | JF | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | JF | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 1 | KD | 19 | ARG | N-CA-C | -5.05 | 105.85 | 111.36 |
| 2 | LA | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | LA | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 1 | DI | 19 | ARG | N-CA-C | -5.05 | 105.86 | 111.36 |
| 1 | FF | 19 | ARG | N-CA-C | -5.05 | 105.86 | 111.36 |
| 2 | IR | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | IR | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 1 | JA | 19 | ARG | N-CA-C | -5.05 | 105.86 | 111.36 |
| 1 | KV | 19 | ARG | N-CA-C | -5.05 | 105.86 | 111.36 |
| 2 | LE | 141 | ASP | CA-C-N | 5.05 | 125.12 | 119.87 |
| 2 | LE | 141 | ASP | C-N-CA | 5.05 | 125.12 | 119.87 |
| 1 | YW | 46 | ARG | CA-C-N | 5.05 | 126.86 | 121.00 |
| 1 | YW | 46 | ARG | C-N-CA | 5.05 | 126.86 | 121.00 |
| 1 | HL | 46 | ARG | CA-C-N | 5.05 | 126.86 | 121.00 |
| 1 | HL | 46 | ARG | C-N-CA | 5.05 | 126.86 | 121.00 |
| 1 | AC | 19 | ARG | N-CA-C | -5.04 | 105.86 | 111.36 |
| 1 | HR | 19 | ARG | N-CA-C | -5.04 | 105.86 | 111.36 |
| 2 | AT | 141 | ASP | CA-C-N | 5.04 | 125.11 | 119.87 |
| 2 | AT | 141 | ASP | C-N-CA | 5.04 | 125.11 | 119.87 |
| 1 | CE | 19 | ARG | N-CA-C | -5.04 | 105.86 | 111.36 |
| 1 | EB | 19 | ARG | N-CA-C | -5.04 | 105.86 | 111.36 |
| 2 | HA | 141 | ASP | CA-C-N | 5.04 | 125.11 | 119.87 |
| 2 | HA | 141 | ASP | C-N-CA | 5.04 | 125.11 | 119.87 |
| 1 | YQ | 19 | ARG | N-CA-C | -5.04 | 105.87 | 111.36 |
| 1 | BS | 46 | ARG | CA-C-N | 5.04 | 126.84 | 121.00 |
| 1 | BS | 46 | ARG | C-N-CA | 5.04 | 126.84 | 121.00 |
| 2 | CB | 141 | ASP | CA-C-N | 5.04 | 125.11 | 119.87 |
| 2 | CB | 141 | ASP | C-N-CA | 5.04 | 125.11 | 119.87 |
| 2 | EW | 141 | ASP | CA-C-N | 5.04 | 125.11 | 119.87 |
| 2 | EW | 141 | ASP | C-N-CA | 5.04 | 125.11 | 119.87 |
| 1 | JG | 19 | ARG | N-CA-C | -5.04 | 105.87 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | ZS | 46 | ARG | CA-C-N | 5.04 | 126.84 | 121.00 |
| 1 | ZS | 46 | ARG | C-N-CA | 5.04 | 126.84 | 121.00 |
| 1 | BY | 19 | ARG | N-CA-C | -5.04 | 105.87 | 111.36 |
| 1 | ET | 19 | ARG | N-CA-C | -5.04 | 105.87 | 111.36 |
| 1 | YW | 19 | ARG | N-CA-C | -5.03 | 105.87 | 111.36 |
| 2 | CD | 141 | ASP | CA-C-N | 5.03 | 125.11 | 119.87 |
| 2 | CD | 141 | ASP | C-N-CA | 5.03 | 125.11 | 119.87 |
| 2 | EY | 141 | ASP | CA-C-N | 5.03 | 125.11 | 119.87 |
| 2 | EY | 141 | ASP | C-N-CA | 5.03 | 125.11 | 119.87 |
| 1 | FX | 46 | ARG | CA-C-N | 5.03 | 126.84 | 121.00 |
| 1 | FX | 46 | ARG | C-N-CA | 5.03 | 126.84 | 121.00 |
| 1 | GD | 19 | ARG | N-CA-C | -5.03 | 105.87 | 111.36 |
| 1 | HL | 19 | ARG | N-CA-C | -5.03 | 105.87 | 111.36 |
| 1 | HX | 19 | ARG | N-CA-C | -5.03 | 105.87 | 111.36 |
| 1 | II | 46 | ARG | CA-C-N | 5.03 | 126.84 | 121.00 |
| 1 | II | 46 | ARG | C-N-CA | 5.03 | 126.84 | 121.00 |
| 2 | AF | 141 | ASP | CA-C-N | 5.03 | 125.10 | 119.87 |
| 2 | AF | 141 | ASP | C-N-CA | 5.03 | 125.10 | 119.87 |
| 2 | HU | 141 | ASP | CA-C-N | 5.03 | 125.10 | 119.87 |
| 2 | HU | 141 | ASP | C-N-CA | 5.03 | 125.10 | 119.87 |
| 2 | IZ | 141 | ASP | CA-C-N | 5.03 | 125.10 | 119.87 |
| 2 | IZ | 141 | ASP | C-N-CA | 5.03 | 125.10 | 119.87 |
| 2 | KU | 141 | ASP | CA-C-N | 5.03 | 125.10 | 119.87 |
| 2 | KU | 141 | ASP | C-N-CA | 5.03 | 125.10 | 119.87 |
| 1 | DI | 46 | ARG | CA-C-N | 5.03 | 126.83 | 121.00 |
| 1 | DI | 46 | ARG | C-N-CA | 5.03 | 126.83 | 121.00 |
| 1 | DU | 46 | ARG | CA-C-N | 5.03 | 126.83 | 121.00 |
| 1 | DU | 46 | ARG | C-N-CA | 5.03 | 126.83 | 121.00 |
| 1 | EZ | 46 | ARG | CA-C-N | 5.03 | 126.83 | 121.00 |
| 1 | EZ | 46 | ARG | C-N-CA | 5.03 | 126.83 | 121.00 |
| 1 | FF | 46 | ARG | CA-C-N | 5.03 | 126.83 | 121.00 |
| 1 | FF | 46 | ARG | C-N-CA | 5.03 | 126.83 | 121.00 |
| 1 | CK | 46 | ARG | CA-C-N | 5.02 | 126.83 | 121.00 |
| 1 | CK | 46 | ARG | C-N-CA | 5.02 | 126.83 | 121.00 |
| 1 | EN | 46 | ARG | CA-C-N | 5.02 | 126.83 | 121.00 |
| 1 | EN | 46 | ARG | C-N-CA | 5.02 | 126.83 | 121.00 |
| 1 | YE | 46 | ARG | CA-C-N | 5.02 | 126.83 | 121.00 |
| 1 | YE | 46 | ARG | C-N-CA | 5.02 | 126.83 | 121.00 |
| 2 | GA | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | GA | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | IL | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | IL | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | JM | 46 | ARG | CA-C-N | 5.02 | 126.83 | 121.00 |
| 1 | JM | 46 | ARG | C-N-CA | 5.02 | 126.83 | 121.00 |
| 2 | AO | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | AO | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | GY | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | GY | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | YP | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | YP | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 1 | AR | 46 | ARG | CA-C-N | 5.02 | 126.82 | 121.00 |
| 1 | AR | 46 | ARG | C-N-CA | 5.02 | 126.82 | 121.00 |
| 2 | AX | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | AX | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 1 | GV | 46 | ARG | CA-C-N | 5.02 | 126.82 | 121.00 |
| 1 | GV | 46 | ARG | C-N-CA | 5.02 | 126.82 | 121.00 |
| 2 | HE | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | HE | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | JW | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | JW | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | KA | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | KA | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | LQ | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | LQ | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | DF | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | DF | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 2 | GM | 141 | ASP | CA-C-N | 5.02 | 125.09 | 119.87 |
| 2 | GM | 141 | ASP | C-N-CA | 5.02 | 125.09 | 119.87 |
| 1 | JX | 46 | ARG | CA-C-N | 5.02 | 126.82 | 121.00 |
| 1 | JX | 46 | ARG | C-N-CA | 5.02 | 126.82 | 121.00 |
| 1 | LN | 46 | ARG | CA-C-N | 5.02 | 126.82 | 121.00 |
| 1 | LN | 46 | ARG | C-N-CA | 5.02 | 126.82 | 121.00 |
| 1 | ZY | 46 | ARG | CA-C-N | 5.01 | 126.82 | 121.00 |
| 1 | ZY | 46 | ARG | C-N-CA | 5.01 | 126.82 | 121.00 |
| 1 | BG | 46 | ARG | CA-C-N | 5.01 | 126.82 | 121.00 |
| 1 | BG | 46 | ARG | C-N-CA | 5.01 | 126.82 | 121.00 |
| 1 | CQ | 19 | ARG | N-CA-C | -5.01 | 105.89 | 111.36 |
| 1 | GP | 19 | ARG | N-CA-C | -5.01 | 105.89 | 111.36 |
| 1 | BA | 46 | ARG | CA-C-N | 5.01 | 126.82 | 121.00 |
| 1 | BA | 46 | ARG | C-N-CA | 5.01 | 126.82 | 121.00 |
| 1 | HG | 46 | ARG | CA-C-N | 5.01 | 126.82 | 121.00 |
| 1 | HG | 46 | ARG | C-N-CA | 5.01 | 126.82 | 121.00 |
| 2 | DH | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | DH | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | DY | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | DY | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 2 | FC | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | FC | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 2 | GO | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | GO | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 1 | BY | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | BY | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | DC | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | DC | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 2 | DL | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | DL | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 1 | ET | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | ET | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 2 | FI | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | FI | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 1 | GJ | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | GJ | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | ZA | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | ZA | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | AI | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | AI | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | AC | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | AC | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 2 | BJ | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | BJ | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 1 | HR | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | HR | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | JA | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | JA | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 1 | KV | 46 | ARG | CA-C-N | 5.01 | 126.81 | 121.00 |
| 1 | KV | 46 | ARG | C-N-CA | 5.01 | 126.81 | 121.00 |
| 2 | YB | 141 | ASP | CA-C-N | 5.01 | 125.08 | 119.87 |
| 2 | YB | 141 | ASP | C-N-CA | 5.01 | 125.08 | 119.87 |
| 2 | YH | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | YH | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |
| 1 | YQ | 46 | ARG | CA-C-N | 5.00 | 126.81 | 121.00 |
| 1 | YQ | 46 | ARG | C-N-CA | 5.00 | 126.81 | 121.00 |
| 2 | CH | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | CH | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |
| 2 | EE | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | EE | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | GD | 46 | ARG | CA-C-N | 5.00 | 126.81 | 121.00 |
| 1 | GD | 46 | ARG | C-N-CA | 5.00 | 126.81 | 121.00 |
| 1 | HX | 46 | ARG | CA-C-N | 5.00 | 126.81 | 121.00 |
| 1 | HX | 46 | ARG | C-N-CA | 5.00 | 126.81 | 121.00 |
| 1 | JG | 46 | ARG | CA-C-N | 5.00 | 126.81 | 121.00 |
| 1 | JG | 46 | ARG | C-N-CA | 5.00 | 126.81 | 121.00 |
| 2 | JP | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | JP | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |
| 1 | CE | 46 | ARG | CA-C-N | 5.00 | 126.80 | 121.00 |
| 1 | CE | 46 | ARG | C-N-CA | 5.00 | 126.80 | 121.00 |
| 1 | EB | 46 | ARG | CA-C-N | 5.00 | 126.80 | 121.00 |
| 1 | EB | 46 | ARG | C-N-CA | 5.00 | 126.80 | 121.00 |
| 2 | JD | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | JD | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |
| 2 | KY | 141 | ASP | CA-C-N | 5.00 | 125.07 | 119.87 |
| 2 | KY | 141 | ASP | C-N-CA | 5.00 | 125.07 | 119.87 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 808 | 0 | 851 | 5 | 0 |
| 1 | AC | 808 | 0 | 851 | 3 | 0 |
| 1 | AE | 808 | 0 | 851 | 6 | 0 |
| 1 | AG | 808 | 0 | 851 | 5 | 0 |
| 1 | AI | 808 | 0 | 851 | 3 | 0 |
| 1 | AK | 808 | 0 | 851 | 7 | 0 |
| 1 | AM | 808 | 0 | 851 | 5 | 0 |
| 1 | AP | 808 | 0 | 851 | 6 | 0 |
| 1 | AR | 808 | 0 | 851 | 4 | 0 |
| 1 | AS | 808 | 0 | 851 | 5 | 0 |
| 1 | AU | 808 | 0 | 851 | 3 | 0 |
| 1 | AW | 808 | 0 | 851 | 7 | 0 |
| 1 | AY | 808 | 0 | 851 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | BA | 808 | 0 | 851 | 3 | 0 |
| 1 | BC | 808 | 0 | 851 | 7 | 0 |
| 1 | BE | 808 | 0 | 851 | 5 | 0 |
| 1 | BG | 808 | 0 | 851 | 4 | 0 |
| 1 | BI | 808 | 0 | 851 | 7 | 0 |
| 1 | BK | 808 | 0 | 851 | 5 | 0 |
| 1 | BM | 808 | 0 | 851 | 3 | 0 |
| 1 | BO | 808 | 0 | 851 | 6 | 0 |
| 1 | BQ | 808 | 0 | 851 | 5 | 0 |
| 1 | BS | 808 | 0 | 851 | 4 | 0 |
| 1 | BU | 808 | 0 | 851 | 6 | 0 |
| 1 | BW | 808 | 0 | 851 | 5 | 0 |
| 1 | BY | 808 | 0 | 851 | 4 | 0 |
| 1 | CA | 808 | 0 | 851 | 7 | 0 |
| 1 | CC | 808 | 0 | 851 | 5 | 0 |
| 1 | CE | 808 | 0 | 851 | 4 | 0 |
| 1 | CG | 808 | 0 | 851 | 6 | 0 |
| 1 | CI | 808 | 0 | 851 | 5 | 0 |
| 1 | CK | 808 | 0 | 851 | 4 | 0 |
| 1 | CM | 808 | 0 | 851 | 6 | 0 |
| 1 | CO | 808 | 0 | 851 | 5 | 0 |
| 1 | CQ | 808 | 0 | 851 | 3 | 0 |
| 1 | CS | 808 | 0 | 851 | 6 | 0 |
| 1 | CU | 808 | 0 | 851 | 5 | 0 |
| 1 | CW | 808 | 0 | 851 | 4 | 0 |
| 1 | CY | 808 | 0 | 851 | 6 | 0 |
| 1 | DA | 808 | 0 | 851 | 4 | 0 |
| 1 | DC | 808 | 0 | 851 | 4 | 0 |
| 1 | DE | 808 | 0 | 851 | 6 | 0 |
| 1 | DG | 808 | 0 | 851 | 5 | 0 |
| 1 | DI | 808 | 0 | 851 | 4 | 0 |
| 1 | DK | 808 | 0 | 851 | 6 | 0 |
| 1 | DM | 808 | 0 | 851 | 5 | 0 |
| 1 | DO | 808 | 0 | 851 | 3 | 0 |
| 1 | DQ | 808 | 0 | 851 | 6 | 0 |
| 1 | DS | 808 | 0 | 851 | 5 | 0 |
| 1 | DU | 808 | 0 | 851 | 4 | 0 |
| 1 | DX | 808 | 0 | 851 | 6 | 0 |
| 1 | DZ | 808 | 0 | 851 | 5 | 0 |
| 1 | EB | 808 | 0 | 851 | 3 | 0 |
| 1 | ED | 808 | 0 | 851 | 6 | 0 |
| 1 | EF | 808 | 0 | 851 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | EH | 808 | 0 | 851 | 4 | 0 |
| 1 | EJ | 808 | 0 | 851 | 6 | 0 |
| 1 | EL | 808 | 0 | 851 | 5 | 0 |
| 1 | EN | 808 | 0 | 851 | 4 | 0 |
| 1 | EP | 808 | 0 | 851 | 6 | 0 |
| 1 | ER | 808 | 0 | 851 | 5 | 0 |
| 1 | ET | 808 | 0 | 851 | 3 | 0 |
| 1 | EV | 808 | 0 | 851 | 7 | 0 |
| 1 | EX | 808 | 0 | 851 | 5 | 0 |
| 1 | EZ | 808 | 0 | 851 | 4 | 0 |
| 1 | FB | 808 | 0 | 851 | 6 | 0 |
| 1 | FD | 808 | 0 | 851 | 5 | 0 |
| 1 | FF | 808 | 0 | 851 | 4 | 0 |
| 1 | FH | 808 | 0 | 851 | 6 | 0 |
| 1 | FJ | 808 | 0 | 851 | 5 | 0 |
| 1 | FL | 808 | 0 | 851 | 4 | 0 |
| 1 | FN | 808 | 0 | 851 | 6 | 0 |
| 1 | FP | 808 | 0 | 851 | 5 | 0 |
| 1 | FR | 808 | 0 | 851 | 3 | 0 |
| 1 | FT | 808 | 0 | 851 | 7 | 0 |
| 1 | FV | 808 | 0 | 851 | 5 | 0 |
| 1 | FX | 808 | 0 | 851 | 4 | 0 |
| 1 | FZ | 808 | 0 | 851 | 6 | 0 |
| 1 | GB | 808 | 0 | 851 | 6 | 0 |
| 1 | GD | 808 | 0 | 851 | 4 | 0 |
| 1 | GF | 808 | 0 | 851 | 6 | 0 |
| 1 | GH | 808 | 0 | 851 | 5 | 0 |
| 1 | GJ | 808 | 0 | 851 | 4 | 0 |
| 1 | GL | 808 | 0 | 851 | 7 | 0 |
| 1 | GN | 808 | 0 | 851 | 5 | 0 |
| 1 | GP | 808 | 0 | 851 | 4 | 0 |
| 1 | GR | 808 | 0 | 851 | 6 | 0 |
| 1 | GT | 808 | 0 | 851 | 5 | 0 |
| 1 | GV | 808 | 0 | 851 | 4 | 0 |
| 1 | GX | 808 | 0 | 851 | 6 | 0 |
| 1 | GZ | 808 | 0 | 851 | 5 | 0 |
| 1 | HB | 808 | 0 | 851 | 3 | 0 |
| 1 | HD | 808 | 0 | 851 | 6 | 0 |
| 1 | HG | 808 | 0 | 851 | 4 | 0 |
| 1 | HI | 808 | 0 | 851 | 6 | 0 |
| 1 | HL | 808 | 0 | 851 | 3 | 0 |
| 1 | HN | 808 | 0 | 851 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | HP | 808 | 0 | 851 | 5 | 0 |
| 1 | HR | 808 | 0 | 851 | 4 | 0 |
| 1 | HT | 808 | 0 | 851 | 6 | 0 |
| 1 | HV | 808 | 0 | 851 | 5 | 0 |
| 1 | HX | 808 | 0 | 851 | 3 | 0 |
| 1 | HZ | 808 | 0 | 851 | 6 | 0 |
| 1 | IC | 808 | 0 | 851 | 3 | 0 |
| 1 | IE | 808 | 0 | 851 | 6 | 0 |
| 1 | IH | 808 | 0 | 851 | 5 | 0 |
| 1 | II | 808 | 0 | 851 | 4 | 0 |
| 1 | IK | 808 | 0 | 851 | 6 | 0 |
| 1 | IM | 808 | 0 | 851 | 5 | 0 |
| 1 | IO | 808 | 0 | 851 | 4 | 0 |
| 1 | IQ | 808 | 0 | 851 | 7 | 0 |
| 1 | IS | 808 | 0 | 851 | 4 | 0 |
| 1 | IU | 808 | 0 | 851 | 4 | 0 |
| 1 | IW | 808 | 0 | 851 | 6 | 0 |
| 1 | IY | 808 | 0 | 851 | 4 | 0 |
| 1 | JA | 808 | 0 | 851 | 4 | 0 |
| 1 | JC | 808 | 0 | 851 | 6 | 0 |
| 1 | JE | 808 | 0 | 851 | 5 | 0 |
| 1 | JG | 808 | 0 | 851 | 4 | 0 |
| 1 | JI | 808 | 0 | 851 | 6 | 0 |
| 1 | JK | 808 | 0 | 851 | 5 | 0 |
| 1 | JM | 808 | 0 | 851 | 3 | 0 |
| 1 | JO | 808 | 0 | 851 | 6 | 0 |
| 1 | JQ | 808 | 0 | 851 | 5 | 0 |
| 1 | JS | 808 | 0 | 851 | 3 | 0 |
| 1 | JV | 808 | 0 | 851 | 5 | 0 |
| 1 | JX | 808 | 0 | 851 | 4 | 0 |
| 1 | JZ | 808 | 0 | 851 | 6 | 0 |
| 1 | KB | 808 | 0 | 851 | 5 | 0 |
| 1 | KD | 808 | 0 | 851 | 3 | 0 |
| 1 | KF | 808 | 0 | 851 | 6 | 0 |
| 1 | KH | 808 | 0 | 851 | 5 | 0 |
| 1 | KJ | 808 | 0 | 851 | 3 | 0 |
| 1 | KL | 808 | 0 | 851 | 7 | 0 |
| 1 | KN | 808 | 0 | 851 | 5 | 0 |
| 1 | KP | 808 | 0 | 851 | 4 | 0 |
| 1 | KR | 808 | 0 | 851 | 7 | 0 |
| 1 | KT | 808 | 0 | 851 | 5 | 0 |
| 1 | KV | 808 | 0 | 851 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | KX | 808 | 0 | 851 | 6 | 0 |
| 1 | KZ | 808 | 0 | 851 | 5 | 0 |
| 1 | LB | 808 | 0 | 851 | 4 | 0 |
| 1 | LD | 808 | 0 | 851 | 7 | 0 |
| 1 | LF | 808 | 0 | 851 | 5 | 0 |
| 1 | LH | 808 | 0 | 851 | 4 | 0 |
| 1 | LJ | 808 | 0 | 851 | 6 | 0 |
| 1 | LL | 808 | 0 | 851 | 5 | 0 |
| 1 | LN | 808 | 0 | 851 | 4 | 0 |
| 1 | LP | 808 | 0 | 851 | 6 | 0 |
| 1 | LR | 808 | 0 | 851 | 5 | 0 |
| 1 | WA | 808 | 0 | 851 | 5 | 0 |
| 1 | WB | 808 | 0 | 851 | 5 | 0 |
| 1 | WC | 808 | 0 | 851 | 5 | 0 |
| 1 | WD | 808 | 0 | 851 | 6 | 0 |
| 1 | YA | 808 | 0 | 851 | 6 | 0 |
| 1 | YC | 808 | 0 | 851 | 5 | 0 |
| 1 | YE | 808 | 0 | 851 | 4 | 0 |
| 1 | YG | 808 | 0 | 851 | 6 | 0 |
| 1 | YI | 808 | 0 | 851 | 5 | 0 |
| 1 | YK | 808 | 0 | 851 | 4 | 0 |
| 1 | YM | 808 | 0 | 851 | 6 | 0 |
| 1 | YO | 808 | 0 | 851 | 5 | 0 |
| 1 | YQ | 808 | 0 | 851 | 4 | 0 |
| 1 | YS | 808 | 0 | 851 | 6 | 0 |
| 1 | YU | 808 | 0 | 851 | 5 | 0 |
| 1 | YW | 808 | 0 | 851 | 4 | 0 |
| 1 | YY | 808 | 0 | 851 | 6 | 0 |
| 1 | ZA | 808 | 0 | 851 | 4 | 0 |
| 1 | ZC | 808 | 0 | 851 | 6 | 0 |
| 1 | ZE | 808 | 0 | 851 | 5 | 0 |
| 1 | ZG | 808 | 0 | 851 | 4 | 0 |
| 1 | ZI | 808 | 0 | 851 | 7 | 0 |
| 1 | ZK | 808 | 0 | 851 | 5 | 0 |
| 1 | ZM | 808 | 0 | 851 | 4 | 0 |
| 1 | ZO | 808 | 0 | 851 | 6 | 0 |
| 1 | ZQ | 808 | 0 | 851 | 5 | 0 |
| 1 | ZS | 808 | 0 | 851 | 3 | 0 |
| 1 | ZU | 808 | 0 | 851 | 6 | 0 |
| 1 | ZW | 808 | 0 | 851 | 5 | 0 |
| 1 | ZY | 808 | 0 | 851 | 3 | 0 |
| 2 | AB | 2267 | 0 | 2393 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | AD | 2267 | 0 | 2393 | 7 | 0 |
| 2 | AF | 2267 | 0 | 2393 | 12 | 0 |
| 2 | AH | 2267 | 0 | 2393 | 10 | 0 |
| 2 | AJ | 2267 | 0 | 2393 | 8 | 0 |
| 2 | AL | 2267 | 0 | 2393 | 11 | 0 |
| 2 | AN | 2267 | 0 | 2393 | 9 | 0 |
| 2 | AO | 2267 | 0 | 2393 | 12 | 0 |
| 2 | AQ | 2267 | 0 | 2393 | 7 | 0 |
| 2 | AT | 2267 | 0 | 2393 | 9 | 0 |
| 2 | AV | 2267 | 0 | 2393 | 7 | 0 |
| 2 | AX | 2267 | 0 | 2393 | 12 | 0 |
| 2 | AZ | 2267 | 0 | 2393 | 10 | 0 |
| 2 | BB | 2267 | 0 | 2393 | 7 | 0 |
| 2 | BD | 2267 | 0 | 2393 | 12 | 0 |
| 2 | BF | 2267 | 0 | 2393 | 10 | 0 |
| 2 | BH | 2267 | 0 | 2393 | 7 | 0 |
| 2 | BJ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | BL | 2267 | 0 | 2393 | 9 | 0 |
| 2 | BN | 2267 | 0 | 2393 | 7 | 0 |
| 2 | BP | 2267 | 0 | 2393 | 11 | 0 |
| 2 | BR | 2267 | 0 | 2393 | 9 | 0 |
| 2 | BT | 2267 | 0 | 2393 | 7 | 0 |
| 2 | BV | 2267 | 0 | 2393 | 12 | 0 |
| 2 | BX | 2267 | 0 | 2393 | 9 | 0 |
| 2 | BZ | 2267 | 0 | 2393 | 7 | 0 |
| 2 | CB | 2267 | 0 | 2393 | 11 | 0 |
| 2 | CD | 2267 | 0 | 2393 | 10 | 0 |
| 2 | CF | 2267 | 0 | 2393 | 8 | 0 |
| 2 | CH | 2267 | 0 | 2393 | 12 | 0 |
| 2 | CJ | 2267 | 0 | 2393 | 9 | 0 |
| 2 | CL | 2267 | 0 | 2393 | 7 | 0 |
| 2 | CN | 2267 | 0 | 2393 | 12 | 0 |
| 2 | CP | 2267 | 0 | 2393 | 9 | 0 |
| 2 | CR | 2267 | 0 | 2393 | 7 | 0 |
| 2 | CT | 2267 | 0 | 2393 | 9 | 0 |
| 2 | CV | 2267 | 0 | 2393 | 9 | 0 |
| 2 | CX | 2267 | 0 | 2393 | 7 | 0 |
| 2 | CZ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | DB | 2267 | 0 | 2393 | 7 | 0 |
| 2 | DD | 2267 | 0 | 2393 | 7 | 0 |
| 2 | DF | 2267 | 0 | 2393 | 12 | 0 |
| 2 | DH | 2267 | 0 | 2393 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | DJ | 2267 | 0 | 2393 | 7 | 0 |
| 2 | DL | 2267 | 0 | 2393 | 10 | 0 |
| 2 | DN | 2267 | 0 | 2393 | 9 | 0 |
| 2 | DP | 2267 | 0 | 2393 | 7 | 0 |
| 2 | DR | 2267 | 0 | 2393 | 11 | 0 |
| 2 | DT | 2267 | 0 | 2393 | 8 | 0 |
| 2 | DW | 2267 | 0 | 2393 | 8 | 0 |
| 2 | DY | 2267 | 0 | 2393 | 13 | 0 |
| 2 | EA | 2267 | 0 | 2393 | 10 | 0 |
| 2 | EC | 2267 | 0 | 2393 | 7 | 0 |
| 2 | EE | 2267 | 0 | 2393 | 11 | 0 |
| 2 | EG | 2267 | 0 | 2393 | 9 | 0 |
| 2 | EI | 2267 | 0 | 2393 | 8 | 0 |
| 2 | EK | 2267 | 0 | 2393 | 10 | 0 |
| 2 | EM | 2267 | 0 | 2393 | 8 | 0 |
| 2 | EO | 2267 | 0 | 2393 | 7 | 0 |
| 2 | EQ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | ES | 2267 | 0 | 2393 | 9 | 0 |
| 2 | EU | 2267 | 0 | 2393 | 7 | 0 |
| 2 | EW | 2267 | 0 | 2393 | 12 | 0 |
| 2 | EY | 2267 | 0 | 2393 | 10 | 0 |
| 2 | FA | 2267 | 0 | 2393 | 8 | 0 |
| 2 | FC | 2267 | 0 | 2393 | 10 | 0 |
| 2 | FE | 2267 | 0 | 2393 | 9 | 0 |
| 2 | FG | 2267 | 0 | 2393 | 7 | 0 |
| 2 | FI | 2267 | 0 | 2393 | 9 | 0 |
| 2 | FK | 2267 | 0 | 2393 | 9 | 0 |
| 2 | FM | 2267 | 0 | 2393 | 8 | 0 |
| 2 | FO | 2267 | 0 | 2393 | 11 | 0 |
| 2 | FQ | 2267 | 0 | 2393 | 8 | 0 |
| 2 | FS | 2267 | 0 | 2393 | 8 | 0 |
| 2 | FU | 2267 | 0 | 2393 | 10 | 0 |
| 2 | FW | 2267 | 0 | 2393 | 9 | 0 |
| 2 | FY | 2267 | 0 | 2393 | 8 | 0 |
| 2 | GA | 2267 | 0 | 2393 | 10 | 0 |
| 2 | GC | 2267 | 0 | 2393 | 8 | 0 |
| 2 | GE | 2267 | 0 | 2393 | 8 | 0 |
| 2 | GG | 2267 | 0 | 2393 | 10 | 0 |
| 2 | GI | 2267 | 0 | 2393 | 8 | 0 |
| 2 | GK | 2267 | 0 | 2393 | 7 | 0 |
| 2 | GM | 2267 | 0 | 2393 | 10 | 0 |
| 2 | GO | 2267 | 0 | 2393 | 7 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | GQ | 2267 | 0 | 2393 | 7 | 0 |
| 2 | GS | 2267 | 0 | 2393 | 11 | 0 |
| 2 | GU | 2267 | 0 | 2393 | 8 | 0 |
| 2 | GW | 2267 | 0 | 2393 | 7 | 0 |
| 2 | GY | 2267 | 0 | 2393 | 10 | 0 |
| 2 | HA | 2267 | 0 | 2393 | 9 | 0 |
| 2 | HC | 2267 | 0 | 2393 | 8 | 0 |
| 2 | HE | 2267 | 0 | 2393 | 10 | 0 |
| 2 | HF | 2267 | 0 | 2393 | 9 | 0 |
| 2 | HH | 2267 | 0 | 2393 | 8 | 0 |
| 2 | HJ | 2267 | 0 | 2393 | 10 | 0 |
| 2 | HK | 2267 | 0 | 2393 | 8 | 0 |
| 2 | HM | 2267 | 0 | 2393 | 8 | 0 |
| 2 | HO | 2267 | 0 | 2393 | 12 | 0 |
| 2 | HQ | 2267 | 0 | 2393 | 9 | 0 |
| 2 | HS | 2267 | 0 | 2393 | 7 | 0 |
| 2 | HU | 2267 | 0 | 2393 | 11 | 0 |
| 2 | HW | 2267 | 0 | 2393 | 10 | 0 |
| 2 | HY | 2267 | 0 | 2393 | 7 | 0 |
| 2 | IA | 2267 | 0 | 2393 | 12 | 0 |
| 2 | IB | 2267 | 0 | 2393 | 9 | 0 |
| 2 | ID | 2267 | 0 | 2393 | 7 | 0 |
| 2 | IF | 2267 | 0 | 2393 | 12 | 0 |
| 2 | IG | 2267 | 0 | 2393 | 7 | 0 |
| 2 | IJ | 2267 | 0 | 2393 | 8 | 0 |
| 2 | IL | 2267 | 0 | 2393 | 11 | 0 |
| 2 | IN | 2267 | 0 | 2393 | 9 | 0 |
| 2 | IP | 2267 | 0 | 2393 | 7 | 0 |
| 2 | IR | 2267 | 0 | 2393 | 9 | 0 |
| 2 | IT | 2267 | 0 | 2393 | 9 | 0 |
| 2 | IV | 2267 | 0 | 2393 | 7 | 0 |
| 2 | IX | 2267 | 0 | 2393 | 12 | 0 |
| 2 | IZ | 2267 | 0 | 2393 | 8 | 0 |
| 2 | JB | 2267 | 0 | 2393 | 7 | 0 |
| 2 | JD | 2267 | 0 | 2393 | 10 | 0 |
| 2 | JF | 2267 | 0 | 2393 | 9 | 0 |
| 2 | JH | 2267 | 0 | 2393 | 8 | 0 |
| 2 | JJ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | JL | 2267 | 0 | 2393 | 9 | 0 |
| 2 | JN | 2267 | 0 | 2393 | 7 | 0 |
| 2 | JP | 2267 | 0 | 2393 | 11 | 0 |
| 2 | JR | 2267 | 0 | 2393 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | JT | 2267 | 0 | 2393 | 7 | 0 |
| 2 | JU | 2267 | 0 | 2393 | 10 | 0 |
| 2 | JW | 2267 | 0 | 2393 | 9 | 0 |
| 2 | JY | 2267 | 0 | 2393 | 7 | 0 |
| 2 | KA | 2267 | 0 | 2393 | 12 | 0 |
| 2 | KC | 2267 | 0 | 2393 | 8 | 0 |
| 2 | KE | 2267 | 0 | 2393 | 7 | 0 |
| 2 | KG | 2267 | 0 | 2393 | 10 | 0 |
| 2 | KI | 2267 | 0 | 2393 | 9 | 0 |
| 2 | KK | 2267 | 0 | 2393 | 8 | 0 |
| 2 | KM | 2267 | 0 | 2393 | 12 | 0 |
| 2 | KO | 2267 | 0 | 2393 | 8 | 0 |
| 2 | KQ | 2267 | 0 | 2393 | 8 | 0 |
| 2 | KS | 2267 | 0 | 2393 | 10 | 0 |
| 2 | KU | 2267 | 0 | 2393 | 9 | 0 |
| 2 | KW | 2267 | 0 | 2393 | 7 | 0 |
| 2 | KY | 2267 | 0 | 2393 | 10 | 0 |
| 2 | LA | 2267 | 0 | 2393 | 8 | 0 |
| 2 | LC | 2267 | 0 | 2393 | 8 | 0 |
| 2 | LE | 2267 | 0 | 2393 | 10 | 0 |
| 2 | LG | 2267 | 0 | 2393 | 9 | 0 |
| 2 | LI | 2267 | 0 | 2393 | 7 | 0 |
| 2 | LK | 2267 | 0 | 2393 | 10 | 0 |
| 2 | LM | 2267 | 0 | 2393 | 9 | 0 |
| 2 | LO | 2267 | 0 | 2393 | 7 | 0 |
| 2 | LQ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | LS | 2267 | 0 | 2393 | 10 | 0 |
| 2 | YB | 2267 | 0 | 2393 | 11 | 0 |
| 2 | YD | 2267 | 0 | 2393 | 10 | 0 |
| 2 | YF | 2267 | 0 | 2393 | 8 | 0 |
| 2 | YH | 2267 | 0 | 2393 | 11 | 0 |
| 2 | YJ | 2267 | 0 | 2393 | 9 | 0 |
| 2 | YL | 2267 | 0 | 2393 | 7 | 0 |
| 2 | YN | 2267 | 0 | 2393 | 11 | 0 |
| 2 | YP | 2267 | 0 | 2393 | 8 | 0 |
| 2 | YR | 2267 | 0 | 2393 | 8 | 0 |
| 2 | YT | 2267 | 0 | 2393 | 10 | 0 |
| 2 | YV | 2267 | 0 | 2393 | 9 | 0 |
| 2 | YX | 2267 | 0 | 2393 | 7 | 0 |
| 2 | YZ | 2267 | 0 | 2393 | 11 | 0 |
| 2 | ZB | 2267 | 0 | 2393 | 8 | 0 |
| 2 | ZD | 2267 | 0 | 2393 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2 | ZF | 2267 | 0 | 2393 | 9 | 0 |
| 2 | ZH | 2267 | 0 | 2393 | 7 | 0 |
| 2 | ZJ | 2267 | 0 | 2393 | 10 | 0 |
| 2 | ZL | 2267 | 0 | 2393 | 10 | 0 |
| 2 | ZN | 2267 | 0 | 2393 | 7 | 0 |
| 2 | ZP | 2267 | 0 | 2393 | 10 | 0 |
| 2 | ZR | 2267 | 0 | 2393 | 8 | 0 |
| 2 | ZT | 2267 | 0 | 2393 | 7 | 0 |
| 2 | ZV | 2267 | 0 | 2393 | 11 | 0 |
| 2 | ZX | 2267 | 0 | 2393 | 10 | 0 |
| 2 | ZZ | 2267 | 0 | 2393 | 8 | 0 |
| All | All | 553500 | 0 | 583920 | 1976 | 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 (1976) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:LB:90:GLU:OE2 | 2:LC:282:LYS:NZ | 2.34 | 0.61 |
| 1:YE:90:GLU:OE2 | 2:YF:282:LYS:NZ | 2.34 | 0.61 |
| 1:BS:90:GLU:OE2 | 2:BT:282:LYS:NZ | 2.34 | 0.61 |
| 1:DC:90:GLU:OE2 | 2:DD:282:LYS:NZ | 2.34 | 0.61 |
| 1:ZG:90:GLU:OE2 | 2:ZH:282:LYS:NZ | 2.34 | 0.61 |
| 1:HL:90:GLU:OE2 | 2:HM:282:LYS:NZ | 2.34 | 0.61 |
| 1:II:90:GLU:OE2 | 2:IJ:282:LYS:NZ | 2.34 | 0.61 |
| 2:AQ:282:LYS:NZ | 1:AR:90:GLU:OE2 | 2.34 | 0.61 |
| 1:EN:90:GLU:OE2 | 2:EO:282:LYS:NZ | 2.34 | 0.61 |
| 1:FR:90:GLU:OE2 | 2:FS:282:LYS:NZ | 2.34 | 0.61 |
| 1:HB:90:GLU:OE2 | 2:HC:282:LYS:NZ | 2.34 | 0.61 |
| 1:JA:90:GLU:OE2 | 2:JB:282:LYS:NZ | 2.34 | 0.61 |
| 1:KP:90:GLU:OE2 | 2:KQ:282:LYS:NZ | 2.34 | 0.61 |
| 1:ZS:90:GLU:OE2 | 2:ZT:282:LYS:NZ | 2.34 | 0.61 |
| 1:AC:90:GLU:OE2 | 2:AD:282:LYS:NZ | 2.34 | 0.61 |
| 1:HG:90:GLU:OE2 | 2:HH:282:LYS:NZ | 2.34 | 0.61 |
| 1:KJ:90:GLU:OE2 | 2:KK:282:LYS:NZ | 2.34 | 0.61 |
| 1:BY:90:GLU:OE2 | 2:BZ:282:LYS:NZ | 2.34 | 0.61 |
| 1:DU:90:GLU:OE2 | 2:DW:282:LYS:NZ | 2.34 | 0.61 |
| 1:EH:90:GLU:OE2 | 2:EI:282:LYS:NZ | 2.34 | 0.61 |
| 1:LH:90:GLU:OE2 | 2:LI:282:LYS:NZ | 2.34 | 0.61 |
| 1:AI:90:GLU:OE2 | 2:AJ:282:LYS:NZ | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:GP:90:GLU:OE2 | 2:GQ:282:LYS:NZ | 2.34 | 0.61 |
| 1:BG:90:GLU:OE2 | 2:BH:282:LYS:NZ | 2.34 | 0.61 |
| 1:CK:90:GLU:OE2 | 2:CL:282:LYS:NZ | 2.34 | 0.61 |
| 1:CQ:90:GLU:OE2 | 2:CR:282:LYS:NZ | 2.34 | 0.61 |
| 1:GD:90:GLU:OE2 | 2:GE:282:LYS:NZ | 2.34 | 0.61 |
| 1:IO:90:GLU:OE2 | 2:IP:282:LYS:NZ | 2.34 | 0.61 |
| 1:IU:90:GLU:OE2 | 2:IV:282:LYS:NZ | 2.34 | 0.61 |
| 1:KV:90:GLU:OE2 | 2:KW:282:LYS:NZ | 2.34 | 0.61 |
| 1:LN:90:GLU:OE2 | 2:LO:282:LYS:NZ | 2.34 | 0.61 |
| 1:YQ:90:GLU:OE2 | 2:YR:282:LYS:NZ | 2.34 | 0.61 |
| 1:AU:90:GLU:OE2 | 2:AV:282:LYS:NZ | 2.34 | 0.61 |
| 1:FL:90:GLU:OE2 | 2:FM:282:LYS:NZ | 2.34 | 0.61 |
| 1:BA:90:GLU:OE2 | 2:BB:282:LYS:NZ | 2.34 | 0.60 |
| 1:EB:90:GLU:OE2 | 2:EC:282:LYS:NZ | 2.34 | 0.60 |
| 1:HX:90:GLU:OE2 | 2:HY:282:LYS:NZ | 2.34 | 0.60 |
| 1:KD:90:GLU:OE2 | 2:KE:282:LYS:NZ | 2.34 | 0.60 |
| 1:ZM:90:GLU:OE2 | 2:ZN:282:LYS:NZ | 2.34 | 0.60 |
| 1:ZY:90:GLU:OE2 | 2:ZZ:282:LYS:NZ | 2.34 | 0.60 |
| 1:CE:90:GLU:OE2 | 2:CF:282:LYS:NZ | 2.34 | 0.60 |
| 1:ZA:90:GLU:OE2 | 2:ZB:282:LYS:NZ | 2.34 | 0.60 |
| 1:DI:90:GLU:OE2 | 2:DJ:282:LYS:NZ | 2.34 | 0.60 |
| 2:FE:123:GLU:OE2 | 2:FE:170:LYS:NZ | 2.34 | 0.60 |
| 1:FX:90:GLU:OE2 | 2:FY:282:LYS:NZ | 2.34 | 0.60 |
| 1:IC:90:GLU:OE2 | 2:ID:282:LYS:NZ | 2.34 | 0.60 |
| 2:IG:123:GLU:OE2 | 2:IG:170:LYS:NZ | 2.34 | 0.60 |
| 1:JS:90:GLU:OE2 | 2:JT:282:LYS:NZ | 2.34 | 0.60 |
| 1:JX:90:GLU:OE2 | 2:JY:282:LYS:NZ | 2.34 | 0.60 |
| 1:FF:90:GLU:OE2 | 2:FG:282:LYS:NZ | 2.34 | 0.60 |
| 1:BM:90:GLU:OE2 | 2:BN:282:LYS:NZ | 2.34 | 0.60 |
| 1:DO:90:GLU:OE2 | 2:DP:282:LYS:NZ | 2.34 | 0.60 |
| 2:EQ:2:ASP:OD2 | 2:ES:101:LYS:NZ | 2.33 | 0.60 |
| 1:ET:90:GLU:OE2 | 2:EU:282:LYS:NZ | 2.34 | 0.60 |
| 2:FW:123:GLU:OE2 | 2:FW:170:LYS:NZ | 2.34 | 0.60 |
| 1:HR:90:GLU:OE2 | 2:HS:282:LYS:NZ | 2.34 | 0.60 |
| 1:JG:90:GLU:OE2 | 2:JH:282:LYS:NZ | 2.34 | 0.60 |
| 1:JM:90:GLU:OE2 | 2:JN:282:LYS:NZ | 2.34 | 0.60 |
| 1:YK:90:GLU:OE2 | 2:YL:282:LYS:NZ | 2.34 | 0.60 |
| 1:CW:90:GLU:OE2 | 2:CX:282:LYS:NZ | 2.34 | 0.60 |
| 1:EZ:90:GLU:OE2 | 2:FA:282:LYS:NZ | 2.34 | 0.60 |
| 2:HW:123:GLU:OE2 | 2:HW:170:LYS:NZ | 2.34 | 0.60 |
| 2:AT:123:GLU:OE2 | 2:AT:170:LYS:NZ | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:GJ:90:GLU:OE2 | 2:GK:282:LYS:NZ | 2.34 | 0.60 |
| 1:GV:90:GLU:OE2 | 2:GW:282:LYS:NZ | 2.34 | 0.60 |
| 2:KO:123:GLU:OE2 | 2:KO:170:LYS:NZ | 2.34 | 0.60 |
| 1:YW:90:GLU:OE2 | 2:YX:282:LYS:NZ | 2.34 | 0.60 |
| 2:DT:123:GLU:OE2 | 2:DT:170:LYS:NZ | 2.34 | 0.60 |
| 2:IL:123:GLU:OE2 | 2:IL:170:LYS:NZ | 2.34 | 0.60 |
| 2:CV:123:GLU:OE2 | 2:CV:170:LYS:NZ | 2.34 | 0.60 |
| 2:FK:123:GLU:OE2 | 2:FK:170:LYS:NZ | 2.34 | 0.60 |
| 2:BD:123:GLU:OE2 | 2:BD:170:LYS:NZ | 2.34 | 0.59 |
| 1:BQ:90:GLU:OE2 | 2:BR:282:LYS:NZ | 2.35 | 0.59 |
| 2:GO:123:GLU:OE2 | 2:GO:170:LYS:NZ | 2.34 | 0.59 |
| 1:GT:90:GLU:OE2 | 2:GU:282:LYS:NZ | 2.35 | 0.59 |
| 1:JE:90:GLU:OE2 | 2:JF:282:LYS:NZ | 2.35 | 0.59 |
| 1:KH:90:GLU:OE2 | 2:KI:282:LYS:NZ | 2.35 | 0.59 |
| 2:LG:123:GLU:OE2 | 2:LG:170:LYS:NZ | 2.34 | 0.59 |
| 2:ZR:123:GLU:OE2 | 2:ZR:170:LYS:NZ | 2.34 | 0.59 |
| 1:YI:90:GLU:OE2 | 2:YJ:282:LYS:NZ | 2.35 | 0.59 |
| 1:AA:90:GLU:OE2 | 2:AB:282:LYS:NZ | 2.35 | 0.59 |
| 1:BE:90:GLU:OE2 | 2:BF:282:LYS:NZ | 2.35 | 0.59 |
| 1:CU:90:GLU:OE2 | 2:CV:282:LYS:NZ | 2.35 | 0.59 |
| 1:FV:90:GLU:OE2 | 2:FW:282:LYS:NZ | 2.36 | 0.59 |
| 1:IM:90:GLU:OE2 | 2:IN:282:LYS:NZ | 2.35 | 0.59 |
| 2:JF:123:GLU:OE2 | 2:JF:170:LYS:NZ | 2.34 | 0.59 |
| 1:JK:90:GLU:OE2 | 2:JL:282:LYS:NZ | 2.35 | 0.59 |
| 1:KT:90:GLU:OE2 | 2:KU:282:LYS:NZ | 2.36 | 0.59 |
| 1:KZ:90:GLU:OE2 | 2:LA:282:LYS:NZ | 2.35 | 0.59 |
| 1:YO:90:GLU:OE2 | 2:YP:282:LYS:NZ | 2.35 | 0.59 |
| 1:AG:90:GLU:OE2 | 2:AH:282:LYS:NZ | 2.35 | 0.59 |
| 1:CC:90:GLU:OE2 | 2:CD:282:LYS:NZ | 2.35 | 0.59 |
| 1:EF:90:GLU:OE2 | 2:EG:282:LYS:NZ | 2.35 | 0.59 |
| 1:HP:90:GLU:OE2 | 2:HQ:282:LYS:NZ | 2.35 | 0.59 |
| 2:IB:123:GLU:OE2 | 2:IB:170:LYS:NZ | 2.34 | 0.59 |
| 1:ZQ:90:GLU:OE2 | 2:ZR:282:LYS:NZ | 2.35 | 0.59 |
| 1:DG:90:GLU:OE2 | 2:DH:282:LYS:NZ | 2.35 | 0.59 |
| 1:LF:90:GLU:OE2 | 2:LG:282:LYS:NZ | 2.35 | 0.59 |
| 2:ZX:123:GLU:OE2 | 2:ZX:170:LYS:NZ | 2.34 | 0.59 |
| 2:BX:123:GLU:OE2 | 2:BX:170:LYS:NZ | 2.34 | 0.59 |
| 1:DA:90:GLU:OE2 | 2:DB:282:LYS:NZ | 2.35 | 0.59 |
| 1:FJ:90:GLU:OE2 | 2:FK:282:LYS:NZ | 2.35 | 0.59 |
| 1:GH:90:GLU:OE2 | 2:GI:282:LYS:NZ | 2.35 | 0.59 |
| 2:IG:282:LYS:NZ | 1:IH:90:GLU:OE2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:KC:123:GLU:OE2 | 2:KC:170:LYS:NZ | 2.34 | 0.59 |
| 2:LK:2:ASP:OD2 | 2:LM:101:LYS:NZ | 2.34 | 0.59 |
| 1:ZW:90:GLU:OE2 | 2:ZX:282:LYS:NZ | 2.35 | 0.59 |
| 1:YU:90:GLU:OE2 | 2:YV:282:LYS:NZ | 2.35 | 0.59 |
| 1:AM:90:GLU:OE2 | 2:AN:282:LYS:NZ | 2.35 | 0.59 |
| 1:CO:90:GLU:OE2 | 2:CP:282:LYS:NZ | 2.35 | 0.59 |
| 1:FD:90:GLU:OE2 | 2:FE:282:LYS:NZ | 2.35 | 0.59 |
| 1:GN:90:GLU:OE2 | 2:GO:282:LYS:NZ | 2.35 | 0.59 |
| 1:GZ:90:GLU:OE2 | 2:HA:282:LYS:NZ | 2.35 | 0.59 |
| 1:HV:90:GLU:OE2 | 2:HW:282:LYS:NZ | 2.35 | 0.59 |
| 1:IS:90:GLU:OE2 | 2:IT:282:LYS:NZ | 2.35 | 0.59 |
| 1:JQ:90:GLU:OE2 | 2:JR:282:LYS:NZ | 2.35 | 0.59 |
| 1:AS:90:GLU:OE2 | 2:AT:282:LYS:NZ | 2.35 | 0.59 |
| 2:CJ:123:GLU:OE2 | 2:CJ:170:LYS:NZ | 2.34 | 0.59 |
| 1:ZE:90:GLU:OE2 | 2:ZF:282:LYS:NZ | 2.35 | 0.59 |
| 1:EL:90:GLU:OE2 | 2:EM:282:LYS:NZ | 2.35 | 0.59 |
| 1:ER:90:GLU:OE2 | 2:ES:282:LYS:NZ | 2.35 | 0.59 |
| 2:HF:282:LYS:NZ | 1:WB:90:GLU:OE2 | 2.35 | 0.59 |
| 2:KI:123:GLU:OE2 | 2:KI:170:LYS:NZ | 2.34 | 0.59 |
| 1:BW:90:GLU:OE2 | 2:BX:282:LYS:NZ | 2.35 | 0.59 |
| 1:DM:90:GLU:OE2 | 2:DN:282:LYS:NZ | 2.35 | 0.59 |
| 2:BF:123:GLU:OE2 | 2:BF:170:LYS:NZ | 2.34 | 0.59 |
| 2:CP:123:GLU:OE2 | 2:CP:170:LYS:NZ | 2.34 | 0.59 |
| 1:KB:90:GLU:OE2 | 2:KC:282:LYS:NZ | 2.35 | 0.59 |
| 1:LL:90:GLU:OE2 | 2:LM:282:LYS:NZ | 2.36 | 0.59 |
| 1:LR:90:GLU:OE2 | 2:LS:282:LYS:NZ | 2.35 | 0.59 |
| 1:EX:90:GLU:OE2 | 2:EY:282:LYS:NZ | 2.35 | 0.59 |
| 2:FQ:123:GLU:OE2 | 2:FQ:170:LYS:NZ | 2.34 | 0.59 |
| 2:IX:2:ASP:OD2 | 2:IZ:101:LYS:NZ | 2.33 | 0.59 |
| 1:ZK:90:GLU:OE2 | 2:ZL:282:LYS:NZ | 2.35 | 0.59 |
| 1:JV:90:GLU:OE2 | 2:JW:282:LYS:NZ | 2.35 | 0.59 |
| 1:YC:90:GLU:OE2 | 2:YD:282:LYS:NZ | 2.36 | 0.58 |
| 2:CZ:2:ASP:OD2 | 2:DB:101:LYS:NZ | 2.34 | 0.58 |
| 1:FP:90:GLU:OE2 | 2:FQ:282:LYS:NZ | 2.35 | 0.58 |
| 2:HA:123:GLU:OE2 | 2:HA:170:LYS:NZ | 2.34 | 0.58 |
| 2:HK:282:LYS:NZ | 1:WA:90:GLU:OE2 | 2.35 | 0.58 |
| 1:CI:90:GLU:OE2 | 2:CJ:282:LYS:NZ | 2.35 | 0.58 |
| 1:DS:90:GLU:OE2 | 2:DT:282:LYS:NZ | 2.35 | 0.58 |
| 1:DZ:90:GLU:OE2 | 2:EA:282:LYS:NZ | 2.35 | 0.58 |
| 2:EM:123:GLU:OE2 | 2:EM:170:LYS:NZ | 2.34 | 0.58 |
| 1:AY:90:GLU:OE2 | 2:AZ:282:LYS:NZ | 2.35 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:GS:2:ASP:OD2 | 2:GU:101:LYS:NZ | 2.33 | 0.58 |
| 2:IB:282:LYS:NZ | 1:WC:90:GLU:OE2 | 2.35 | 0.58 |
| 1:IY:90:GLU:OE2 | 2:IZ:282:LYS:NZ | 2.36 | 0.58 |
| 2:IX:123:GLU:OE2 | 2:IX:170:LYS:NZ | 2.34 | 0.58 |
| 2:YJ:123:GLU:OE2 | 2:YJ:170:LYS:NZ | 2.34 | 0.58 |
| 1:BK:90:GLU:OE2 | 2:BL:282:LYS:NZ | 2.36 | 0.58 |
| 2:CD:123:GLU:OE2 | 2:CD:170:LYS:NZ | 2.34 | 0.58 |
| 1:GB:90:GLU:OE2 | 2:GC:282:LYS:NZ | 2.35 | 0.58 |
| 2:GC:123:GLU:OE2 | 2:GC:170:LYS:NZ | 2.34 | 0.58 |
| 2:GI:123:GLU:OE2 | 2:GI:170:LYS:NZ | 2.34 | 0.58 |
| 1:KN:90:GLU:OE2 | 2:KO:282:LYS:NZ | 2.36 | 0.58 |
| 2:DB:123:GLU:OE2 | 2:DB:170:LYS:NZ | 2.34 | 0.58 |
| 2:EY:123:GLU:OE2 | 2:EY:170:LYS:NZ | 2.34 | 0.58 |
| 2:HQ:123:GLU:OE2 | 2:HQ:170:LYS:NZ | 2.34 | 0.58 |
| 2:EA:123:GLU:OE2 | 2:EA:170:LYS:NZ | 2.34 | 0.58 |
| 2:GA:2:ASP:OD2 | 2:GC:101:LYS:NZ | 2.34 | 0.58 |
| 2:IT:123:GLU:OE2 | 2:IT:170:LYS:NZ | 2.34 | 0.58 |
| 2:JL:123:GLU:OE2 | 2:JL:170:LYS:NZ | 2.34 | 0.58 |
| 2:ZP:123:GLU:OE2 | 2:ZP:170:LYS:NZ | 2.34 | 0.58 |
| 2:GG:123:GLU:OE2 | 2:GG:170:LYS:NZ | 2.34 | 0.58 |
| 2:YH:123:GLU:OE2 | 2:YH:170:LYS:NZ | 2.34 | 0.58 |
| 2:AN:123:GLU:OE2 | 2:AN:170:LYS:NZ | 2.34 | 0.57 |
| 2:DH:123:GLU:OE2 | 2:DH:170:LYS:NZ | 2.34 | 0.57 |
| 2:FU:2:ASP:OD2 | 2:FW:101:LYS:NZ | 2.34 | 0.57 |
| 2:ZF:123:GLU:OE2 | 2:ZF:170:LYS:NZ | 2.34 | 0.57 |
| 2:BJ:123:GLU:OE2 | 2:BJ:170:LYS:NZ | 2.34 | 0.57 |
| 2:GM:123:GLU:OE2 | 2:GM:170:LYS:NZ | 2.34 | 0.57 |
| 2:ZL:123:GLU:OE2 | 2:ZL:170:LYS:NZ | 2.34 | 0.57 |
| 2:YZ:123:GLU:OE2 | 2:YZ:170:LYS:NZ | 2.34 | 0.57 |
| 2:AL:123:GLU:OE2 | 2:AL:170:LYS:NZ | 2.34 | 0.57 |
| 2:GA:123:GLU:OE2 | 2:GA:170:LYS:NZ | 2.34 | 0.57 |
| 2:JW:123:GLU:OE2 | 2:JW:170:LYS:NZ | 2.34 | 0.57 |
| 2:KS:2:ASP:OD2 | 2:KU:101:LYS:NZ | 2.33 | 0.57 |
| 2:LS:123:GLU:OE2 | 2:LS:170:LYS:NZ | 2.34 | 0.57 |
| 2:YZ:134:ASP:OD1 | 2:YZ:138:LYS:NZ | 2.38 | 0.57 |
| 2:DN:123:GLU:OE2 | 2:DN:170:LYS:NZ | 2.34 | 0.57 |
| 1:YG:92:GLU:OE2 | 2:YH:282:LYS:NZ | 2.38 | 0.57 |
| 2:AF:134:ASP:OD1 | 2:AF:138:LYS:NZ | 2.38 | 0.57 |
| 1:CS:92:GLU:OE2 | 2:CT:282:LYS:NZ | 2.38 | 0.57 |
| 2:CZ:134:ASP:OD1 | 2:CZ:138:LYS:NZ | 2.38 | 0.57 |
| 1:DK:92:GLU:OE2 | 2:DL:282:LYS:NZ | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:DL:134:ASP:OD1 | 2:DL:138:LYS:NZ | 2.38 | 0.57 |
| 2:DR:134:ASP:OD1 | 2:DR:138:LYS:NZ | 2.38 | 0.57 |
| 1:FN:92:GLU:OE2 | 2:FO:282:LYS:NZ | 2.38 | 0.57 |
| 2:FO:134:ASP:OD1 | 2:FO:138:LYS:NZ | 2.38 | 0.57 |
| 2:GM:134:ASP:OD1 | 2:GM:138:LYS:NZ | 2.38 | 0.57 |
| 2:HJ:134:ASP:OD1 | 2:HJ:138:LYS:NZ | 2.38 | 0.57 |
| 2:HO:134:ASP:OD1 | 2:HO:138:LYS:NZ | 2.38 | 0.57 |
| 2:JU:134:ASP:OD1 | 2:JU:138:LYS:NZ | 2.38 | 0.57 |
| 2:KY:134:ASP:OD1 | 2:KY:138:LYS:NZ | 2.38 | 0.57 |
| 2:ZP:134:ASP:OD1 | 2:ZP:138:LYS:NZ | 2.38 | 0.57 |
| 1:YS:92:GLU:OE2 | 2:YT:282:LYS:NZ | 2.38 | 0.57 |
| 2:BL:123:GLU:OE2 | 2:BL:170:LYS:NZ | 2.34 | 0.57 |
| 1:DE:92:GLU:OE2 | 2:DF:282:LYS:NZ | 2.38 | 0.57 |
| 1:DQ:92:GLU:OE2 | 2:DR:282:LYS:NZ | 2.38 | 0.57 |
| 2:DY:134:ASP:OD1 | 2:DY:138:LYS:NZ | 2.38 | 0.57 |
| 2:EK:134:ASP:OD1 | 2:EK:138:LYS:NZ | 2.38 | 0.57 |
| 1:FZ:92:GLU:OE2 | 2:GA:282:LYS:NZ | 2.38 | 0.57 |
| 2:GU:123:GLU:OE2 | 2:GU:170:LYS:NZ | 2.34 | 0.57 |
| 1:ZI:92:GLU:OE2 | 2:ZJ:282:LYS:NZ | 2.38 | 0.57 |
| 2:IZ:123:GLU:OE2 | 2:IZ:170:LYS:NZ | 2.34 | 0.57 |
| 1:JI:92:GLU:OE2 | 2:JJ:282:LYS:NZ | 2.38 | 0.57 |
| 1:ZC:92:GLU:OE2 | 2:ZD:282:LYS:NZ | 2.38 | 0.57 |
| 2:ZD:134:ASP:OD1 | 2:ZD:138:LYS:NZ | 2.38 | 0.57 |
| 2:DF:134:ASP:OD1 | 2:DF:138:LYS:NZ | 2.38 | 0.57 |
| 2:EE:134:ASP:OD1 | 2:EE:138:LYS:NZ | 2.38 | 0.57 |
| 1:EJ:92:GLU:OE2 | 2:EK:282:LYS:NZ | 2.38 | 0.57 |
| 1:HD:92:GLU:OE2 | 2:HE:282:LYS:NZ | 2.38 | 0.57 |
| 2:YV:123:GLU:OE2 | 2:YV:170:LYS:NZ | 2.34 | 0.57 |
| 2:AH:123:GLU:OE2 | 2:AH:170:LYS:NZ | 2.34 | 0.57 |
| 2:AL:134:ASP:OD1 | 2:AL:138:LYS:NZ | 2.38 | 0.57 |
| 2:AO:2:ASP:OD2 | 2:AT:101:LYS:NZ | 2.34 | 0.57 |
| 1:AW:92:GLU:OE2 | 2:AX:282:LYS:NZ | 2.38 | 0.57 |
| 2:BD:134:ASP:OD1 | 2:BD:138:LYS:NZ | 2.38 | 0.57 |
| 2:CH:134:ASP:OD1 | 2:CH:138:LYS:NZ | 2.38 | 0.57 |
| 1:CM:92:GLU:OE2 | 2:CN:282:LYS:NZ | 2.38 | 0.57 |
| 2:EQ:134:ASP:OD1 | 2:EQ:138:LYS:NZ | 2.38 | 0.57 |
| 2:EW:2:ASP:OD2 | 2:EY:101:LYS:NZ | 2.34 | 0.57 |
| 1:GL:92:GLU:OE2 | 2:GM:282:LYS:NZ | 2.38 | 0.57 |
| 2:GY:134:ASP:OD1 | 2:GY:138:LYS:NZ | 2.38 | 0.57 |
| 2:HE:134:ASP:OD1 | 2:HE:138:LYS:NZ | 2.38 | 0.57 |
| 1:HT:92:GLU:OE2 | 2:HU:282:LYS:NZ | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:HZ:92:GLU:OE2 | 2:IA:282:LYS:NZ | 2.38 | 0.57 |
| 2:JD:134:ASP:OD1 | 2:JD:138:LYS:NZ | 2.38 | 0.57 |
| 2:LK:123:GLU:OE2 | 2:LK:170:LYS:NZ | 2.34 | 0.57 |
| 2:LQ:134:ASP:OD1 | 2:LQ:138:LYS:NZ | 2.38 | 0.57 |
| 2:AB:123:GLU:OE2 | 2:AB:170:LYS:NZ | 2.34 | 0.56 |
| 1:EV:92:GLU:OE2 | 2:EW:282:LYS:NZ | 2.38 | 0.56 |
| 2:FU:134:ASP:OD1 | 2:FU:138:LYS:NZ | 2.38 | 0.56 |
| 2:HU:123:GLU:OE2 | 2:HU:170:LYS:NZ | 2.34 | 0.56 |
| 1:IW:92:GLU:OE2 | 2:IX:282:LYS:NZ | 2.38 | 0.56 |
| 1:KF:92:GLU:OE2 | 2:KG:282:LYS:NZ | 2.38 | 0.56 |
| 2:YH:134:ASP:OD1 | 2:YH:138:LYS:NZ | 2.38 | 0.56 |
| 1:YM:92:GLU:OE2 | 2:YN:282:LYS:NZ | 2.38 | 0.56 |
| 1:BO:92:GLU:OE2 | 2:BP:282:LYS:NZ | 2.38 | 0.56 |
| 2:BV:134:ASP:OD1 | 2:BV:138:LYS:NZ | 2.38 | 0.56 |
| 2:CT:123:GLU:OE2 | 2:CT:170:LYS:NZ | 2.34 | 0.56 |
| 1:CY:92:GLU:OE2 | 2:CZ:282:LYS:NZ | 2.38 | 0.56 |
| 1:DX:92:GLU:OE2 | 2:DY:282:LYS:NZ | 2.38 | 0.56 |
| 2:EW:134:ASP:OD1 | 2:EW:138:LYS:NZ | 2.38 | 0.56 |
| 2:FC:134:ASP:OD1 | 2:FC:138:LYS:NZ | 2.38 | 0.56 |
| 1:HI:92:GLU:OE2 | 2:HJ:282:LYS:NZ | 2.38 | 0.56 |
| 1:HN:92:GLU:OE2 | 2:HO:282:LYS:NZ | 2.38 | 0.56 |
| 2:HU:134:ASP:OD1 | 2:HU:138:LYS:NZ | 2.38 | 0.56 |
| 2:IF:134:ASP:OD1 | 2:IF:138:LYS:NZ | 2.38 | 0.56 |
| 2:IR:134:ASP:OD1 | 2:IR:138:LYS:NZ | 2.38 | 0.56 |
| 1:JC:92:GLU:OE2 | 2:JD:282:LYS:NZ | 2.38 | 0.56 |
| 2:KS:134:ASP:OD1 | 2:KS:138:LYS:NZ | 2.38 | 0.56 |
| 1:KX:92:GLU:OE2 | 2:KY:282:LYS:NZ | 2.38 | 0.56 |
| 1:LJ:92:GLU:OE2 | 2:LK:282:LYS:NZ | 2.38 | 0.56 |
| 2:ZP:2:ASP:OD2 | 2:ZR:101:LYS:NZ | 2.34 | 0.56 |
| 2:YD:123:GLU:OE2 | 2:YD:170:LYS:NZ | 2.34 | 0.56 |
| 1:AK:92:GLU:OE2 | 2:AL:282:LYS:NZ | 2.38 | 0.56 |
| 2:BD:2:ASP:OD2 | 2:BF:101:LYS:NZ | 2.33 | 0.56 |
| 1:BI:92:GLU:OE2 | 2:BJ:282:LYS:NZ | 2.38 | 0.56 |
| 2:BJ:134:ASP:OD1 | 2:BJ:138:LYS:NZ | 2.38 | 0.56 |
| 2:CN:134:ASP:OD1 | 2:CN:138:LYS:NZ | 2.38 | 0.56 |
| 2:CT:134:ASP:OD1 | 2:CT:138:LYS:NZ | 2.38 | 0.56 |
| 1:ED:92:GLU:OE2 | 2:EE:282:LYS:NZ | 2.38 | 0.56 |
| 1:FT:92:GLU:OE2 | 2:FU:282:LYS:NZ | 2.38 | 0.56 |
| 2:GA:134:ASP:OD1 | 2:GA:138:LYS:NZ | 2.38 | 0.56 |
| 1:GR:92:GLU:OE2 | 2:GS:282:LYS:NZ | 2.38 | 0.56 |
| 2:GS:134:ASP:OD1 | 2:GS:138:LYS:NZ | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:GX:92:GLU:OE2 | 2:GY:282:LYS:NZ | 2.38 | 0.56 |
| 2:ZJ:134:ASP:OD1 | 2:ZJ:138:LYS:NZ | 2.38 | 0.56 |
| 2:IF:2:ASP:OD2 | 2:IG:101:LYS:NZ | 2.34 | 0.56 |
| 1:IK:92:GLU:OE2 | 2:IL:282:LYS:NZ | 2.38 | 0.56 |
| 2:IL:134:ASP:OD1 | 2:IL:138:LYS:NZ | 2.38 | 0.56 |
| 2:IX:134:ASP:OD1 | 2:IX:138:LYS:NZ | 2.38 | 0.56 |
| 2:KA:2:ASP:OD2 | 2:KC:101:LYS:NZ | 2.33 | 0.56 |
| 1:KL:92:GLU:OE2 | 2:KM:282:LYS:NZ | 2.38 | 0.56 |
| 1:KR:92:GLU:OE2 | 2:KS:282:LYS:NZ | 2.38 | 0.56 |
| 2:KU:123:GLU:OE2 | 2:KU:170:LYS:NZ | 2.34 | 0.56 |
| 1:YA:92:GLU:OE2 | 2:YB:282:LYS:NZ | 2.38 | 0.56 |
| 2:YT:134:ASP:OD1 | 2:YT:138:LYS:NZ | 2.38 | 0.56 |
| 2:AO:134:ASP:OD1 | 2:AO:138:LYS:NZ | 2.38 | 0.56 |
| 2:BP:134:ASP:OD1 | 2:BP:138:LYS:NZ | 2.38 | 0.56 |
| 2:CB:134:ASP:OD1 | 2:CB:138:LYS:NZ | 2.38 | 0.56 |
| 2:GY:2:ASP:OD2 | 2:HA:101:LYS:NZ | 2.34 | 0.56 |
| 2:IA:134:ASP:OD1 | 2:IA:138:LYS:NZ | 2.38 | 0.56 |
| 1:IE:92:GLU:OE2 | 2:IF:282:LYS:NZ | 2.38 | 0.56 |
| 1:JZ:92:GLU:OE2 | 2:KA:282:LYS:NZ | 2.38 | 0.56 |
| 1:LP:92:GLU:OE2 | 2:LQ:282:LYS:NZ | 2.38 | 0.56 |
| 1:YY:92:GLU:OE2 | 2:YZ:282:LYS:NZ | 2.38 | 0.56 |
| 1:AE:92:GLU:OE2 | 2:AF:282:LYS:NZ | 2.38 | 0.56 |
| 1:BU:92:GLU:OE2 | 2:BV:282:LYS:NZ | 2.38 | 0.56 |
| 2:ZD:2:ASP:OD2 | 2:ZF:101:LYS:NZ | 2.33 | 0.56 |
| 1:CA:92:GLU:OE2 | 2:CB:282:LYS:NZ | 2.38 | 0.56 |
| 1:CG:92:GLU:OE2 | 2:CH:282:LYS:NZ | 2.38 | 0.56 |
| 1:EP:92:GLU:OE2 | 2:EQ:282:LYS:NZ | 2.38 | 0.56 |
| 2:IA:123:GLU:OE2 | 2:IA:170:LYS:NZ | 2.34 | 0.56 |
| 2:LE:123:GLU:OE2 | 2:LE:170:LYS:NZ | 2.34 | 0.56 |
| 2:IR:123:GLU:OE2 | 2:IR:170:LYS:NZ | 2.34 | 0.56 |
| 2:LE:134:ASP:OD1 | 2:LE:138:LYS:NZ | 2.38 | 0.56 |
| 2:LK:134:ASP:OD1 | 2:LK:138:LYS:NZ | 2.38 | 0.56 |
| 1:ZO:92:GLU:OE2 | 2:ZP:282:LYS:NZ | 2.38 | 0.56 |
| 2:FI:134:ASP:OD1 | 2:FI:138:LYS:NZ | 2.38 | 0.56 |
| 2:JJ:134:ASP:OD1 | 2:JJ:138:LYS:NZ | 2.38 | 0.56 |
| 1:JO:92:GLU:OE2 | 2:JP:282:LYS:NZ | 2.38 | 0.56 |
| 2:KA:134:ASP:OD1 | 2:KA:138:LYS:NZ | 2.38 | 0.56 |
| 2:ZV:134:ASP:OD1 | 2:ZV:138:LYS:NZ | 2.38 | 0.56 |
| 2:YB:134:ASP:OD1 | 2:YB:138:LYS:NZ | 2.38 | 0.56 |
| 2:YP:123:GLU:OE2 | 2:YP:170:LYS:NZ | 2.34 | 0.56 |
| 2:YT:2:ASP:OD2 | 2:YV:101:LYS:NZ | 2.33 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:AO:282:LYS:NZ | 1:AP:92:GLU:OE2 | 2.38 | 0.56 |
| 2:AX:134:ASP:OD1 | 2:AX:138:LYS:NZ | 2.38 | 0.56 |
| 1:FB:92:GLU:OE2 | 2:FC:282:LYS:NZ | 2.38 | 0.56 |
| 2:FO:2:ASP:OD2 | 2:FQ:101:LYS:NZ | 2.33 | 0.56 |
| 1:GF:92:GLU:OE2 | 2:GG:282:LYS:NZ | 2.38 | 0.56 |
| 1:IQ:92:GLU:OE2 | 2:IR:282:LYS:NZ | 2.38 | 0.56 |
| 2:JR:123:GLU:OE2 | 2:JR:170:LYS:NZ | 2.34 | 0.56 |
| 2:JU:282:LYS:NZ | 1:WD:92:GLU:OE2 | 2.38 | 0.56 |
| 2:AZ:123:GLU:OE2 | 2:AZ:170:LYS:NZ | 2.34 | 0.56 |
| 1:BC:92:GLU:OE2 | 2:BD:282:LYS:NZ | 2.38 | 0.56 |
| 1:FH:92:GLU:OE2 | 2:FI:282:LYS:NZ | 2.38 | 0.56 |
| 2:LM:123:GLU:OE2 | 2:LM:170:LYS:NZ | 2.34 | 0.56 |
| 2:YN:134:ASP:OD1 | 2:YN:138:LYS:NZ | 2.38 | 0.56 |
| 2:GG:134:ASP:OD1 | 2:GG:138:LYS:NZ | 2.38 | 0.56 |
| 2:HJ:123:GLU:OE2 | 2:HJ:170:LYS:NZ | 2.34 | 0.56 |
| 2:HW:160:ASP:OD1 | 2:HW:168:LYS:NZ | 2.36 | 0.56 |
| 2:KM:134:ASP:OD1 | 2:KM:138:LYS:NZ | 2.38 | 0.56 |
| 1:ZU:92:GLU:OE2 | 2:ZV:282:LYS:NZ | 2.38 | 0.56 |
| 2:LQ:2:ASP:OD2 | 2:LS:101:LYS:NZ | 2.33 | 0.55 |
| 2:CH:123:GLU:OE2 | 2:CH:170:LYS:NZ | 2.34 | 0.55 |
| 2:GG:2:ASP:OD2 | 2:GI:101:LYS:NZ | 2.33 | 0.55 |
| 2:HF:123:GLU:OE2 | 2:HF:170:LYS:NZ | 2.34 | 0.55 |
| 2:JP:134:ASP:OD1 | 2:JP:138:LYS:NZ | 2.38 | 0.55 |
| 2:LA:123:GLU:OE2 | 2:LA:170:LYS:NZ | 2.34 | 0.55 |
| 2:HU:2:ASP:OD2 | 2:HW:101:LYS:NZ | 2.34 | 0.55 |
| 2:IR:2:ASP:OD2 | 2:IT:101:LYS:NZ | 2.33 | 0.55 |
| 2:JU:2:ASP:OD2 | 2:JW:101:LYS:NZ | 2.34 | 0.55 |
| 2:KG:134:ASP:OD1 | 2:KG:138:LYS:NZ | 2.38 | 0.55 |
| 2:KS:123:GLU:OE2 | 2:KS:170:LYS:NZ | 2.34 | 0.55 |
| 2:ZJ:2:ASP:OD2 | 2:ZL:101:LYS:NZ | 2.33 | 0.55 |
| 1:LD:92:GLU:OE2 | 2:LE:282:LYS:NZ | 2.38 | 0.55 |
| 2:ZV:2:ASP:OD2 | 2:ZX:101:LYS:NZ | 2.34 | 0.55 |
| 2:ZV:123:GLU:OE2 | 2:ZV:170:LYS:NZ | 2.34 | 0.55 |
| 2:FU:123:GLU:OE2 | 2:FU:170:LYS:NZ | 2.34 | 0.55 |
| 2:JJ:123:GLU:OE2 | 2:JJ:170:LYS:NZ | 2.34 | 0.55 |
| 2:KM:2:ASP:OD2 | 2:KO:101:LYS:NZ | 2.34 | 0.55 |
| 2:BR:123:GLU:OE2 | 2:BR:170:LYS:NZ | 2.34 | 0.55 |
| 2:DR:123:GLU:OE2 | 2:DR:170:LYS:NZ | 2.34 | 0.55 |
| 2:ES:123:GLU:OE2 | 2:ES:170:LYS:NZ | 2.34 | 0.55 |
| 2:YN:123:GLU:OE2 | 2:YN:170:LYS:NZ | 2.34 | 0.55 |
| 2:FO:123:GLU:OE2 | 2:FO:170:LYS:NZ | 2.34 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:KG:2:ASP:OD2 | 2:KI:101:LYS:NZ | 2.33 | 0.55 |
| 2:EG:123:GLU:OE2 | 2:EG:170:LYS:NZ | 2.34 | 0.54 |
| 2:AX:123:GLU:OE2 | 2:AX:170:LYS:NZ | 2.34 | 0.54 |
| 2:HK:123:GLU:OE2 | 2:HK:170:LYS:NZ | 2.34 | 0.54 |
| 2:HO:2:ASP:OD2 | 2:HQ:101:LYS:NZ | 2.33 | 0.54 |
| 2:IN:123:GLU:OE2 | 2:IN:170:LYS:NZ | 2.34 | 0.54 |
| 2:FC:2:ASP:OD2 | 2:FE:101:LYS:NZ | 2.34 | 0.54 |
| 2:HO:123:GLU:OE2 | 2:HO:170:LYS:NZ | 2.34 | 0.54 |
| 2:CH:2:ASP:OD2 | 2:CJ:101:LYS:NZ | 2.33 | 0.54 |
| 2:EK:123:GLU:OE2 | 2:EK:170:LYS:NZ | 2.34 | 0.54 |
| 2:YH:2:ASP:OD2 | 2:YJ:101:LYS:NZ | 2.34 | 0.54 |
| 2:AF:123:GLU:OE2 | 2:AF:170:LYS:NZ | 2.34 | 0.54 |
| 2:BJ:2:ASP:OD2 | 2:BL:101:LYS:NZ | 2.33 | 0.54 |
| 2:KY:2:ASP:OD2 | 2:LA:101:LYS:NZ | 2.33 | 0.54 |
| 2:GY:123:GLU:OE2 | 2:GY:170:LYS:NZ | 2.34 | 0.54 |
| 2:DF:2:ASP:OD2 | 2:DH:101:LYS:NZ | 2.33 | 0.53 |
| 2:JD:2:ASP:OD2 | 2:JF:101:LYS:NZ | 2.33 | 0.53 |
| 2:KM:123:GLU:OE2 | 2:KM:170:LYS:NZ | 2.34 | 0.53 |
| 2:HE:2:ASP:OD2 | 2:HF:101:LYS:NZ | 2.33 | 0.53 |
| 2:YN:2:ASP:OD2 | 2:YP:101:LYS:NZ | 2.34 | 0.53 |
| 2:EK:2:ASP:OD2 | 2:EM:101:LYS:NZ | 2.34 | 0.53 |
| 2:AF:2:ASP:OD2 | 2:AH:101:LYS:NZ | 2.34 | 0.53 |
| 2:EQ:123:GLU:OE2 | 2:EQ:170:LYS:NZ | 2.34 | 0.53 |
| 2:JP:123:GLU:OE2 | 2:JP:170:LYS:NZ | 2.34 | 0.53 |
| 2:AX:2:ASP:OD2 | 2:AZ:101:LYS:NZ | 2.33 | 0.53 |
| 2:YD:101:LYS:NZ | 2:YB:2:ASP:OD2 | 2.33 | 0.53 |
| 2:CT:2:ASP:OD2 | 2:CV:101:LYS:NZ | 2.33 | 0.53 |
| 2:CB:123:GLU:OE2 | 2:CB:170:LYS:NZ | 2.34 | 0.53 |
| 2:FI:2:ASP:OD2 | 2:FK:101:LYS:NZ | 2.33 | 0.53 |
| 2:EA:160:ASP:OD1 | 2:EA:168:LYS:NZ | 2.36 | 0.52 |
| 2:FI:123:GLU:OE2 | 2:FI:170:LYS:NZ | 2.34 | 0.52 |
| 2:JJ:2:ASP:OD2 | 2:JL:101:LYS:NZ | 2.33 | 0.52 |
| 2:IA:2:ASP:OD2 | 2:IB:101:LYS:NZ | 2.33 | 0.52 |
| 2:KY:123:GLU:OE2 | 2:KY:170:LYS:NZ | 2.34 | 0.52 |
| 2:ZD:123:GLU:OE2 | 2:ZD:170:LYS:NZ | 2.34 | 0.52 |
| 2:FC:123:GLU:OE2 | 2:FC:170:LYS:NZ | 2.34 | 0.52 |
| 2:HJ:2:ASP:OD2 | 2:HK:101:LYS:NZ | 2.33 | 0.52 |
| 2:CN:123:GLU:OE2 | 2:CN:170:LYS:NZ | 2.34 | 0.52 |
| 2:DL:2:ASP:OD2 | 2:DN:101:LYS:NZ | 2.33 | 0.52 |
| 2:AZ:160:ASP:OD1 | 2:AZ:168:LYS:NZ | 2.36 | 0.52 |
| 2:GM:2:ASP:OD2 | 2:GO:101:LYS:NZ | 2.33 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:JP:2:ASP:OD2 | 2:JR:101:LYS:NZ | 2.34 | 0.52 |
| 2:CN:2:ASP:OD2 | 2:CP:101:LYS:NZ | 2.33 | 0.52 |
| 2:LE:2:ASP:OD2 | 2:LG:101:LYS:NZ | 2.33 | 0.52 |
| 2:BP:2:ASP:OD2 | 2:BR:101:LYS:NZ | 2.34 | 0.51 |
| 2:DF:123:GLU:OE2 | 2:DF:170:LYS:NZ | 2.34 | 0.51 |
| 2:BP:123:GLU:OE2 | 2:BP:170:LYS:NZ | 2.34 | 0.51 |
| 2:JU:123:GLU:OE2 | 2:JU:170:LYS:NZ | 2.34 | 0.51 |
| 2:GS:123:GLU:OE2 | 2:GS:170:LYS:NZ | 2.34 | 0.51 |
| 2:IL:2:ASP:OD2 | 2:IN:101:LYS:NZ | 2.34 | 0.51 |
| 2:KA:123:GLU:OE2 | 2:KA:170:LYS:NZ | 2.34 | 0.51 |
| 2:CB:2:ASP:OD2 | 2:CD:101:LYS:NZ | 2.34 | 0.51 |
| 1:DS:43:VAL:HG13 | 1:DS:50:VAL:HG11 | 1.93 | 0.51 |
| 2:HE:123:GLU:OE2 | 2:HE:170:LYS:NZ | 2.34 | 0.51 |
| 1:JE:43:VAL:HG13 | 1:JE:50:VAL:HG11 | 1.93 | 0.51 |
| 1:LR:43:VAL:HG13 | 1:LR:50:VAL:HG11 | 1.93 | 0.51 |
| 1:DZ:43:VAL:HG13 | 1:DZ:50:VAL:HG11 | 1.93 | 0.51 |
| 2:FU:228:TYR:CD1 | 2:FU:228:TYR:C | 2.89 | 0.51 |
| 1:HP:43:VAL:HG13 | 1:HP:50:VAL:HG11 | 1.93 | 0.51 |
| 1:IY:43:VAL:HG13 | 1:IY:50:VAL:HG11 | 1.93 | 0.51 |
| 2:JD:228:TYR:CD1 | 2:JD:228:TYR:C | 2.89 | 0.51 |
| 2:LE:228:TYR:CD1 | 2:LE:228:TYR:C | 2.89 | 0.51 |
| 1:YC:43:VAL:HG13 | 1:YC:50:VAL:HG11 | 1.93 | 0.51 |
| 2:YN:228:TYR:CD1 | 2:YN:228:TYR:C | 2.89 | 0.51 |
| 2:AF:228:TYR:C | 2:AF:228:TYR:CD1 | 2.89 | 0.51 |
| 2:AL:228:TYR:C | 2:AL:228:TYR:CD1 | 2.89 | 0.51 |
| 1:BE:43:VAL:HG13 | 1:BE:50:VAL:HG11 | 1.93 | 0.51 |
| 1:BK:43:VAL:HG13 | 1:BK:50:VAL:HG11 | 1.93 | 0.51 |
| 2:BP:228:TYR:C | 2:BP:228:TYR:CD1 | 2.89 | 0.51 |
| 2:CZ:123:GLU:OE2 | 2:CZ:170:LYS:NZ | 2.34 | 0.51 |
| 2:EE:123:GLU:OE2 | 2:EE:170:LYS:NZ | 2.34 | 0.51 |
| 2:EK:228:TYR:CD1 | 2:EK:228:TYR:C | 2.89 | 0.51 |
| 1:GN:43:VAL:HG13 | 1:GN:50:VAL:HG11 | 1.93 | 0.51 |
| 1:HV:43:VAL:HG13 | 1:HV:50:VAL:HG11 | 1.93 | 0.51 |
| 2:JD:123:GLU:OE2 | 2:JD:170:LYS:NZ | 2.34 | 0.51 |
| 1:ZQ:43:VAL:HG13 | 1:ZQ:50:VAL:HG11 | 1.93 | 0.51 |
| 1:AM:43:VAL:HG13 | 1:AM:50:VAL:HG11 | 1.93 | 0.51 |
| 2:CH:228:TYR:CD1 | 2:CH:228:TYR:C | 2.89 | 0.51 |
| 1:WA:43:VAL:HG13 | 1:WA:50:VAL:HG11 | 1.93 | 0.51 |
| 2:ZJ:123:GLU:OE2 | 2:ZJ:170:LYS:NZ | 2.34 | 0.51 |
| 2:KS:228:TYR:CD1 | 2:KS:228:TYR:C | 2.89 | 0.51 |
| 2:YH:228:TYR:CD1 | 2:YH:228:TYR:C | 2.89 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:YT:228:TYR:CD1 | 2:YT:228:TYR:C | 2.89 | 0.51 |
| 1:CU:43:VAL:HG13 | 1:CU:50:VAL:HG11 | 1.93 | 0.51 |
| 1:DG:43:VAL:HG13 | 1:DG:50:VAL:HG11 | 1.93 | 0.51 |
| 1:EF:43:VAL:HG13 | 1:EF:50:VAL:HG11 | 1.93 | 0.51 |
| 1:GB:43:VAL:HG13 | 1:GB:50:VAL:HG11 | 1.93 | 0.51 |
| 2:GG:228:TYR:CD1 | 2:GG:228:TYR:C | 2.89 | 0.51 |
| 1:WB:43:VAL:HG13 | 1:WB:50:VAL:HG11 | 1.93 | 0.51 |
| 1:IM:43:VAL:HG13 | 1:IM:50:VAL:HG11 | 1.93 | 0.51 |
| 2:KG:228:TYR:C | 2:KG:228:TYR:CD1 | 2.89 | 0.51 |
| 2:BL:160:ASP:OD1 | 2:BL:168:LYS:NZ | 2.36 | 0.50 |
| 2:BV:2:ASP:OD2 | 2:BX:101:LYS:NZ | 2.34 | 0.50 |
| 1:BW:43:VAL:HG13 | 1:BW:50:VAL:HG11 | 1.93 | 0.50 |
| 2:CT:228:TYR:CD1 | 2:CT:228:TYR:C | 2.89 | 0.50 |
| 1:ER:43:VAL:HG13 | 1:ER:50:VAL:HG11 | 1.93 | 0.50 |
| 2:HO:228:TYR:CD1 | 2:HO:228:TYR:C | 2.89 | 0.50 |
| 1:WC:43:VAL:HG13 | 1:WC:50:VAL:HG11 | 1.93 | 0.50 |
| 2:IF:123:GLU:OE2 | 2:IF:170:LYS:NZ | 2.34 | 0.50 |
| 2:JJ:228:TYR:CD1 | 2:JJ:228:TYR:C | 2.89 | 0.50 |
| 1:JK:43:VAL:HG13 | 1:JK:50:VAL:HG11 | 1.93 | 0.50 |
| 2:LQ:228:TYR:CD1 | 2:LQ:228:TYR:C | 2.89 | 0.50 |
| 1:YI:43:VAL:HG13 | 1:YI:50:VAL:HG11 | 1.93 | 0.50 |
| 2:YT:123:GLU:OE2 | 2:YT:170:LYS:NZ | 2.34 | 0.50 |
| 2:AO:123:GLU:OE2 | 2:AO:170:LYS:NZ | 2.34 | 0.50 |
| 2:BV:228:TYR:CD1 | 2:BV:228:TYR:C | 2.89 | 0.50 |
| 2:GY:228:TYR:C | 2:GY:228:TYR:CD1 | 2.89 | 0.50 |
| 2:HU:228:TYR:C | 2:HU:228:TYR:CD1 | 2.89 | 0.50 |
| 1:KH:43:VAL:HG13 | 1:KH:50:VAL:HG11 | 1.93 | 0.50 |
| 2:AO:228:TYR:C | 2:AO:228:TYR:CD1 | 2.89 | 0.50 |
| 2:EW:228:TYR:CD1 | 2:EW:228:TYR:C | 2.89 | 0.50 |
| 2:FC:228:TYR:CD1 | 2:FC:228:TYR:C | 2.89 | 0.50 |
| 1:LL:43:VAL:HG13 | 1:LL:50:VAL:HG11 | 1.93 | 0.50 |
| 2:AX:228:TYR:CD1 | 2:AX:228:TYR:C | 2.89 | 0.50 |
| 2:BV:123:GLU:OE2 | 2:BV:170:LYS:NZ | 2.34 | 0.50 |
| 2:CN:228:TYR:CD1 | 2:CN:228:TYR:C | 2.89 | 0.50 |
| 1:FJ:43:VAL:HG13 | 1:FJ:50:VAL:HG11 | 1.93 | 0.50 |
| 2:IL:228:TYR:C | 2:IL:228:TYR:CD1 | 2.89 | 0.50 |
| 2:JU:228:TYR:CD1 | 2:JU:228:TYR:C | 2.89 | 0.50 |
| 2:LK:228:TYR:CD1 | 2:LK:228:TYR:C | 2.89 | 0.50 |
| 2:AL:2:ASP:OD2 | 2:AN:101:LYS:NZ | 2.33 | 0.50 |
| 2:DY:228:TYR:CD1 | 2:DY:228:TYR:C | 2.89 | 0.50 |
| 2:EE:2:ASP:OD2 | 2:EG:101:LYS:NZ | 2.33 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:GT:43:VAL:HG13 | 1:GT:50:VAL:HG11 | 1.93 | 0.50 |
| 2:HE:228:TYR:CD1 | 2:HE:228:TYR:C | 2.89 | 0.50 |
| 2:IX:228:TYR:CD1 | 2:IX:228:TYR:C | 2.89 | 0.50 |
| 1:KB:43:VAL:HG13 | 1:KB:50:VAL:HG11 | 1.93 | 0.50 |
| 1:AA:43:VAL:HG13 | 1:AA:50:VAL:HG11 | 1.93 | 0.50 |
| 2:ZD:228:TYR:CD1 | 2:ZD:228:TYR:C | 2.89 | 0.50 |
| 2:DF:228:TYR:CD1 | 2:DF:228:TYR:C | 2.89 | 0.50 |
| 2:FO:228:TYR:C | 2:FO:228:TYR:CD1 | 2.89 | 0.50 |
| 2:GA:228:TYR:CD1 | 2:GA:228:TYR:C | 2.89 | 0.50 |
| 2:GM:228:TYR:CD1 | 2:GM:228:TYR:C | 2.89 | 0.50 |
| 2:KG:123:GLU:OE2 | 2:KG:170:LYS:NZ | 2.34 | 0.50 |
| 1:ZW:43:VAL:HG13 | 1:ZW:50:VAL:HG11 | 1.93 | 0.50 |
| 2:YB:123:GLU:OE2 | 2:YB:170:LYS:NZ | 2.34 | 0.50 |
| 2:AB:101:LYS:NZ | 2:YZ:2:ASP:OD2 | 2.33 | 0.50 |
| 2:YZ:228:TYR:C | 2:YZ:228:TYR:CD1 | 2.89 | 0.50 |
| 2:CB:228:TYR:CD1 | 2:CB:228:TYR:C | 2.89 | 0.50 |
| 2:DL:228:TYR:CD1 | 2:DL:228:TYR:C | 2.89 | 0.50 |
| 2:DR:228:TYR:CD1 | 2:DR:228:TYR:C | 2.89 | 0.50 |
| 2:EE:228:TYR:C | 2:EE:228:TYR:CD1 | 2.89 | 0.50 |
| 2:FI:228:TYR:CD1 | 2:FI:228:TYR:C | 2.89 | 0.50 |
| 1:GH:43:VAL:HG13 | 1:GH:50:VAL:HG11 | 1.93 | 0.50 |
| 2:IF:228:TYR:C | 2:IF:228:TYR:CD1 | 2.89 | 0.50 |
| 1:JV:43:VAL:HG13 | 1:JV:50:VAL:HG11 | 1.93 | 0.50 |
| 2:YB:228:TYR:CD1 | 2:YB:228:TYR:C | 2.89 | 0.50 |
| 2:DL:123:GLU:OE2 | 2:DL:170:LYS:NZ | 2.34 | 0.50 |
| 2:EW:123:GLU:OE2 | 2:EW:170:LYS:NZ | 2.34 | 0.50 |
| 1:EX:43:VAL:HG13 | 1:EX:50:VAL:HG11 | 1.93 | 0.50 |
| 1:GF:11:ALA:HB1 | 1:GF:43:VAL:O | 2.12 | 0.50 |
| 2:GS:228:TYR:CD1 | 2:GS:228:TYR:C | 2.89 | 0.50 |
| 1:IS:43:VAL:HG13 | 1:IS:50:VAL:HG11 | 1.93 | 0.50 |
| 1:ZK:43:VAL:HG13 | 1:ZK:50:VAL:HG11 | 1.93 | 0.50 |
| 1:JQ:43:VAL:HG13 | 1:JQ:50:VAL:HG11 | 1.93 | 0.50 |
| 1:LP:11:ALA:HB1 | 1:LP:43:VAL:O | 2.12 | 0.50 |
| 1:YG:11:ALA:HB1 | 1:YG:43:VAL:O | 2.12 | 0.50 |
| 1:AP:11:ALA:HB1 | 1:AP:43:VAL:O | 2.12 | 0.50 |
| 1:BC:11:ALA:HB1 | 1:BC:43:VAL:O | 2.12 | 0.50 |
| 2:BJ:228:TYR:CD1 | 2:BJ:228:TYR:C | 2.89 | 0.50 |
| 1:BU:11:ALA:HB1 | 1:BU:43:VAL:O | 2.12 | 0.50 |
| 1:CA:11:ALA:HB1 | 1:CA:43:VAL:O | 2.12 | 0.50 |
| 1:CM:11:ALA:HB1 | 1:CM:43:VAL:O | 2.12 | 0.50 |
| 1:FT:11:ALA:HB1 | 1:FT:43:VAL:O | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:IA:228:TYR:C | 2:IA:228:TYR:CD1 | 2.89 | 0.50 |
| 2:ZJ:228:TYR:CD1 | 2:ZJ:228:TYR:C | 2.89 | 0.50 |
| 1:IH:43:VAL:HG13 | 1:IH:50:VAL:HG11 | 1.93 | 0.50 |
| 2:JP:228:TYR:CD1 | 2:JP:228:TYR:C | 2.89 | 0.50 |
| 2:KA:228:TYR:CD1 | 2:KA:228:TYR:C | 2.89 | 0.50 |
| 2:ZL:160:ASP:OD1 | 2:ZL:168:LYS:NZ | 2.36 | 0.50 |
| 1:KL:11:ALA:HB1 | 1:KL:43:VAL:O | 2.12 | 0.50 |
| 1:KN:43:VAL:HG13 | 1:KN:50:VAL:HG11 | 1.93 | 0.50 |
| 1:KZ:43:VAL:HG13 | 1:KZ:50:VAL:HG11 | 1.93 | 0.50 |
| 1:AY:43:VAL:HG13 | 1:AY:50:VAL:HG11 | 1.93 | 0.49 |
| 1:BO:11:ALA:HB1 | 1:BO:43:VAL:O | 2.12 | 0.49 |
| 1:DM:43:VAL:HG13 | 1:DM:50:VAL:HG11 | 1.93 | 0.49 |
| 1:EP:11:ALA:HB1 | 1:EP:43:VAL:O | 2.12 | 0.49 |
| 2:EQ:228:TYR:CD1 | 2:EQ:228:TYR:C | 2.89 | 0.49 |
| 1:FV:43:VAL:HG13 | 1:FV:50:VAL:HG11 | 1.93 | 0.49 |
| 1:ZO:11:ALA:HB1 | 1:ZO:43:VAL:O | 2.12 | 0.49 |
| 1:BI:11:ALA:HB1 | 1:BI:43:VAL:O | 2.12 | 0.49 |
| 1:BQ:43:VAL:HG13 | 1:BQ:50:VAL:HG11 | 1.93 | 0.49 |
| 1:CO:43:VAL:HG13 | 1:CO:50:VAL:HG11 | 1.93 | 0.49 |
| 1:DQ:11:ALA:HB1 | 1:DQ:43:VAL:O | 2.12 | 0.49 |
| 1:DX:11:ALA:HB1 | 1:DX:43:VAL:O | 2.12 | 0.49 |
| 1:FD:43:VAL:HG13 | 1:FD:50:VAL:HG11 | 1.93 | 0.49 |
| 1:FN:11:ALA:HB1 | 1:FN:43:VAL:O | 2.12 | 0.49 |
| 1:FP:43:VAL:HG13 | 1:FP:50:VAL:HG11 | 1.93 | 0.49 |
| 1:GL:11:ALA:HB1 | 1:GL:43:VAL:O | 2.12 | 0.49 |
| 2:HJ:228:TYR:C | 2:HJ:228:TYR:CD1 | 2.89 | 0.49 |
| 1:HZ:11:ALA:HB1 | 1:HZ:43:VAL:O | 2.12 | 0.49 |
| 1:IQ:11:ALA:HB1 | 1:IQ:43:VAL:O | 2.12 | 0.49 |
| 1:KT:43:VAL:HG13 | 1:KT:50:VAL:HG11 | 1.93 | 0.49 |
| 1:LF:43:VAL:HG13 | 1:LF:50:VAL:HG11 | 1.93 | 0.49 |
| 1:YO:43:VAL:HG13 | 1:YO:50:VAL:HG11 | 1.93 | 0.49 |
| 1:YS:11:ALA:HB1 | 1:YS:43:VAL:O | 2.12 | 0.49 |
| 2:CZ:228:TYR:CD1 | 2:CZ:228:TYR:C | 2.89 | 0.49 |
| 1:DA:43:VAL:HG13 | 1:DA:50:VAL:HG11 | 1.93 | 0.49 |
| 1:DK:11:ALA:HB1 | 1:DK:43:VAL:O | 2.12 | 0.49 |
| 2:DY:123:GLU:OE2 | 2:DY:170:LYS:NZ | 2.34 | 0.49 |
| 1:EV:11:ALA:HB1 | 1:EV:43:VAL:O | 2.12 | 0.49 |
| 1:HN:11:ALA:HB1 | 1:HN:43:VAL:O | 2.12 | 0.49 |
| 1:KF:11:ALA:HB1 | 1:KF:43:VAL:O | 2.12 | 0.49 |
| 2:KY:228:TYR:CD1 | 2:KY:228:TYR:C | 2.89 | 0.49 |
| 2:ZP:228:TYR:CD1 | 2:ZP:228:TYR:C | 2.89 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:ZV:228:TYR:C | 2:ZV:228:TYR:CD1 | 2.89 | 0.49 |
| 1:YM:11:ALA:HB1 | 1:YM:43:VAL:O | 2.12 | 0.49 |
| 1:AS:43:VAL:HG13 | 1:AS:50:VAL:HG11 | 1.93 | 0.49 |
| 1:AW:11:ALA:HB1 | 1:AW:43:VAL:O | 2.12 | 0.49 |
| 1:IW:11:ALA:HB1 | 1:IW:43:VAL:O | 2.12 | 0.49 |
| 1:AG:43:VAL:HG13 | 1:AG:50:VAL:HG11 | 1.93 | 0.49 |
| 2:BD:228:TYR:CD1 | 2:BD:228:TYR:C | 2.89 | 0.49 |
| 1:GZ:43:VAL:HG13 | 1:GZ:50:VAL:HG11 | 1.93 | 0.49 |
| 1:ZI:11:ALA:HB1 | 1:ZI:43:VAL:O | 2.12 | 0.49 |
| 1:HI:11:ALA:HB1 | 1:HI:43:VAL:O | 2.12 | 0.49 |
| 2:KM:228:TYR:C | 2:KM:228:TYR:CD1 | 2.89 | 0.49 |
| 1:CG:11:ALA:HB1 | 1:CG:43:VAL:O | 2.12 | 0.49 |
| 2:DY:2:ASP:OD2 | 2:EA:101:LYS:NZ | 2.34 | 0.49 |
| 1:FZ:11:ALA:HB1 | 1:FZ:43:VAL:O | 2.12 | 0.49 |
| 2:IF:6:LYS:NZ | 2:IF:10:GLU:OE2 | 2.45 | 0.49 |
| 2:IR:228:TYR:CD1 | 2:IR:228:TYR:C | 2.89 | 0.49 |
| 1:WD:11:ALA:HB1 | 1:WD:43:VAL:O | 2.12 | 0.49 |
| 1:AE:11:ALA:HB1 | 1:AE:43:VAL:O | 2.12 | 0.49 |
| 1:CY:11:ALA:HB1 | 1:CY:43:VAL:O | 2.12 | 0.49 |
| 1:EJ:11:ALA:HB1 | 1:EJ:43:VAL:O | 2.12 | 0.49 |
| 1:EL:43:VAL:HG13 | 1:EL:50:VAL:HG11 | 1.93 | 0.49 |
| 1:GR:11:ALA:HB1 | 1:GR:43:VAL:O | 2.12 | 0.49 |
| 1:HT:11:ALA:HB1 | 1:HT:43:VAL:O | 2.12 | 0.49 |
| 1:ZE:43:VAL:HG13 | 1:ZE:50:VAL:HG11 | 1.93 | 0.49 |
| 1:FH:11:ALA:HB1 | 1:FH:43:VAL:O | 2.12 | 0.49 |
| 1:JC:11:ALA:HB1 | 1:JC:43:VAL:O | 2.12 | 0.49 |
| 1:LD:11:ALA:HB1 | 1:LD:43:VAL:O | 2.12 | 0.49 |
| 1:CI:43:VAL:HG13 | 1:CI:50:VAL:HG11 | 1.93 | 0.49 |
| 2:ZJ:6:LYS:NZ | 2:ZJ:10:GLU:OE2 | 2.45 | 0.49 |
| 2:KY:6:LYS:NZ | 2:KY:10:GLU:OE2 | 2.45 | 0.49 |
| 1:LJ:11:ALA:HB1 | 1:LJ:43:VAL:O | 2.12 | 0.49 |
| 1:YY:11:ALA:HB1 | 1:YY:43:VAL:O | 2.12 | 0.49 |
| 1:CC:43:VAL:HG13 | 1:CC:50:VAL:HG11 | 1.93 | 0.49 |
| 1:ED:11:ALA:HB1 | 1:ED:43:VAL:O | 2.12 | 0.49 |
| 1:IK:11:ALA:HB1 | 1:IK:43:VAL:O | 2.12 | 0.49 |
| 1:JO:11:ALA:HB1 | 1:JO:43:VAL:O | 2.12 | 0.49 |
| 1:YA:11:ALA:HB1 | 1:YA:43:VAL:O | 2.12 | 0.49 |
| 2:CH:6:LYS:NZ | 2:CH:10:GLU:OE2 | 2.45 | 0.48 |
| 2:KS:6:LYS:NZ | 2:KS:10:GLU:OE2 | 2.45 | 0.48 |
| 1:YU:43:VAL:HG13 | 1:YU:50:VAL:HG11 | 1.93 | 0.48 |
| 2:BT:228:TYR:CD1 | 2:BT:228:TYR:C | 2.92 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:DJ:228:TYR:CD1 | 2:DJ:228:TYR:C | 2.92 | 0.48 |
| 2:DL:6:LYS:NZ | 2:DL:10:GLU:OE2 | 2.45 | 0.48 |
| 2:FM:228:TYR:CD1 | 2:FM:228:TYR:C | 2.92 | 0.48 |
| 1:GX:11:ALA:HB1 | 1:GX:43:VAL:O | 2.12 | 0.48 |
| 2:HH:228:TYR:CD1 | 2:HH:228:TYR:C | 2.92 | 0.48 |
| 1:JZ:11:ALA:HB1 | 1:JZ:43:VAL:O | 2.12 | 0.48 |
| 2:KK:228:TYR:CD1 | 2:KK:228:TYR:C | 2.92 | 0.48 |
| 1:KR:11:ALA:HB1 | 1:KR:43:VAL:O | 2.12 | 0.48 |
| 2:LI:228:TYR:CD1 | 2:LI:228:TYR:C | 2.92 | 0.48 |
| 1:AK:11:ALA:HB1 | 1:AK:43:VAL:O | 2.12 | 0.48 |
| 1:ZC:11:ALA:HB1 | 1:ZC:43:VAL:O | 2.12 | 0.48 |
| 2:EC:228:TYR:CD1 | 2:EC:228:TYR:C | 2.92 | 0.48 |
| 2:FO:6:LYS:NZ | 2:FO:10:GLU:OE2 | 2.45 | 0.48 |
| 2:FY:228:TYR:CD1 | 2:FY:228:TYR:C | 2.92 | 0.48 |
| 2:ZH:228:TYR:C | 2:ZH:228:TYR:CD1 | 2.92 | 0.48 |
| 2:IA:6:LYS:NZ | 2:IA:10:GLU:OE2 | 2.45 | 0.48 |
| 1:IE:11:ALA:HB1 | 1:IE:43:VAL:O | 2.12 | 0.48 |
| 1:JI:11:ALA:HB1 | 1:JI:43:VAL:O | 2.12 | 0.48 |
| 2:YN:6:LYS:NZ | 2:YN:10:GLU:OE2 | 2.45 | 0.48 |
| 2:DD:228:TYR:CD1 | 2:DD:228:TYR:C | 2.91 | 0.48 |
| 2:DP:228:TYR:CD1 | 2:DP:228:TYR:C | 2.92 | 0.48 |
| 2:EE:6:LYS:NZ | 2:EE:10:GLU:OE2 | 2.45 | 0.48 |
| 2:EI:228:TYR:CD1 | 2:EI:228:TYR:C | 2.92 | 0.48 |
| 2:EO:228:TYR:CD1 | 2:EO:228:TYR:C | 2.92 | 0.48 |
| 1:FB:11:ALA:HB1 | 1:FB:43:VAL:O | 2.12 | 0.48 |
| 2:GY:6:LYS:NZ | 2:GY:10:GLU:OE2 | 2.45 | 0.48 |
| 1:HD:11:ALA:HB1 | 1:HD:43:VAL:O | 2.12 | 0.48 |
| 2:IP:228:TYR:CD1 | 2:IP:228:TYR:C | 2.92 | 0.48 |
| 2:ZZ:228:TYR:CD1 | 2:ZZ:228:TYR:C | 2.92 | 0.48 |
| 2:EW:6:LYS:NZ | 2:EW:10:GLU:OE2 | 2.45 | 0.48 |
| 2:KQ:228:TYR:CD1 | 2:KQ:228:TYR:C | 2.92 | 0.48 |
| 2:LO:228:TYR:CD1 | 2:LO:228:TYR:C | 2.91 | 0.48 |
| 2:AQ:228:TYR:C | 2:AQ:228:TYR:CD1 | 2.92 | 0.48 |
| 1:CS:11:ALA:HB1 | 1:CS:43:VAL:O | 2.12 | 0.48 |
| 2:CX:228:TYR:C | 2:CX:228:TYR:CD1 | 2.92 | 0.48 |
| 2:FS:228:TYR:CD1 | 2:FS:228:TYR:C | 2.92 | 0.48 |
| 1:KX:11:ALA:HB1 | 1:KX:43:VAL:O | 2.12 | 0.48 |
| 2:AJ:228:TYR:CD1 | 2:AJ:228:TYR:C | 2.92 | 0.48 |
| 2:BZ:228:TYR:CD1 | 2:BZ:228:TYR:C | 2.92 | 0.48 |
| 2:CL:228:TYR:CD1 | 2:CL:228:TYR:C | 2.92 | 0.48 |
| 2:HM:78:LYS:NZ | 2:HQ:73:GLU:OE1 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:HY:228:TYR:CD1 | 2:HY:228:TYR:C | 2.92 | 0.48 |
| 1:ZU:11:ALA:HB1 | 1:ZU:43:VAL:O | 2.12 | 0.48 |
| 2:YL:228:TYR:CD1 | 2:YL:228:TYR:C | 2.92 | 0.48 |
| 2:YT:6:LYS:NZ | 2:YT:10:GLU:OE2 | 2.45 | 0.48 |
| 2:AB:73:GLU:OE1 | 2:YX:78:LYS:NZ | 2.47 | 0.48 |
| 2:AV:78:LYS:NZ | 2:AZ:73:GLU:OE1 | 2.47 | 0.48 |
| 2:BB:228:TYR:C | 2:BB:228:TYR:CD1 | 2.92 | 0.48 |
| 2:CT:6:LYS:NZ | 2:CT:10:GLU:OE2 | 2.45 | 0.48 |
| 2:DW:228:TYR:C | 2:DW:228:TYR:CD1 | 2.91 | 0.48 |
| 2:GC:160:ASP:OD1 | 2:GC:168:LYS:NZ | 2.36 | 0.48 |
| 2:GQ:228:TYR:C | 2:GQ:228:TYR:CD1 | 2.92 | 0.48 |
| 2:GS:6:LYS:NZ | 2:GS:10:GLU:OE2 | 2.45 | 0.48 |
| 2:HM:228:TYR:CD1 | 2:HM:228:TYR:C | 2.92 | 0.48 |
| 2:JH:228:TYR:CD1 | 2:JH:228:TYR:C | 2.92 | 0.48 |
| 2:ZT:78:LYS:NZ | 2:ZX:73:GLU:OE1 | 2.47 | 0.48 |
| 2:ZT:228:TYR:CD1 | 2:ZT:228:TYR:C | 2.92 | 0.48 |
| 2:YD:73:GLU:OE1 | 2:ZZ:78:LYS:NZ | 2.47 | 0.48 |
| 2:YF:78:LYS:NZ | 2:YJ:73:GLU:OE1 | 2.47 | 0.48 |
| 2:ZB:228:TYR:CD1 | 2:ZB:228:TYR:C | 2.92 | 0.48 |
| 2:CF:78:LYS:NZ | 2:CJ:73:GLU:OE1 | 2.47 | 0.48 |
| 2:DD:78:LYS:NZ | 2:DH:73:GLU:OE1 | 2.47 | 0.48 |
| 1:DE:11:ALA:HB1 | 1:DE:43:VAL:O | 2.12 | 0.48 |
| 2:EI:78:LYS:NZ | 2:EM:73:GLU:OE1 | 2.47 | 0.48 |
| 2:FG:78:LYS:NZ | 2:FK:73:GLU:OE1 | 2.47 | 0.48 |
| 2:FU:6:LYS:NZ | 2:FU:10:GLU:OE2 | 2.45 | 0.48 |
| 2:GA:6:LYS:NZ | 2:GA:10:GLU:OE2 | 2.45 | 0.48 |
| 2:GK:78:LYS:NZ | 2:GO:73:GLU:OE1 | 2.47 | 0.48 |
| 2:GQ:78:LYS:NZ | 2:GU:73:GLU:OE1 | 2.47 | 0.48 |
| 2:HO:6:LYS:NZ | 2:HO:10:GLU:OE2 | 2.45 | 0.48 |
| 2:ID:78:LYS:NZ | 2:IG:73:GLU:OE1 | 2.47 | 0.48 |
| 2:JB:78:LYS:NZ | 2:JF:73:GLU:OE1 | 2.47 | 0.48 |
| 2:JN:78:LYS:NZ | 2:JR:73:GLU:OE1 | 2.47 | 0.48 |
| 2:KW:228:TYR:CD1 | 2:KW:228:TYR:C | 2.91 | 0.48 |
| 2:LI:78:LYS:NZ | 2:LM:73:GLU:OE1 | 2.47 | 0.48 |
| 2:ZP:6:LYS:NZ | 2:ZP:10:GLU:OE2 | 2.45 | 0.48 |
| 2:YF:228:TYR:CD1 | 2:YF:228:TYR:C | 2.92 | 0.48 |
| 2:AF:6:LYS:NZ | 2:AF:10:GLU:OE2 | 2.45 | 0.48 |
| 2:BB:78:LYS:NZ | 2:BF:73:GLU:OE1 | 2.47 | 0.48 |
| 2:CR:78:LYS:NZ | 2:CV:73:GLU:OE1 | 2.47 | 0.48 |
| 2:CR:228:TYR:C | 2:CR:228:TYR:CD1 | 2.92 | 0.48 |
| 2:DR:6:LYS:NZ | 2:DR:10:GLU:OE2 | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:ZH:78:LYS:NZ | 2:ZL:73:GLU:OE1 | 2.47 | 0.48 |
| 2:GW:78:LYS:NZ | 2:HA:73:GLU:OE1 | 2.47 | 0.48 |
| 2:IR:6:LYS:NZ | 2:IR:10:GLU:OE2 | 2.45 | 0.48 |
| 2:IV:78:LYS:NZ | 2:IZ:73:GLU:OE1 | 2.47 | 0.48 |
| 2:KW:78:LYS:NZ | 2:LA:73:GLU:OE1 | 2.47 | 0.48 |
| 2:LC:78:LYS:NZ | 2:LG:73:GLU:OE1 | 2.47 | 0.48 |
| 2:LO:78:LYS:NZ | 2:LS:73:GLU:OE1 | 2.47 | 0.48 |
| 2:LQ:123:GLU:OE2 | 2:LQ:170:LYS:NZ | 2.34 | 0.48 |
| 2:AV:228:TYR:CD1 | 2:AV:228:TYR:C | 2.92 | 0.47 |
| 2:BN:228:TYR:C | 2:BN:228:TYR:CD1 | 2.92 | 0.47 |
| 2:BT:78:LYS:NZ | 2:BX:73:GLU:OE1 | 2.47 | 0.47 |
| 2:CL:78:LYS:NZ | 2:CP:73:GLU:OE1 | 2.47 | 0.47 |
| 2:DP:78:LYS:NZ | 2:DT:73:GLU:OE1 | 2.47 | 0.47 |
| 2:FG:228:TYR:C | 2:FG:228:TYR:CD1 | 2.92 | 0.47 |
| 2:HC:228:TYR:CD1 | 2:HC:228:TYR:C | 2.92 | 0.47 |
| 2:IV:228:TYR:CD1 | 2:IV:228:TYR:C | 2.92 | 0.47 |
| 2:IX:6:LYS:NZ | 2:IX:10:GLU:OE2 | 2.45 | 0.47 |
| 2:ZN:228:TYR:C | 2:ZN:228:TYR:CD1 | 2.92 | 0.47 |
| 2:AJ:78:LYS:NZ | 2:AN:73:GLU:OE1 | 2.47 | 0.47 |
| 2:EU:78:LYS:NZ | 2:EY:73:GLU:OE1 | 2.47 | 0.47 |
| 2:FM:78:LYS:NZ | 2:FQ:73:GLU:OE1 | 2.47 | 0.47 |
| 2:GE:228:TYR:CD1 | 2:GE:228:TYR:C | 2.92 | 0.47 |
| 2:GK:228:TYR:CD1 | 2:GK:228:TYR:C | 2.91 | 0.47 |
| 2:HC:78:LYS:NZ | 2:HF:73:GLU:OE1 | 2.47 | 0.47 |
| 2:HH:78:LYS:NZ | 2:HK:73:GLU:OE1 | 2.47 | 0.47 |
| 2:JU:6:LYS:NZ | 2:JU:10:GLU:OE2 | 2.45 | 0.47 |
| 2:JY:78:LYS:NZ | 2:KC:73:GLU:OE1 | 2.47 | 0.47 |
| 2:JY:228:TYR:C | 2:JY:228:TYR:CD1 | 2.91 | 0.47 |
| 2:KE:228:TYR:CD1 | 2:KE:228:TYR:C | 2.92 | 0.47 |
| 2:LA:160:ASP:OD1 | 2:LA:168:LYS:NZ | 2.36 | 0.47 |
| 2:ZV:6:LYS:NZ | 2:ZV:10:GLU:OE2 | 2.45 | 0.47 |
| 2:YR:228:TYR:C | 2:YR:228:TYR:CD1 | 2.92 | 0.47 |
| 1:AW:94:GLU:OE1 | 2:AX:278:ARG:NH2 | 2.48 | 0.47 |
| 2:FS:78:LYS:NZ | 2:FW:73:GLU:OE1 | 2.47 | 0.47 |
| 1:GR:94:GLU:OE1 | 2:GS:278:ARG:NH2 | 2.48 | 0.47 |
| 2:HS:228:TYR:CD1 | 2:HS:228:TYR:C | 2.92 | 0.47 |
| 1:HT:94:GLU:OE1 | 2:HU:278:ARG:NH2 | 2.48 | 0.47 |
| 2:ID:228:TYR:CD1 | 2:ID:228:TYR:C | 2.92 | 0.47 |
| 2:IJ:78:LYS:NZ | 2:IN:73:GLU:OE1 | 2.47 | 0.47 |
| 2:IJ:228:TYR:CD1 | 2:IJ:228:TYR:C | 2.92 | 0.47 |
| 1:IW:94:GLU:OE1 | 2:IX:278:ARG:NH2 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:JT:78:LYS:NZ | 2:JW:73:GLU:OE1 | 2.47 | 0.47 |
| 2:KE:78:LYS:NZ | 2:KI:73:GLU:OE1 | 2.47 | 0.47 |
| 2:KQ:78:LYS:NZ | 2:KU:73:GLU:OE1 | 2.47 | 0.47 |
| 2:LC:228:TYR:C | 2:LC:228:TYR:CD1 | 2.92 | 0.47 |
| 2:ZN:78:LYS:NZ | 2:ZR:73:GLU:OE1 | 2.47 | 0.47 |
| 2:ZB:78:LYS:NZ | 2:ZF:73:GLU:OE1 | 2.47 | 0.47 |
| 2:BH:228:TYR:C | 2:BH:228:TYR:CD1 | 2.92 | 0.47 |
| 1:BU:94:GLU:OE1 | 2:BV:278:ARG:NH2 | 2.48 | 0.47 |
| 2:BZ:78:LYS:NZ | 2:CD:73:GLU:OE1 | 2.47 | 0.47 |
| 2:ZD:6:LYS:NZ | 2:ZD:10:GLU:OE2 | 2.45 | 0.47 |
| 1:CG:94:GLU:OE1 | 2:CH:278:ARG:NH2 | 2.48 | 0.47 |
| 1:CS:94:GLU:OE1 | 2:CT:278:ARG:NH2 | 2.48 | 0.47 |
| 2:DR:2:ASP:OD2 | 2:DT:101:LYS:NZ | 2.33 | 0.47 |
| 2:EU:228:TYR:CD1 | 2:EU:228:TYR:C | 2.92 | 0.47 |
| 2:FA:78:LYS:NZ | 2:FE:73:GLU:OE1 | 2.47 | 0.47 |
| 2:GW:228:TYR:CD1 | 2:GW:228:TYR:C | 2.92 | 0.47 |
| 2:HQ:160:ASP:OD1 | 2:HQ:168:LYS:NZ | 2.36 | 0.47 |
| 2:IP:78:LYS:NZ | 2:IT:73:GLU:OE1 | 2.47 | 0.47 |
| 1:JC:94:GLU:OE1 | 2:JD:278:ARG:NH2 | 2.48 | 0.47 |
| 2:JN:228:TYR:C | 2:JN:228:TYR:CD1 | 2.92 | 0.47 |
| 2:JU:278:ARG:NH2 | 1:WD:94:GLU:OE1 | 2.48 | 0.47 |
| 1:KL:94:GLU:OE1 | 2:KM:278:ARG:NH2 | 2.48 | 0.47 |
| 2:YR:78:LYS:NZ | 2:YV:73:GLU:OE1 | 2.47 | 0.47 |
| 1:YS:94:GLU:OE1 | 2:YT:278:ARG:NH2 | 2.48 | 0.47 |
| 2:AD:78:LYS:NZ | 2:AH:73:GLU:OE1 | 2.47 | 0.47 |
| 2:AD:228:TYR:CD1 | 2:AD:228:TYR:C | 2.92 | 0.47 |
| 2:AO:278:ARG:NH2 | 1:AP:94:GLU:OE1 | 2.48 | 0.47 |
| 1:BI:94:GLU:OE1 | 2:BJ:278:ARG:NH2 | 2.48 | 0.47 |
| 2:CF:228:TYR:CD1 | 2:CF:228:TYR:C | 2.92 | 0.47 |
| 2:CX:78:LYS:NZ | 2:DB:73:GLU:OE1 | 2.47 | 0.47 |
| 1:HZ:94:GLU:OE1 | 2:IA:278:ARG:NH2 | 2.48 | 0.47 |
| 2:JH:78:LYS:NZ | 2:JL:73:GLU:OE1 | 2.47 | 0.47 |
| 2:JT:228:TYR:CD1 | 2:JT:228:TYR:C | 2.92 | 0.47 |
| 1:JZ:94:GLU:OE1 | 2:KA:278:ARG:NH2 | 2.48 | 0.47 |
| 1:KR:94:GLU:OE1 | 2:KS:278:ARG:NH2 | 2.48 | 0.47 |
| 2:LK:6:LYS:NZ | 2:LK:10:GLU:OE2 | 2.45 | 0.47 |
| 1:ZO:94:GLU:OE1 | 2:ZP:278:ARG:NH2 | 2.48 | 0.47 |
| 2:EO:78:LYS:NZ | 2:ES:73:GLU:OE1 | 2.47 | 0.47 |
| 1:EP:94:GLU:OE1 | 2:EQ:278:ARG:NH2 | 2.48 | 0.47 |
| 2:EQ:6:LYS:NZ | 2:EQ:10:GLU:OE2 | 2.45 | 0.47 |
| 1:GL:94:GLU:OE1 | 2:GM:278:ARG:NH2 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:GX:94:GLU:OE1 | 2:GY:278:ARG:NH2 | 2.48 | 0.47 |
| 2:HU:6:LYS:NZ | 2:HU:10:GLU:OE2 | 2.45 | 0.47 |
| 2:HY:78:LYS:NZ | 2:IB:73:GLU:OE1 | 2.47 | 0.47 |
| 1:JO:94:GLU:OE1 | 2:JP:278:ARG:NH2 | 2.48 | 0.47 |
| 1:LP:94:GLU:OE1 | 2:LQ:278:ARG:NH2 | 2.48 | 0.47 |
| 1:YC:33:ALA:N | 1:YC:34:PRO:CD | 2.78 | 0.47 |
| 1:YM:94:GLU:OE1 | 2:YN:278:ARG:NH2 | 2.48 | 0.47 |
| 1:YY:94:GLU:OE1 | 2:YZ:278:ARG:NH2 | 2.48 | 0.47 |
| 2:AQ:78:LYS:NZ | 2:AT:73:GLU:OE1 | 2.47 | 0.47 |
| 1:ZC:94:GLU:OE1 | 2:ZD:278:ARG:NH2 | 2.48 | 0.47 |
| 2:BN:231:VAL:HG11 | 2:BN:238:MET:HB2 | 1.97 | 0.47 |
| 2:BP:6:LYS:NZ | 2:BP:10:GLU:OE2 | 2.45 | 0.47 |
| 2:DJ:78:LYS:NZ | 2:DN:73:GLU:OE1 | 2.47 | 0.47 |
| 2:DW:78:LYS:NZ | 2:EA:73:GLU:OE1 | 2.47 | 0.47 |
| 1:EL:33:ALA:N | 1:EL:34:PRO:CD | 2.78 | 0.47 |
| 1:EV:94:GLU:OE1 | 2:EW:278:ARG:NH2 | 2.48 | 0.47 |
| 1:EX:33:ALA:N | 1:EX:34:PRO:CD | 2.78 | 0.47 |
| 1:FH:94:GLU:OE1 | 2:FI:278:ARG:NH2 | 2.48 | 0.47 |
| 1:FN:94:GLU:OE1 | 2:FO:278:ARG:NH2 | 2.48 | 0.47 |
| 1:FP:33:ALA:N | 1:FP:34:PRO:CD | 2.78 | 0.47 |
| 1:FT:94:GLU:OE1 | 2:FU:278:ARG:NH2 | 2.48 | 0.47 |
| 2:FY:78:LYS:NZ | 2:GC:73:GLU:OE1 | 2.47 | 0.47 |
| 2:GM:6:LYS:NZ | 2:GM:10:GLU:OE2 | 2.45 | 0.47 |
| 1:ZI:94:GLU:OE1 | 2:ZJ:278:ARG:NH2 | 2.48 | 0.47 |
| 1:KH:33:ALA:N | 1:KH:34:PRO:CD | 2.78 | 0.47 |
| 2:KM:6:LYS:NZ | 2:KM:10:GLU:OE2 | 2.45 | 0.47 |
| 1:LD:94:GLU:OE1 | 2:LE:278:ARG:NH2 | 2.48 | 0.47 |
| 2:YX:228:TYR:CD1 | 2:YX:228:TYR:C | 2.92 | 0.47 |
| 1:AE:94:GLU:OE1 | 2:AF:278:ARG:NH2 | 2.48 | 0.47 |
| 1:AK:94:GLU:OE1 | 2:AL:278:ARG:NH2 | 2.48 | 0.47 |
| 1:BO:94:GLU:OE1 | 2:BP:278:ARG:NH2 | 2.48 | 0.47 |
| 1:DQ:94:GLU:OE1 | 2:DR:278:ARG:NH2 | 2.48 | 0.47 |
| 2:EC:78:LYS:NZ | 2:EG:73:GLU:OE1 | 2.47 | 0.47 |
| 1:ED:94:GLU:OE1 | 2:EE:278:ARG:NH2 | 2.48 | 0.47 |
| 1:FB:94:GLU:OE1 | 2:FC:278:ARG:NH2 | 2.48 | 0.47 |
| 1:GT:33:ALA:N | 1:GT:34:PRO:CD | 2.78 | 0.47 |
| 1:HP:33:ALA:N | 1:HP:34:PRO:CD | 2.78 | 0.47 |
| 2:HS:78:LYS:NZ | 2:HW:73:GLU:OE1 | 2.47 | 0.47 |
| 2:JB:228:TYR:CD1 | 2:JB:228:TYR:C | 2.91 | 0.47 |
| 1:JK:33:ALA:N | 1:JK:34:PRO:CD | 2.78 | 0.47 |
| 2:KK:78:LYS:NZ | 2:KO:73:GLU:OE1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:LJ:94:GLU:OE1 | 2:LK:278:ARG:NH2 | 2.48 | 0.47 |
| 2:ZN:231:VAL:HG11 | 2:ZN:238:MET:HB2 | 1.97 | 0.47 |
| 1:AG:33:ALA:N | 1:AG:34:PRO:CD | 2.78 | 0.47 |
| 1:AS:33:ALA:N | 1:AS:34:PRO:CD | 2.78 | 0.47 |
| 1:BK:33:ALA:N | 1:BK:34:PRO:CD | 2.78 | 0.47 |
| 1:CC:33:ALA:N | 1:CC:34:PRO:CD | 2.78 | 0.47 |
| 2:CX:231:VAL:HG11 | 2:CX:238:MET:HB2 | 1.97 | 0.47 |
| 1:IK:94:GLU:OE1 | 2:IL:278:ARG:NH2 | 2.48 | 0.47 |
| 1:IQ:94:GLU:OE1 | 2:IR:278:ARG:NH2 | 2.48 | 0.47 |
| 1:KX:94:GLU:OE1 | 2:KY:278:ARG:NH2 | 2.48 | 0.47 |
| 1:KZ:33:ALA:N | 1:KZ:34:PRO:CD | 2.78 | 0.47 |
| 1:CU:33:ALA:N | 1:CU:34:PRO:CD | 2.78 | 0.47 |
| 1:CY:94:GLU:OE1 | 2:CZ:278:ARG:NH2 | 2.48 | 0.47 |
| 1:DX:94:GLU:OE1 | 2:DY:278:ARG:NH2 | 2.48 | 0.47 |
| 2:FA:228:TYR:CD1 | 2:FA:228:TYR:C | 2.91 | 0.47 |
| 2:FY:231:VAL:HG11 | 2:FY:238:MET:HB2 | 1.97 | 0.47 |
| 2:GE:78:LYS:NZ | 2:GI:73:GLU:OE1 | 2.47 | 0.47 |
| 1:GF:94:GLU:OE1 | 2:GG:278:ARG:NH2 | 2.48 | 0.47 |
| 2:GW:231:VAL:HG11 | 2:GW:238:MET:HB2 | 1.97 | 0.47 |
| 1:HD:94:GLU:OE1 | 2:HE:278:ARG:NH2 | 2.48 | 0.47 |
| 1:WB:33:ALA:N | 1:WB:34:PRO:CD | 2.78 | 0.47 |
| 2:HH:231:VAL:HG11 | 2:HH:238:MET:HB2 | 1.97 | 0.47 |
| 2:ID:231:VAL:HG11 | 2:ID:238:MET:HB2 | 1.97 | 0.47 |
| 1:IE:94:GLU:OE1 | 2:IF:278:ARG:NH2 | 2.48 | 0.47 |
| 1:JE:33:ALA:N | 1:JE:34:PRO:CD | 2.78 | 0.47 |
| 1:KF:94:GLU:OE1 | 2:KG:278:ARG:NH2 | 2.48 | 0.47 |
| 1:YA:94:GLU:OE1 | 2:YB:278:ARG:NH2 | 2.48 | 0.47 |
| 1:YI:33:ALA:N | 1:YI:34:PRO:CD | 2.78 | 0.46 |
| 2:YZ:6:LYS:NZ | 2:YZ:10:GLU:OE2 | 2.45 | 0.46 |
| 2:AJ:231:VAL:HG11 | 2:AJ:238:MET:HB2 | 1.97 | 0.46 |
| 1:BE:33:ALA:N | 1:BE:34:PRO:CD | 2.78 | 0.46 |
| 2:BZ:231:VAL:HG11 | 2:BZ:238:MET:HB2 | 1.97 | 0.46 |
| 1:CA:94:GLU:OE1 | 2:CB:278:ARG:NH2 | 2.48 | 0.46 |
| 1:DK:94:GLU:OE1 | 2:DL:278:ARG:NH2 | 2.48 | 0.46 |
| 1:EJ:94:GLU:OE1 | 2:EK:278:ARG:NH2 | 2.48 | 0.46 |
| 2:EO:231:VAL:HG11 | 2:EO:238:MET:HB2 | 1.97 | 0.46 |
| 2:FS:231:VAL:HG11 | 2:FS:238:MET:HB2 | 1.97 | 0.46 |
| 1:FZ:94:GLU:OE1 | 2:GA:278:ARG:NH2 | 2.48 | 0.46 |
| 1:HV:33:ALA:N | 1:HV:34:PRO:CD | 2.78 | 0.46 |
| 2:JH:231:VAL:HG11 | 2:JH:238:MET:HB2 | 1.97 | 0.46 |
| 2:KQ:231:VAL:HG11 | 2:KQ:238:MET:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:KW:231:VAL:HG11 | 2:KW:238:MET:HB2 | 1.97 | 0.46 |
| 1:ZW:33:ALA:N | 1:ZW:34:PRO:CD | 2.78 | 0.46 |
| 2:YH:6:LYS:NZ | 2:YH:10:GLU:OE2 | 2.45 | 0.46 |
| 2:YL:78:LYS:NZ | 2:YP:73:GLU:OE1 | 2.47 | 0.46 |
| 2:YL:231:VAL:HG11 | 2:YL:238:MET:HB2 | 1.97 | 0.46 |
| 1:AY:33:ALA:N | 1:AY:34:PRO:CD | 2.78 | 0.46 |
| 1:BC:94:GLU:OE1 | 2:BD:278:ARG:NH2 | 2.48 | 0.46 |
| 2:BH:78:LYS:NZ | 2:BL:73:GLU:OE1 | 2.47 | 0.46 |
| 2:BJ:6:LYS:NZ | 2:BJ:10:GLU:OE2 | 2.45 | 0.46 |
| 2:EU:231:VAL:HG11 | 2:EU:238:MET:HB2 | 1.97 | 0.46 |
| 1:FD:33:ALA:N | 1:FD:34:PRO:CD | 2.78 | 0.46 |
| 1:IS:33:ALA:N | 1:IS:34:PRO:CD | 2.78 | 0.46 |
| 1:JQ:33:ALA:N | 1:JQ:34:PRO:CD | 2.78 | 0.46 |
| 2:JT:231:VAL:HG11 | 2:JT:238:MET:HB2 | 1.97 | 0.46 |
| 1:KB:33:ALA:N | 1:KB:34:PRO:CD | 2.78 | 0.46 |
| 1:ZU:94:GLU:OE1 | 2:ZV:278:ARG:NH2 | 2.48 | 0.46 |
| 2:ZZ:231:VAL:HG11 | 2:ZZ:238:MET:HB2 | 1.97 | 0.46 |
| 2:AD:231:VAL:HG11 | 2:AD:238:MET:HB2 | 1.97 | 0.46 |
| 1:CM:94:GLU:OE1 | 2:CN:278:ARG:NH2 | 2.48 | 0.46 |
| 2:DD:231:VAL:HG11 | 2:DD:238:MET:HB2 | 1.97 | 0.46 |
| 1:ER:33:ALA:N | 1:ER:34:PRO:CD | 2.78 | 0.46 |
| 1:FV:33:ALA:N | 1:FV:34:PRO:CD | 2.78 | 0.46 |
| 1:GZ:33:ALA:N | 1:GZ:34:PRO:CD | 2.78 | 0.46 |
| 2:HY:231:VAL:HG11 | 2:HY:238:MET:HB2 | 1.97 | 0.46 |
| 1:WC:33:ALA:N | 1:WC:34:PRO:CD | 2.78 | 0.46 |
| 1:KT:33:ALA:N | 1:KT:34:PRO:CD | 2.78 | 0.46 |
| 2:LE:6:LYS:NZ | 2:LE:10:GLU:OE2 | 2.45 | 0.46 |
| 1:YG:94:GLU:OE1 | 2:YH:278:ARG:NH2 | 2.48 | 0.46 |
| 1:YO:33:ALA:N | 1:YO:34:PRO:CD | 2.78 | 0.46 |
| 2:YR:231:VAL:HG11 | 2:YR:238:MET:HB2 | 1.97 | 0.46 |
| 1:BA:11:ALA:HB1 | 1:BA:43:VAL:O | 2.16 | 0.46 |
| 2:CR:231:VAL:HG11 | 2:CR:238:MET:HB2 | 1.97 | 0.46 |
| 1:DZ:33:ALA:N | 1:DZ:34:PRO:CD | 2.78 | 0.46 |
| 2:EC:231:VAL:HG11 | 2:EC:238:MET:HB2 | 1.97 | 0.46 |
| 2:FG:231:VAL:HG11 | 2:FG:238:MET:HB2 | 1.97 | 0.46 |
| 1:HN:94:GLU:OE1 | 2:HO:278:ARG:NH2 | 2.48 | 0.46 |
| 2:JN:231:VAL:HG11 | 2:JN:238:MET:HB2 | 1.97 | 0.46 |
| 1:KN:33:ALA:N | 1:KN:34:PRO:CD | 2.78 | 0.46 |
| 1:LF:33:ALA:N | 1:LF:34:PRO:CD | 2.78 | 0.46 |
| 1:LL:33:ALA:N | 1:LL:34:PRO:CD | 2.78 | 0.46 |
| 2:ZB:231:VAL:HG11 | 2:ZB:238:MET:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BQ:33:ALA:N | 1:BQ:34:PRO:CD | 2.78 | 0.46 |
| 1:CO:33:ALA:N | 1:CO:34:PRO:CD | 2.78 | 0.46 |
| 1:DE:94:GLU:OE1 | 2:DF:278:ARG:NH2 | 2.48 | 0.46 |
| 1:DG:33:ALA:N | 1:DG:34:PRO:CD | 2.78 | 0.46 |
| 1:EF:33:ALA:N | 1:EF:34:PRO:CD | 2.78 | 0.46 |
| 2:EK:6:LYS:NZ | 2:EK:10:GLU:OE2 | 2.45 | 0.46 |
| 1:GN:33:ALA:N | 1:GN:34:PRO:CD | 2.78 | 0.46 |
| 2:HE:6:LYS:NZ | 2:HE:10:GLU:OE2 | 2.45 | 0.46 |
| 1:WA:33:ALA:N | 1:WA:34:PRO:CD | 2.78 | 0.46 |
| 1:IM:33:ALA:N | 1:IM:34:PRO:CD | 2.78 | 0.46 |
| 2:JY:231:VAL:HG11 | 2:JY:238:MET:HB2 | 1.97 | 0.46 |
| 1:KP:11:ALA:HB1 | 1:KP:43:VAL:O | 2.16 | 0.46 |
| 1:ZA:11:ALA:HB1 | 1:ZA:43:VAL:O | 2.16 | 0.46 |
| 2:BT:231:VAL:HG11 | 2:BT:238:MET:HB2 | 1.97 | 0.46 |
| 2:CL:231:VAL:HG11 | 2:CL:238:MET:HB2 | 1.97 | 0.46 |
| 2:EI:231:VAL:HG11 | 2:EI:238:MET:HB2 | 1.97 | 0.46 |
| 1:EZ:11:ALA:HB1 | 1:EZ:43:VAL:O | 2.16 | 0.46 |
| 1:GD:11:ALA:HB1 | 1:GD:43:VAL:O | 2.16 | 0.46 |
| 1:HX:11:ALA:HB1 | 1:HX:43:VAL:O | 2.16 | 0.46 |
| 1:IH:33:ALA:N | 1:IH:34:PRO:CD | 2.78 | 0.46 |
| 1:IU:11:ALA:HB1 | 1:IU:43:VAL:O | 2.16 | 0.46 |
| 1:IY:33:ALA:N | 1:IY:34:PRO:CD | 2.78 | 0.46 |
| 1:ZK:33:ALA:N | 1:ZK:34:PRO:CD | 2.78 | 0.46 |
| 2:KG:6:LYS:NZ | 2:KG:10:GLU:OE2 | 2.45 | 0.46 |
| 1:KJ:11:ALA:HB1 | 1:KJ:43:VAL:O | 2.16 | 0.46 |
| 2:LC:231:VAL:HG11 | 2:LC:238:MET:HB2 | 1.97 | 0.46 |
| 2:LQ:6:LYS:NZ | 2:LQ:10:GLU:OE2 | 2.45 | 0.46 |
| 1:ZQ:33:ALA:N | 1:ZQ:34:PRO:CD | 2.78 | 0.46 |
| 1:ZS:11:ALA:HB1 | 1:ZS:43:VAL:O | 2.16 | 0.46 |
| 1:AC:11:ALA:HB1 | 1:AC:43:VAL:O | 2.16 | 0.46 |
| 1:BM:11:ALA:HB1 | 1:BM:43:VAL:O | 2.16 | 0.46 |
| 1:CI:33:ALA:N | 1:CI:34:PRO:CD | 2.78 | 0.46 |
| 2:FI:6:LYS:NZ | 2:FI:10:GLU:OE2 | 2.45 | 0.46 |
| 2:GG:6:LYS:NZ | 2:GG:10:GLU:OE2 | 2.45 | 0.46 |
| 1:GV:11:ALA:HB1 | 1:GV:43:VAL:O | 2.16 | 0.46 |
| 1:HB:11:ALA:HB1 | 1:HB:43:VAL:O | 2.16 | 0.46 |
| 1:HI:94:GLU:OE1 | 2:HJ:278:ARG:NH2 | 2.48 | 0.46 |
| 2:HS:231:VAL:HG11 | 2:HS:238:MET:HB2 | 1.97 | 0.46 |
| 1:IC:11:ALA:HB1 | 1:IC:43:VAL:O | 2.16 | 0.46 |
| 2:IV:231:VAL:HG11 | 2:IV:238:MET:HB2 | 1.97 | 0.46 |
| 1:JI:94:GLU:OE1 | 2:JJ:278:ARG:NH2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:JJ:6:LYS:NZ | 2:JJ:10:GLU:OE2 | 2.45 | 0.46 |
| 1:LH:11:ALA:HB1 | 1:LH:43:VAL:O | 2.16 | 0.46 |
| 1:LR:33:ALA:N | 1:LR:34:PRO:CD | 2.78 | 0.46 |
| 2:AQ:231:VAL:HG11 | 2:AQ:238:MET:HB2 | 1.97 | 0.46 |
| 2:BB:231:VAL:HG11 | 2:BB:238:MET:HB2 | 1.97 | 0.46 |
| 2:BN:78:LYS:NZ | 2:BR:73:GLU:OE1 | 2.47 | 0.46 |
| 1:CQ:11:ALA:HB1 | 1:CQ:43:VAL:O | 2.16 | 0.46 |
| 1:DS:33:ALA:N | 1:DS:34:PRO:CD | 2.78 | 0.46 |
| 2:DY:6:LYS:NZ | 2:DY:10:GLU:OE2 | 2.45 | 0.46 |
| 1:GP:11:ALA:HB1 | 1:GP:43:VAL:O | 2.16 | 0.46 |
| 2:KK:231:VAL:HG11 | 2:KK:238:MET:HB2 | 1.97 | 0.46 |
| 1:YE:11:ALA:HB1 | 1:YE:43:VAL:O | 2.16 | 0.46 |
| 1:CW:11:ALA:HB1 | 1:CW:43:VAL:O | 2.16 | 0.46 |
| 1:ET:11:ALA:HB1 | 1:ET:43:VAL:O | 2.16 | 0.46 |
| 1:FJ:33:ALA:N | 1:FJ:34:PRO:CD | 2.78 | 0.46 |
| 1:GB:33:ALA:N | 1:GB:34:PRO:CD | 2.78 | 0.46 |
| 1:GH:33:ALA:N | 1:GH:34:PRO:CD | 2.78 | 0.46 |
| 2:GQ:231:VAL:HG11 | 2:GQ:238:MET:HB2 | 1.97 | 0.46 |
| 1:HL:11:ALA:HB1 | 1:HL:43:VAL:O | 2.16 | 0.46 |
| 2:JD:6:LYS:NZ | 2:JD:10:GLU:OE2 | 2.45 | 0.46 |
| 1:JV:33:ALA:N | 1:JV:34:PRO:CD | 2.78 | 0.46 |
| 1:ZM:11:ALA:HB1 | 1:ZM:43:VAL:O | 2.16 | 0.46 |
| 2:ZV:160:ASP:OD1 | 2:ZV:168:LYS:NZ | 2.45 | 0.46 |
| 1:YQ:11:ALA:HB1 | 1:YQ:43:VAL:O | 2.16 | 0.46 |
| 1:YU:33:ALA:N | 1:YU:34:PRO:CD | 2.78 | 0.46 |
| 1:YW:11:ALA:HB1 | 1:YW:43:VAL:O | 2.16 | 0.46 |
| 2:YX:231:VAL:HG11 | 2:YX:238:MET:HB2 | 1.97 | 0.46 |
| 1:AM:33:ALA:N | 1:AM:34:PRO:CD | 2.78 | 0.46 |
| 1:DA:33:ALA:N | 1:DA:34:PRO:CD | 2.78 | 0.46 |
| 1:EH:11:ALA:HB1 | 1:EH:43:VAL:O | 2.16 | 0.46 |
| 1:FL:11:ALA:HB1 | 1:FL:43:VAL:O | 2.16 | 0.46 |
| 2:GK:231:VAL:HG11 | 2:GK:238:MET:HB2 | 1.97 | 0.46 |
| 2:HJ:6:LYS:NZ | 2:HJ:10:GLU:OE2 | 2.45 | 0.46 |
| 2:IJ:231:VAL:HG11 | 2:IJ:238:MET:HB2 | 1.97 | 0.46 |
| 2:IL:6:LYS:NZ | 2:IL:10:GLU:OE2 | 2.45 | 0.46 |
| 1:JX:11:ALA:HB1 | 1:JX:43:VAL:O | 2.16 | 0.46 |
| 2:BD:6:LYS:NZ | 2:BD:10:GLU:OE2 | 2.45 | 0.45 |
| 1:EB:11:ALA:HB1 | 1:EB:43:VAL:O | 2.16 | 0.45 |
| 2:FM:231:VAL:HG11 | 2:FM:238:MET:HB2 | 1.97 | 0.45 |
| 1:FX:11:ALA:HB1 | 1:FX:43:VAL:O | 2.16 | 0.45 |
| 1:GJ:11:ALA:HB1 | 1:GJ:43:VAL:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:HM:231:VAL:HG11 | 2:HM:238:MET:HB2 | 1.97 | 0.45 |
| 1:HR:11:ALA:HB1 | 1:HR:43:VAL:O | 2.16 | 0.45 |
| 2:JB:231:VAL:HG11 | 2:JB:238:MET:HB2 | 1.97 | 0.45 |
| 1:AA:33:ALA:N | 1:AA:34:PRO:CD | 2.78 | 0.45 |
| 1:BG:11:ALA:HB1 | 1:BG:43:VAL:O | 2.16 | 0.45 |
| 1:BW:33:ALA:N | 1:BW:34:PRO:CD | 2.78 | 0.45 |
| 1:CE:11:ALA:HB1 | 1:CE:43:VAL:O | 2.16 | 0.45 |
| 1:ZE:33:ALA:N | 1:ZE:34:PRO:CD | 2.78 | 0.45 |
| 1:DC:11:ALA:HB1 | 1:DC:43:VAL:O | 2.16 | 0.45 |
| 1:DM:33:ALA:N | 1:DM:34:PRO:CD | 2.78 | 0.45 |
| 2:DW:231:VAL:HG11 | 2:DW:238:MET:HB2 | 1.97 | 0.45 |
| 2:FA:231:VAL:HG11 | 2:FA:238:MET:HB2 | 1.97 | 0.45 |
| 2:ZH:231:VAL:HG11 | 2:ZH:238:MET:HB2 | 1.97 | 0.45 |
| 2:HC:231:VAL:HG11 | 2:HC:238:MET:HB2 | 1.97 | 0.45 |
| 1:IO:11:ALA:HB1 | 1:IO:43:VAL:O | 2.16 | 0.45 |
| 2:IP:231:VAL:HG11 | 2:IP:238:MET:HB2 | 1.97 | 0.45 |
| 1:ZY:11:ALA:HB1 | 1:ZY:43:VAL:O | 2.16 | 0.45 |
| 1:YK:11:ALA:HB1 | 1:YK:43:VAL:O | 2.16 | 0.45 |
| 2:CN:6:LYS:NZ | 2:CN:10:GLU:OE2 | 2.45 | 0.45 |
| 2:DJ:231:VAL:HG11 | 2:DJ:238:MET:HB2 | 1.97 | 0.45 |
| 1:FR:11:ALA:HB1 | 1:FR:43:VAL:O | 2.16 | 0.45 |
| 2:HM:9:LEU:HD11 | 2:HO:71:VAL:HG21 | 1.99 | 0.45 |
| 1:KV:11:ALA:HB1 | 1:KV:43:VAL:O | 2.16 | 0.45 |
| 1:LB:11:ALA:HB1 | 1:LB:43:VAL:O | 2.16 | 0.45 |
| 1:LP:77:TYR:N | 1:LP:77:TYR:CD1 | 2.84 | 0.45 |
| 2:AO:6:LYS:NZ | 2:AO:10:GLU:OE2 | 2.45 | 0.45 |
| 2:AV:231:VAL:HG11 | 2:AV:238:MET:HB2 | 1.97 | 0.45 |
| 1:BY:11:ALA:HB1 | 1:BY:43:VAL:O | 2.16 | 0.45 |
| 1:CK:11:ALA:HB1 | 1:CK:43:VAL:O | 2.16 | 0.45 |
| 2:DJ:9:LEU:HD11 | 2:DL:71:VAL:HG21 | 1.99 | 0.45 |
| 2:GE:231:VAL:HG11 | 2:GE:238:MET:HB2 | 1.97 | 0.45 |
| 1:AR:11:ALA:HB1 | 1:AR:43:VAL:O | 2.16 | 0.45 |
| 2:BH:9:LEU:HD11 | 2:BJ:71:VAL:HG21 | 1.99 | 0.45 |
| 2:CZ:6:LYS:NZ | 2:CZ:10:GLU:OE2 | 2.45 | 0.45 |
| 1:DI:11:ALA:HB1 | 1:DI:43:VAL:O | 2.16 | 0.45 |
| 1:ZG:11:ALA:HB1 | 1:ZG:43:VAL:O | 2.16 | 0.45 |
| 1:FF:11:ALA:HB1 | 1:FF:43:VAL:O | 2.16 | 0.45 |
| 1:GL:77:TYR:N | 1:GL:77:TYR:CD1 | 2.84 | 0.45 |
| 1:JM:11:ALA:HB1 | 1:JM:43:VAL:O | 2.16 | 0.45 |
| 1:KD:11:ALA:HB1 | 1:KD:43:VAL:O | 2.16 | 0.45 |
| 2:KE:231:VAL:HG11 | 2:KE:238:MET:HB2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:YM:77:TYR:N | 1:YM:77:TYR:CD1 | 2.84 | 0.45 |
| 2:AO:160:ASP:OD1 | 2:AO:168:LYS:NZ | 2.45 | 0.45 |
| 1:BI:77:TYR:N | 1:BI:77:TYR:CD1 | 2.84 | 0.45 |
| 1:BS:11:ALA:HB1 | 1:BS:43:VAL:O | 2.16 | 0.45 |
| 2:FA:9:LEU:HD11 | 2:FC:71:VAL:HG21 | 1.99 | 0.45 |
| 1:HG:11:ALA:HB1 | 1:HG:43:VAL:O | 2.16 | 0.45 |
| 1:HI:77:TYR:N | 1:HI:77:TYR:CD1 | 2.84 | 0.45 |
| 2:LC:9:LEU:HD11 | 2:LE:71:VAL:HG21 | 1.99 | 0.45 |
| 1:LJ:77:TYR:N | 1:LJ:77:TYR:CD1 | 2.84 | 0.45 |
| 2:YF:9:LEU:HD11 | 2:YH:71:VAL:HG21 | 1.99 | 0.45 |
| 2:YF:231:VAL:HG11 | 2:YF:238:MET:HB2 | 1.97 | 0.45 |
| 1:AI:11:ALA:HB1 | 1:AI:43:VAL:O | 2.16 | 0.45 |
| 2:BN:9:LEU:HD11 | 2:BP:71:VAL:HG21 | 1.99 | 0.45 |
| 1:BO:77:TYR:CD1 | 1:BO:77:TYR:N | 2.84 | 0.45 |
| 2:CF:231:VAL:HG11 | 2:CF:238:MET:HB2 | 1.97 | 0.45 |
| 1:DU:11:ALA:HB1 | 1:DU:43:VAL:O | 2.16 | 0.45 |
| 1:DX:77:TYR:CD1 | 1:DX:77:TYR:N | 2.84 | 0.45 |
| 1:EN:11:ALA:HB1 | 1:EN:43:VAL:O | 2.16 | 0.45 |
| 2:GE:9:LEU:HD11 | 2:GG:71:VAL:HG21 | 1.99 | 0.45 |
| 2:HY:9:LEU:HD11 | 2:IA:71:VAL:HG21 | 1.99 | 0.45 |
| 1:II:11:ALA:HB1 | 1:II:43:VAL:O | 2.16 | 0.45 |
| 1:JS:11:ALA:HB1 | 1:JS:43:VAL:O | 2.16 | 0.45 |
| 2:KE:9:LEU:HD11 | 2:KG:71:VAL:HG21 | 1.99 | 0.45 |
| 1:KL:77:TYR:N | 1:KL:77:TYR:CD1 | 2.84 | 0.45 |
| 2:KW:9:LEU:HD11 | 2:KY:71:VAL:HG21 | 1.99 | 0.45 |
| 2:LI:231:VAL:HG11 | 2:LI:238:MET:HB2 | 1.97 | 0.45 |
| 2:LO:231:VAL:HG11 | 2:LO:238:MET:HB2 | 1.97 | 0.45 |
| 2:YX:9:LEU:HD11 | 2:YZ:71:VAL:HG21 | 1.99 | 0.45 |
| 2:BH:231:VAL:HG11 | 2:BH:238:MET:HB2 | 1.97 | 0.45 |
| 2:HC:9:LEU:HD11 | 2:HE:71:VAL:HG21 | 1.99 | 0.45 |
| 1:LN:11:ALA:HB1 | 1:LN:43:VAL:O | 2.16 | 0.45 |
| 2:ZT:231:VAL:HG11 | 2:ZT:238:MET:HB2 | 1.97 | 0.45 |
| 2:ZZ:9:LEU:HD11 | 2:YB:71:VAL:HG21 | 1.99 | 0.45 |
| 2:BX:160:ASP:OD1 | 2:BX:168:LYS:NZ | 2.36 | 0.45 |
| 2:EI:9:LEU:HD11 | 2:EK:71:VAL:HG21 | 1.99 | 0.45 |
| 2:FS:9:LEU:HD11 | 2:FU:71:VAL:HG21 | 1.99 | 0.45 |
| 1:JG:11:ALA:HB1 | 1:JG:43:VAL:O | 2.16 | 0.45 |
| 2:JP:6:LYS:NZ | 2:JP:10:GLU:OE2 | 2.45 | 0.45 |
| 2:LI:9:LEU:HD11 | 2:LK:71:VAL:HG21 | 1.99 | 0.45 |
| 2:ZT:9:LEU:HD11 | 2:ZV:71:VAL:HG21 | 1.99 | 0.45 |
| 2:ZB:9:LEU:HD11 | 2:ZD:71:VAL:HG21 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:BB:9:LEU:HD11 | 2:BD:71:VAL:HG21 | 1.99 | 0.45 |
| 2:DP:231:VAL:HG11 | 2:DP:238:MET:HB2 | 1.97 | 0.45 |
| 1:FZ:77:TYR:N | 1:FZ:77:TYR:CD1 | 2.84 | 0.45 |
| 1:JA:11:ALA:HB1 | 1:JA:43:VAL:O | 2.16 | 0.45 |
| 2:KQ:9:LEU:HD11 | 2:KS:71:VAL:HG21 | 1.99 | 0.45 |
| 1:LD:77:TYR:N | 1:LD:77:TYR:CD1 | 2.84 | 0.45 |
| 2:DF:6:LYS:NZ | 2:DF:10:GLU:OE2 | 2.45 | 0.44 |
| 2:DP:9:LEU:HD11 | 2:DR:71:VAL:HG21 | 1.99 | 0.44 |
| 1:GF:77:TYR:N | 1:GF:77:TYR:CD1 | 2.84 | 0.44 |
| 2:JY:9:LEU:HD11 | 2:KA:71:VAL:HG21 | 1.99 | 0.44 |
| 2:AD:9:LEU:HD11 | 2:AF:71:VAL:HG21 | 1.99 | 0.44 |
| 2:AH:160:ASP:OD1 | 2:AH:168:LYS:NZ | 2.36 | 0.44 |
| 1:DO:11:ALA:HB1 | 1:DO:43:VAL:O | 2.16 | 0.44 |
| 1:AU:11:ALA:HB1 | 1:AU:43:VAL:O | 2.16 | 0.44 |
| 2:EC:9:LEU:HD11 | 2:EE:71:VAL:HG21 | 1.99 | 0.44 |
| 1:FB:77:TYR:N | 1:FB:77:TYR:CD1 | 2.84 | 0.44 |
| 2:FC:6:LYS:NZ | 2:FC:10:GLU:OE2 | 2.45 | 0.44 |
| 2:FY:9:LEU:HD11 | 2:GA:71:VAL:HG21 | 1.99 | 0.44 |
| 2:ZH:9:LEU:HD11 | 2:ZJ:71:VAL:HG21 | 1.99 | 0.44 |
| 2:IF:160:ASP:OD1 | 2:IF:168:LYS:NZ | 2.45 | 0.44 |
| 1:IW:77:TYR:N | 1:IW:77:TYR:CD1 | 2.84 | 0.44 |
| 2:AO:71:VAL:HG21 | 2:AQ:9:LEU:HD11 | 1.99 | 0.44 |
| 1:CO:81:ARG:NH2 | 2:CP:281:PHE:O | 2.51 | 0.44 |
| 1:JK:81:ARG:NH2 | 2:JL:281:PHE:O | 2.51 | 0.44 |
| 1:KN:81:ARG:NH2 | 2:KO:281:PHE:O | 2.51 | 0.44 |
| 1:CU:81:ARG:NH2 | 2:CV:281:PHE:O | 2.51 | 0.44 |
| 1:DM:81:ARG:NH2 | 2:DN:281:PHE:O | 2.51 | 0.44 |
| 1:DQ:77:TYR:N | 1:DQ:77:TYR:CD1 | 2.84 | 0.44 |
| 2:FG:9:LEU:HD11 | 2:FI:71:VAL:HG21 | 1.99 | 0.44 |
| 2:FM:9:LEU:HD11 | 2:FO:71:VAL:HG21 | 1.99 | 0.44 |
| 1:JZ:31:LYS:O | 1:JZ:87:GLN:NE2 | 2.51 | 0.44 |
| 2:LO:9:LEU:HD11 | 2:LQ:71:VAL:HG21 | 1.99 | 0.44 |
| 2:YR:9:LEU:HD11 | 2:YT:71:VAL:HG21 | 1.99 | 0.44 |
| 1:YY:77:TYR:N | 1:YY:77:TYR:CD1 | 2.84 | 0.44 |
| 1:BI:31:LYS:O | 1:BI:87:GLN:NE2 | 2.51 | 0.44 |
| 2:DW:9:LEU:HD11 | 2:DY:71:VAL:HG21 | 1.99 | 0.44 |
| 2:EU:9:LEU:HD11 | 2:EW:71:VAL:HG21 | 1.99 | 0.44 |
| 2:GQ:9:LEU:HD11 | 2:GS:71:VAL:HG21 | 1.99 | 0.44 |
| 1:GR:31:LYS:O | 1:GR:87:GLN:NE2 | 2.51 | 0.44 |
| 1:IE:77:TYR:N | 1:IE:77:TYR:CD1 | 2.84 | 0.44 |
| 1:ZO:31:LYS:O | 1:ZO:87:GLN:NE2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:YG:31:LYS:O | 1:YG:87:GLN:NE2 | 2.51 | 0.44 |
| 2:AJ:9:LEU:HD11 | 2:AL:71:VAL:HG21 | 1.99 | 0.44 |
| 1:ZC:31:LYS:O | 1:ZC:87:GLN:NE2 | 2.51 | 0.44 |
| 2:BF:160:ASP:OD1 | 2:BF:168:LYS:NZ | 2.36 | 0.44 |
| 1:CM:31:LYS:O | 1:CM:87:GLN:NE2 | 2.51 | 0.44 |
| 1:CM:77:TYR:N | 1:CM:77:TYR:CD1 | 2.84 | 0.44 |
| 1:CS:31:LYS:O | 1:CS:87:GLN:NE2 | 2.51 | 0.44 |
| 1:DE:31:LYS:O | 1:DE:87:GLN:NE2 | 2.51 | 0.44 |
| 1:GZ:81:ARG:NH2 | 2:HA:281:PHE:O | 2.51 | 0.44 |
| 1:IK:31:LYS:O | 1:IK:87:GLN:NE2 | 2.51 | 0.44 |
| 1:ZW:81:ARG:NH2 | 2:ZX:281:PHE:O | 2.51 | 0.44 |
| 2:YB:6:LYS:NZ | 2:YB:10:GLU:OE2 | 2.45 | 0.44 |
| 1:YC:81:ARG:NH2 | 2:YD:281:PHE:O | 2.51 | 0.44 |
| 1:AP:31:LYS:O | 1:AP:87:GLN:NE2 | 2.51 | 0.44 |
| 1:CA:31:LYS:O | 1:CA:87:GLN:NE2 | 2.51 | 0.44 |
| 2:CB:6:LYS:NZ | 2:CB:10:GLU:OE2 | 2.45 | 0.44 |
| 1:CG:31:LYS:O | 1:CG:87:GLN:NE2 | 2.51 | 0.44 |
| 1:FB:31:LYS:O | 1:FB:87:GLN:NE2 | 2.51 | 0.44 |
| 1:GX:21:VAL:HG11 | 1:GX:54:VAL:HG11 | 2.00 | 0.44 |
| 2:HS:9:LEU:HD11 | 2:HU:71:VAL:HG21 | 1.99 | 0.44 |
| 1:HZ:31:LYS:O | 1:HZ:87:GLN:NE2 | 2.51 | 0.44 |
| 2:ID:149:GLN:HG2 | 2:ID:178:ALA:HB3 | 2.00 | 0.44 |
| 2:IV:9:LEU:HD11 | 2:IX:71:VAL:HG21 | 1.99 | 0.44 |
| 1:IW:31:LYS:O | 1:IW:87:GLN:NE2 | 2.51 | 0.44 |
| 2:JN:9:LEU:HD11 | 2:JP:71:VAL:HG21 | 1.99 | 0.44 |
| 1:KT:81:ARG:NH2 | 2:KU:281:PHE:O | 2.51 | 0.44 |
| 1:LL:81:ARG:NH2 | 2:LM:281:PHE:O | 2.51 | 0.44 |
| 1:ZU:31:LYS:O | 1:ZU:87:GLN:NE2 | 2.51 | 0.44 |
| 2:YF:149:GLN:HG2 | 2:YF:178:ALA:HB3 | 2.00 | 0.44 |
| 1:ZC:21:VAL:HG11 | 1:ZC:54:VAL:HG11 | 2.00 | 0.44 |
| 2:CL:149:GLN:HG2 | 2:CL:178:ALA:HB3 | 2.00 | 0.44 |
| 2:CX:9:LEU:HD11 | 2:CZ:71:VAL:HG21 | 1.99 | 0.44 |
| 2:CX:149:GLN:HG2 | 2:CX:178:ALA:HB3 | 2.00 | 0.44 |
| 2:DP:149:GLN:HG2 | 2:DP:178:ALA:HB3 | 2.00 | 0.44 |
| 2:EO:149:GLN:HG2 | 2:EO:178:ALA:HB3 | 2.00 | 0.44 |
| 1:EV:21:VAL:HG11 | 1:EV:54:VAL:HG11 | 2.00 | 0.44 |
| 1:FB:21:VAL:HG11 | 1:FB:54:VAL:HG11 | 2.00 | 0.44 |
| 2:FG:45:HIS:CE1 | 2:FI:46:ASN:HD21 | 2.36 | 0.44 |
| 1:FT:31:LYS:O | 1:FT:87:GLN:NE2 | 2.51 | 0.44 |
| 1:GF:31:LYS:O | 1:GF:87:GLN:NE2 | 2.51 | 0.44 |
| 1:GL:31:LYS:O | 1:GL:87:GLN:NE2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:ZI:31:LYS:O | 1:ZI:87:GLN:NE2 | 2.51 | 0.44 |
| 2:HH:9:LEU:HD11 | 2:HJ:71:VAL:HG21 | 1.99 | 0.44 |
| 1:HN:31:LYS:O | 1:HN:87:GLN:NE2 | 2.51 | 0.44 |
| 1:HT:31:LYS:O | 1:HT:87:GLN:NE2 | 2.51 | 0.44 |
| 1:IE:31:LYS:O | 1:IE:87:GLN:NE2 | 2.51 | 0.44 |
| 2:IP:9:LEU:HD11 | 2:IR:71:VAL:HG21 | 1.99 | 0.44 |
| 2:IV:149:GLN:HG2 | 2:IV:178:ALA:HB3 | 2.00 | 0.44 |
| 2:JH:9:LEU:HD11 | 2:JJ:71:VAL:HG21 | 1.99 | 0.44 |
| 1:JI:77:TYR:N | 1:JI:77:TYR:CD1 | 2.84 | 0.44 |
| 1:KF:31:LYS:O | 1:KF:87:GLN:NE2 | 2.51 | 0.44 |
| 1:KR:21:VAL:HG11 | 1:KR:54:VAL:HG11 | 2.00 | 0.44 |
| 2:LI:149:GLN:HG2 | 2:LI:178:ALA:HB3 | 2.00 | 0.44 |
| 2:ZN:9:LEU:HD11 | 2:ZP:71:VAL:HG21 | 1.99 | 0.44 |
| 2:ZZ:149:GLN:HG2 | 2:ZZ:178:ALA:HB3 | 2.00 | 0.43 |
| 1:YS:21:VAL:HG11 | 1:YS:54:VAL:HG11 | 2.00 | 0.43 |
| 2:CL:9:LEU:HD11 | 2:CN:71:VAL:HG21 | 1.99 | 0.43 |
| 2:EI:149:GLN:HG2 | 2:EI:178:ALA:HB3 | 2.00 | 0.43 |
| 1:EJ:31:LYS:O | 1:EJ:87:GLN:NE2 | 2.51 | 0.43 |
| 1:FH:21:VAL:HG11 | 1:FH:54:VAL:HG11 | 2.00 | 0.43 |
| 1:FT:77:TYR:CD1 | 1:FT:77:TYR:N | 2.84 | 0.43 |
| 2:GE:149:GLN:HG2 | 2:GE:178:ALA:HB3 | 2.00 | 0.43 |
| 2:GK:9:LEU:HD11 | 2:GM:71:VAL:HG21 | 1.99 | 0.43 |
| 2:GQ:45:HIS:CE1 | 2:GS:46:ASN:HD21 | 2.36 | 0.43 |
| 1:GX:31:LYS:O | 1:GX:87:GLN:NE2 | 2.51 | 0.43 |
| 1:ZI:21:VAL:HG11 | 1:ZI:54:VAL:HG11 | 2.00 | 0.43 |
| 2:HH:149:GLN:HG2 | 2:HH:178:ALA:HB3 | 2.00 | 0.43 |
| 2:HM:149:GLN:HG2 | 2:HM:178:ALA:HB3 | 2.00 | 0.43 |
| 1:IQ:31:LYS:O | 1:IQ:87:GLN:NE2 | 2.51 | 0.43 |
| 2:JB:9:LEU:HD11 | 2:JD:71:VAL:HG21 | 1.99 | 0.43 |
| 1:JC:31:LYS:O | 1:JC:87:GLN:NE2 | 2.51 | 0.43 |
| 2:JN:149:GLN:HG2 | 2:JN:178:ALA:HB3 | 2.00 | 0.43 |
| 1:KF:21:VAL:HG11 | 1:KF:54:VAL:HG11 | 2.00 | 0.43 |
| 1:KH:81:ARG:NH2 | 2:KI:281:PHE:O | 2.51 | 0.43 |
| 1:KX:31:LYS:O | 1:KX:87:GLN:NE2 | 2.51 | 0.43 |
| 1:ZO:21:VAL:HG11 | 1:ZO:54:VAL:HG11 | 2.00 | 0.43 |
| 1:YA:31:LYS:O | 1:YA:87:GLN:NE2 | 2.51 | 0.43 |
| 2:YL:9:LEU:HD11 | 2:YN:71:VAL:HG21 | 1.99 | 0.43 |
| 2:YX:149:GLN:HG2 | 2:YX:178:ALA:HB3 | 2.00 | 0.43 |
| 1:YY:21:VAL:HG11 | 1:YY:54:VAL:HG11 | 2.00 | 0.43 |
| 1:YY:31:LYS:O | 1:YY:87:GLN:NE2 | 2.51 | 0.43 |
| 1:AW:31:LYS:O | 1:AW:87:GLN:NE2 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:BB:149:GLN:HG2 | 2:BB:178:ALA:HB3 | 2.00 | 0.43 |
| 1:BC:77:TYR:N | 1:BC:77:TYR:CD1 | 2.84 | 0.43 |
| 1:BE:81:ARG:NH2 | 2:BF:281:PHE:O | 2.51 | 0.43 |
| 1:BI:21:VAL:HG11 | 1:BI:54:VAL:HG11 | 2.01 | 0.43 |
| 2:BT:9:LEU:HD11 | 2:BV:71:VAL:HG21 | 1.99 | 0.43 |
| 1:CG:21:VAL:HG11 | 1:CG:54:VAL:HG11 | 2.00 | 0.43 |
| 1:EP:31:LYS:O | 1:EP:87:GLN:NE2 | 2.51 | 0.43 |
| 1:FN:21:VAL:HG11 | 1:FN:54:VAL:HG11 | 2.00 | 0.43 |
| 1:FZ:31:LYS:O | 1:FZ:87:GLN:NE2 | 2.51 | 0.43 |
| 1:GR:77:TYR:N | 1:GR:77:TYR:CD1 | 2.84 | 0.43 |
| 2:GW:9:LEU:HD11 | 2:GY:71:VAL:HG21 | 1.99 | 0.43 |
| 2:HS:45:HIS:CE1 | 2:HU:46:ASN:HD21 | 2.37 | 0.43 |
| 1:IK:21:VAL:HG11 | 1:IK:54:VAL:HG11 | 2.00 | 0.43 |
| 1:JO:31:LYS:O | 1:JO:87:GLN:NE2 | 2.51 | 0.43 |
| 2:KA:6:LYS:NZ | 2:KA:10:GLU:OE2 | 2.45 | 0.43 |
| 1:KR:31:LYS:O | 1:KR:87:GLN:NE2 | 2.51 | 0.43 |
| 2:LC:149:GLN:HG2 | 2:LC:178:ALA:HB3 | 2.00 | 0.43 |
| 1:LP:31:LYS:O | 1:LP:87:GLN:NE2 | 2.51 | 0.43 |
| 2:ZN:45:HIS:CE1 | 2:ZP:46:ASN:HD21 | 2.37 | 0.43 |
| 1:ZU:21:VAL:HG11 | 1:ZU:54:VAL:HG11 | 2.00 | 0.43 |
| 1:YA:77:TYR:N | 1:YA:77:TYR:CD1 | 2.84 | 0.43 |
| 2:YR:45:HIS:CE1 | 2:YT:46:ASN:HD21 | 2.37 | 0.43 |
| 1:YS:77:TYR:CD1 | 1:YS:77:TYR:N | 2.84 | 0.43 |
| 2:ZB:149:GLN:HG2 | 2:ZB:178:ALA:HB3 | 2.00 | 0.43 |
| 1:AE:77:TYR:N | 1:AE:77:TYR:CD1 | 2.84 | 0.43 |
| 2:AV:45:HIS:CE1 | 2:AX:46:ASN:HD21 | 2.37 | 0.43 |
| 1:BC:21:VAL:HG11 | 1:BC:54:VAL:HG11 | 2.00 | 0.43 |
| 2:BH:149:GLN:HG2 | 2:BH:178:ALA:HB3 | 2.00 | 0.43 |
| 2:CF:9:LEU:HD11 | 2:CH:71:VAL:HG21 | 1.99 | 0.43 |
| 2:CF:149:GLN:HG2 | 2:CF:178:ALA:HB3 | 2.00 | 0.43 |
| 2:CR:9:LEU:HD11 | 2:CT:71:VAL:HG21 | 1.99 | 0.43 |
| 2:CR:45:HIS:CE1 | 2:CT:46:ASN:HD21 | 2.36 | 0.43 |
| 1:CY:77:TYR:CD1 | 1:CY:77:TYR:N | 2.84 | 0.43 |
| 2:DJ:45:HIS:CE1 | 2:DL:46:ASN:HD21 | 2.36 | 0.43 |
| 1:FH:31:LYS:O | 1:FH:87:GLN:NE2 | 2.51 | 0.43 |
| 1:GH:81:ARG:NH2 | 2:GI:281:PHE:O | 2.51 | 0.43 |
| 2:GQ:149:GLN:HG2 | 2:GQ:178:ALA:HB3 | 2.00 | 0.43 |
| 1:HT:21:VAL:HG11 | 1:HT:54:VAL:HG11 | 2.00 | 0.43 |
| 2:IP:45:HIS:CE1 | 2:IR:46:ASN:HD21 | 2.36 | 0.43 |
| 1:WD:21:VAL:HG11 | 1:WD:54:VAL:HG11 | 2.00 | 0.43 |
| 2:KK:9:LEU:HD11 | 2:KM:71:VAL:HG21 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:KK:149:GLN:HG2 | 2:KK:178:ALA:HB3 | 2.00 | 0.43 |
| 1:LF:81:ARG:NH2 | 2:LG:281:PHE:O | 2.51 | 0.43 |
| 2:YR:149:GLN:HG2 | 2:YR:178:ALA:HB3 | 2.00 | 0.43 |
| 1:AW:21:VAL:HG11 | 1:AW:54:VAL:HG11 | 2.00 | 0.43 |
| 1:DZ:81:ARG:NH2 | 2:EA:281:PHE:O | 2.51 | 0.43 |
| 1:ED:31:LYS:O | 1:ED:87:GLN:NE2 | 2.51 | 0.43 |
| 1:EL:81:ARG:NH2 | 2:EM:281:PHE:O | 2.51 | 0.43 |
| 1:FN:31:LYS:O | 1:FN:87:GLN:NE2 | 2.51 | 0.43 |
| 2:FS:149:GLN:HG2 | 2:FS:178:ALA:HB3 | 2.00 | 0.43 |
| 1:ZI:77:TYR:N | 1:ZI:77:TYR:CD1 | 2.84 | 0.43 |
| 1:IQ:98:ASP:OD1 | 1:IQ:98:ASP:N | 2.52 | 0.43 |
| 1:ZK:81:ARG:NH2 | 2:ZL:281:PHE:O | 2.51 | 0.43 |
| 2:JB:45:HIS:CE1 | 2:JD:46:ASN:HD21 | 2.37 | 0.43 |
| 1:JC:21:VAL:HG11 | 1:JC:54:VAL:HG11 | 2.00 | 0.43 |
| 2:LC:45:HIS:CE1 | 2:LE:46:ASN:HD21 | 2.36 | 0.43 |
| 2:AD:149:GLN:HG2 | 2:AD:178:ALA:HB3 | 2.00 | 0.43 |
| 1:AK:77:TYR:N | 1:AK:77:TYR:CD1 | 2.84 | 0.43 |
| 2:AV:9:LEU:HD11 | 2:AX:71:VAL:HG21 | 1.99 | 0.43 |
| 2:AV:149:GLN:HG2 | 2:AV:178:ALA:HB3 | 2.00 | 0.43 |
| 1:AW:77:TYR:N | 1:AW:77:TYR:CD1 | 2.84 | 0.43 |
| 2:DJ:149:GLN:HG2 | 2:DJ:178:ALA:HB3 | 2.00 | 0.43 |
| 1:DK:21:VAL:HG11 | 1:DK:54:VAL:HG11 | 2.00 | 0.43 |
| 2:DW:45:HIS:CE1 | 2:DY:46:ASN:HD21 | 2.37 | 0.43 |
| 2:DY:160:ASP:OD1 | 2:DY:168:LYS:NZ | 2.45 | 0.43 |
| 2:FM:149:GLN:HG2 | 2:FM:178:ALA:HB3 | 2.00 | 0.43 |
| 1:FV:81:ARG:NH2 | 2:FW:281:PHE:O | 2.51 | 0.43 |
| 2:ZH:149:GLN:HG2 | 2:ZH:178:ALA:HB3 | 2.00 | 0.43 |
| 1:GR:21:VAL:HG11 | 1:GR:54:VAL:HG11 | 2.00 | 0.43 |
| 1:HD:31:LYS:O | 1:HD:87:GLN:NE2 | 2.51 | 0.43 |
| 1:HI:31:LYS:O | 1:HI:87:GLN:NE2 | 2.51 | 0.43 |
| 1:JE:81:ARG:NH2 | 2:JF:281:PHE:O | 2.51 | 0.43 |
| 2:JT:9:LEU:HD11 | 2:JU:71:VAL:HG21 | 1.99 | 0.43 |
| 1:WD:77:TYR:N | 1:WD:77:TYR:CD1 | 2.84 | 0.43 |
| 1:LJ:21:VAL:HG11 | 1:LJ:54:VAL:HG11 | 2.00 | 0.43 |
| 1:LP:21:VAL:HG11 | 1:LP:54:VAL:HG11 | 2.00 | 0.43 |
| 1:ZO:77:TYR:N | 1:ZO:77:TYR:CD1 | 2.84 | 0.43 |
| 2:YL:45:HIS:CE1 | 2:YN:46:ASN:HD21 | 2.37 | 0.43 |
| 1:YO:81:ARG:NH2 | 2:YP:281:PHE:O | 2.51 | 0.43 |
| 1:YS:31:LYS:O | 1:YS:87:GLN:NE2 | 2.51 | 0.43 |
| 2:ZB:45:HIS:CE1 | 2:ZD:46:ASN:HD21 | 2.37 | 0.43 |
| 1:ZC:77:TYR:N | 1:ZC:77:TYR:CD1 | 2.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:BC:31:LYS:O | 1:BC:87:GLN:NE2 | 2.51 | 0.43 |
| 2:BT:45:HIS:CE1 | 2:BV:46:ASN:HD21 | 2.37 | 0.43 |
| 1:CG:77:TYR:N | 1:CG:77:TYR:CD1 | 2.84 | 0.43 |
| 1:CS:21:VAL:HG11 | 1:CS:54:VAL:HG11 | 2.00 | 0.43 |
| 2:DD:9:LEU:HD11 | 2:DF:71:VAL:HG21 | 1.99 | 0.43 |
| 1:DK:31:LYS:O | 1:DK:87:GLN:NE2 | 2.51 | 0.43 |
| 1:DQ:31:LYS:O | 1:DQ:87:GLN:NE2 | 2.51 | 0.43 |
| 1:EF:81:ARG:NH2 | 2:EG:281:PHE:O | 2.51 | 0.43 |
| 1:EV:31:LYS:O | 1:EV:87:GLN:NE2 | 2.51 | 0.43 |
| 1:FH:77:TYR:CD1 | 1:FH:77:TYR:N | 2.84 | 0.43 |
| 1:FZ:21:VAL:HG11 | 1:FZ:54:VAL:HG11 | 2.00 | 0.43 |
| 2:GE:45:HIS:CE1 | 2:GG:46:ASN:HD21 | 2.36 | 0.43 |
| 2:GW:45:HIS:CE1 | 2:GY:46:ASN:HD21 | 2.37 | 0.43 |
| 2:HC:45:HIS:CE1 | 2:HE:46:ASN:HD21 | 2.37 | 0.43 |
| 2:ID:9:LEU:HD11 | 2:IF:71:VAL:HG21 | 1.99 | 0.43 |
| 2:IJ:9:LEU:HD11 | 2:IL:71:VAL:HG21 | 1.99 | 0.43 |
| 2:IJ:45:HIS:CE1 | 2:IL:46:ASN:HD21 | 2.37 | 0.43 |
| 1:WD:31:LYS:O | 1:WD:87:GLN:NE2 | 2.51 | 0.43 |
| 1:KL:31:LYS:O | 1:KL:87:GLN:NE2 | 2.51 | 0.43 |
| 2:KQ:149:GLN:HG2 | 2:KQ:178:ALA:HB3 | 2.00 | 0.43 |
| 1:KX:77:TYR:N | 1:KX:77:TYR:CD1 | 2.84 | 0.43 |
| 1:LJ:31:LYS:O | 1:LJ:87:GLN:NE2 | 2.51 | 0.43 |
| 2:ZZ:45:HIS:CE1 | 2:YB:46:ASN:HD21 | 2.36 | 0.43 |
| 2:YF:45:HIS:CE1 | 2:YH:46:ASN:HD21 | 2.37 | 0.43 |
| 1:YM:21:VAL:HG11 | 1:YM:54:VAL:HG11 | 2.00 | 0.43 |
| 1:AW:98:ASP:OD1 | 1:AW:98:ASP:N | 2.52 | 0.43 |
| 1:AY:81:ARG:NH2 | 2:AZ:281:PHE:O | 2.51 | 0.43 |
| 1:BO:31:LYS:O | 1:BO:87:GLN:NE2 | 2.51 | 0.43 |
| 2:EO:9:LEU:HD11 | 2:EQ:71:VAL:HG21 | 1.99 | 0.43 |
| 1:HD:21:VAL:HG11 | 1:HD:54:VAL:HG11 | 2.00 | 0.43 |
| 1:JZ:21:VAL:HG11 | 1:JZ:54:VAL:HG11 | 2.00 | 0.43 |
| 2:LI:45:HIS:CE1 | 2:LK:46:ASN:HD21 | 2.36 | 0.43 |
| 2:ZT:149:GLN:HG2 | 2:ZT:178:ALA:HB3 | 2.00 | 0.43 |
| 1:ZU:77:TYR:N | 1:ZU:77:TYR:CD1 | 2.84 | 0.43 |
| 1:AE:21:VAL:HG11 | 1:AE:54:VAL:HG11 | 2.00 | 0.43 |
| 1:AE:31:LYS:O | 1:AE:87:GLN:NE2 | 2.51 | 0.43 |
| 1:AP:77:TYR:CD1 | 1:AP:77:TYR:N | 2.84 | 0.43 |
| 1:AS:81:ARG:NH2 | 2:AT:281:PHE:O | 2.51 | 0.43 |
| 1:BU:21:VAL:HG11 | 1:BU:54:VAL:HG11 | 2.00 | 0.43 |
| 1:BU:77:TYR:N | 1:BU:77:TYR:CD1 | 2.84 | 0.43 |
| 1:CA:98:ASP:OD1 | 1:CA:98:ASP:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:DS:81:ARG:NH2 | 2:DT:281:PHE:O | 2.51 | 0.43 |
| 1:DX:31:LYS:O | 1:DX:87:GLN:NE2 | 2.51 | 0.43 |
| 2:EI:45:HIS:CE1 | 2:EK:46:ASN:HD21 | 2.36 | 0.43 |
| 2:HH:45:HIS:CE1 | 2:HJ:46:ASN:HD21 | 2.37 | 0.43 |
| 1:JI:31:LYS:O | 1:JI:87:GLN:NE2 | 2.51 | 0.43 |
| 1:JO:77:TYR:CD1 | 1:JO:77:TYR:N | 2.84 | 0.43 |
| 1:JQ:81:ARG:NH2 | 2:JR:281:PHE:O | 2.51 | 0.43 |
| 2:JT:149:GLN:HG2 | 2:JT:178:ALA:HB3 | 2.00 | 0.43 |
| 1:JZ:77:TYR:N | 1:JZ:77:TYR:CD1 | 2.84 | 0.43 |
| 1:LD:31:LYS:O | 1:LD:87:GLN:NE2 | 2.51 | 0.43 |
| 2:YL:149:GLN:HG2 | 2:YL:178:ALA:HB3 | 2.00 | 0.43 |
| 1:YM:31:LYS:O | 1:YM:87:GLN:NE2 | 2.51 | 0.43 |
| 2:BH:45:HIS:CE1 | 2:BJ:46:ASN:HD21 | 2.36 | 0.43 |
| 1:DE:21:VAL:HG11 | 1:DE:54:VAL:HG11 | 2.00 | 0.43 |
| 1:DQ:21:VAL:HG11 | 1:DQ:54:VAL:HG11 | 2.00 | 0.43 |
| 1:FP:81:ARG:NH2 | 2:FQ:281:PHE:O | 2.51 | 0.43 |
| 1:HP:81:ARG:NH2 | 2:HQ:281:PHE:O | 2.51 | 0.43 |
| 1:IK:77:TYR:N | 1:IK:77:TYR:CD1 | 2.84 | 0.43 |
| 2:JH:45:HIS:CE1 | 2:JJ:46:ASN:HD21 | 2.37 | 0.43 |
| 2:JY:149:GLN:HG2 | 2:JY:178:ALA:HB3 | 2.00 | 0.43 |
| 2:LO:45:HIS:CE1 | 2:LQ:46:ASN:HD21 | 2.37 | 0.43 |
| 2:BZ:9:LEU:HD11 | 2:CB:71:VAL:HG21 | 1.99 | 0.43 |
| 2:BZ:149:GLN:HG2 | 2:BZ:178:ALA:HB3 | 2.00 | 0.43 |
| 2:DD:45:HIS:CE1 | 2:DF:46:ASN:HD21 | 2.37 | 0.43 |
| 1:DG:81:ARG:NH2 | 2:DH:281:PHE:O | 2.51 | 0.43 |
| 1:EJ:21:VAL:HG11 | 1:EJ:54:VAL:HG11 | 2.01 | 0.43 |
| 2:FS:45:HIS:CE1 | 2:FU:46:ASN:HD21 | 2.37 | 0.43 |
| 2:ZH:45:HIS:CE1 | 2:ZJ:46:ASN:HD21 | 2.36 | 0.43 |
| 2:HY:45:HIS:CE1 | 2:IA:46:ASN:HD21 | 2.36 | 0.43 |
| 1:IM:81:ARG:NH2 | 2:IN:281:PHE:O | 2.51 | 0.43 |
| 1:JV:81:ARG:NH2 | 2:JW:281:PHE:O | 2.51 | 0.43 |
| 2:KK:45:HIS:CE1 | 2:KM:46:ASN:HD21 | 2.36 | 0.43 |
| 1:AK:21:VAL:HG11 | 1:AK:54:VAL:HG11 | 2.00 | 0.42 |
| 1:BQ:81:ARG:NH2 | 2:BR:281:PHE:O | 2.51 | 0.42 |
| 2:BZ:45:HIS:CE1 | 2:CB:46:ASN:HD21 | 2.37 | 0.42 |
| 2:DD:149:GLN:HG2 | 2:DD:178:ALA:HB3 | 2.00 | 0.42 |
| 1:DE:77:TYR:N | 1:DE:77:TYR:CD1 | 2.84 | 0.42 |
| 1:ED:21:VAL:HG11 | 1:ED:54:VAL:HG11 | 2.00 | 0.42 |
| 2:EU:45:HIS:CE1 | 2:EW:46:ASN:HD21 | 2.37 | 0.42 |
| 2:FG:149:GLN:HG2 | 2:FG:178:ALA:HB3 | 2.00 | 0.42 |
| 1:GT:81:ARG:NH2 | 2:GU:281:PHE:O | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GX:77:TYR:N | 1:GX:77:TYR:CD1 | 2.84 | 0.42 |
| 2:HS:149:GLN:HG2 | 2:HS:178:ALA:HB3 | 2.00 | 0.42 |
| 1:HT:77:TYR:N | 1:HT:77:TYR:CD1 | 2.84 | 0.42 |
| 1:HZ:21:VAL:HG11 | 1:HZ:54:VAL:HG11 | 2.00 | 0.42 |
| 2:IP:149:GLN:HG2 | 2:IP:178:ALA:HB3 | 2.00 | 0.42 |
| 2:JB:149:GLN:HG2 | 2:JB:178:ALA:HB3 | 2.00 | 0.42 |
| 1:JO:21:VAL:HG11 | 1:JO:54:VAL:HG11 | 2.00 | 0.42 |
| 1:LD:21:VAL:HG11 | 1:LD:54:VAL:HG11 | 2.00 | 0.42 |
| 2:ZT:45:HIS:CE1 | 2:ZV:46:ASN:HD21 | 2.37 | 0.42 |
| 2:AJ:45:HIS:CE1 | 2:AL:46:ASN:HD21 | 2.37 | 0.42 |
| 1:AK:31:LYS:O | 1:AK:87:GLN:NE2 | 2.51 | 0.42 |
| 2:BN:149:GLN:HG2 | 2:BN:178:ALA:HB3 | 2.00 | 0.42 |
| 1:BU:31:LYS:O | 1:BU:87:GLN:NE2 | 2.51 | 0.42 |
| 1:BW:81:ARG:NH2 | 2:BX:281:PHE:O | 2.51 | 0.42 |
| 1:CA:21:VAL:HG11 | 1:CA:54:VAL:HG11 | 2.00 | 0.42 |
| 2:CF:45:HIS:CE1 | 2:CH:46:ASN:HD21 | 2.36 | 0.42 |
| 1:CM:21:VAL:HG11 | 1:CM:54:VAL:HG11 | 2.00 | 0.42 |
| 2:DW:149:GLN:HG2 | 2:DW:178:ALA:HB3 | 2.00 | 0.42 |
| 2:EE:160:ASP:OD1 | 2:EE:168:LYS:NZ | 2.45 | 0.42 |
| 1:FJ:81:ARG:NH2 | 2:FK:281:PHE:O | 2.51 | 0.42 |
| 1:FT:21:VAL:HG11 | 1:FT:54:VAL:HG11 | 2.00 | 0.42 |
| 2:FY:149:GLN:HG2 | 2:FY:178:ALA:HB3 | 2.00 | 0.42 |
| 2:IT:133:ILE:HG21 | 2:IT:181:ILE:HD13 | 2.02 | 0.42 |
| 1:KR:98:ASP:OD1 | 1:KR:98:ASP:N | 2.52 | 0.42 |
| 1:LR:81:ARG:NH2 | 2:LS:281:PHE:O | 2.51 | 0.42 |
| 2:ZR:133:ILE:HG21 | 2:ZR:181:ILE:HD13 | 2.02 | 0.42 |
| 2:YP:133:ILE:HG21 | 2:YP:181:ILE:HD13 | 2.02 | 0.42 |
| 2:YX:45:HIS:CE1 | 2:YZ:46:ASN:HD21 | 2.37 | 0.42 |
| 2:AT:133:ILE:HG21 | 2:AT:181:ILE:HD13 | 2.02 | 0.42 |
| 1:BO:21:VAL:HG11 | 1:BO:54:VAL:HG11 | 2.00 | 0.42 |
| 2:BT:149:GLN:HG2 | 2:BT:178:ALA:HB3 | 2.00 | 0.42 |
| 1:ZE:81:ARG:NH2 | 2:ZF:281:PHE:O | 2.51 | 0.42 |
| 2:FA:45:HIS:CE1 | 2:FC:46:ASN:HD21 | 2.37 | 0.42 |
| 2:FA:149:GLN:HG2 | 2:FA:178:ALA:HB3 | 2.00 | 0.42 |
| 2:FM:45:HIS:CE1 | 2:FO:46:ASN:HD21 | 2.36 | 0.42 |
| 2:FQ:133:ILE:HG21 | 2:FQ:181:ILE:HD13 | 2.01 | 0.42 |
| 2:FY:45:HIS:CE1 | 2:GA:46:ASN:HD21 | 2.37 | 0.42 |
| 2:GI:133:ILE:HG21 | 2:GI:181:ILE:HD13 | 2.02 | 0.42 |
| 2:GK:149:GLN:HG2 | 2:GK:178:ALA:HB3 | 2.00 | 0.42 |
| 2:GO:133:ILE:HG21 | 2:GO:181:ILE:HD13 | 2.02 | 0.42 |
| 2:HW:133:ILE:HG21 | 2:HW:181:ILE:HD13 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:IQ:21:VAL:HG11 | 1:IQ:54:VAL:HG11 | 2.00 | 0.42 |
| 2:IV:45:HIS:CE1 | 2:IX:46:ASN:HD21 | 2.36 | 0.42 |
| 1:JC:77:TYR:N | 1:JC:77:TYR:CD1 | 2.84 | 0.42 |
| 2:KW:149:GLN:HG2 | 2:KW:178:ALA:HB3 | 2.00 | 0.42 |
| 1:LD:98:ASP:OD1 | 1:LD:98:ASP:N | 2.52 | 0.42 |
| 1:AP:21:VAL:HG11 | 1:AP:54:VAL:HG11 | 2.00 | 0.42 |
| 2:BB:45:HIS:CE1 | 2:BD:46:ASN:HD21 | 2.37 | 0.42 |
| 2:BD:160:ASP:OD1 | 2:BD:168:LYS:NZ | 2.45 | 0.42 |
| 2:CX:45:HIS:CE1 | 2:CZ:46:ASN:HD21 | 2.36 | 0.42 |
| 1:CY:31:LYS:O | 1:CY:87:GLN:NE2 | 2.51 | 0.42 |
| 2:DN:133:ILE:HG21 | 2:DN:181:ILE:HD13 | 2.02 | 0.42 |
| 2:DP:45:HIS:CE1 | 2:DR:46:ASN:HD21 | 2.36 | 0.42 |
| 1:DX:21:VAL:HG11 | 1:DX:54:VAL:HG11 | 2.00 | 0.42 |
| 2:ES:133:ILE:HG21 | 2:ES:181:ILE:HD13 | 2.02 | 0.42 |
| 2:EU:149:GLN:HG2 | 2:EU:178:ALA:HB3 | 2.00 | 0.42 |
| 2:EY:160:ASP:OD1 | 2:EY:168:LYS:NZ | 2.35 | 0.42 |
| 2:GC:133:ILE:HG21 | 2:GC:181:ILE:HD13 | 2.02 | 0.42 |
| 2:GK:45:HIS:CE1 | 2:GM:46:ASN:HD21 | 2.37 | 0.42 |
| 2:IB:133:ILE:HG21 | 2:IB:181:ILE:HD13 | 2.02 | 0.42 |
| 1:JI:21:VAL:HG11 | 1:JI:54:VAL:HG11 | 2.00 | 0.42 |
| 2:JR:133:ILE:HG21 | 2:JR:181:ILE:HD13 | 2.02 | 0.42 |
| 2:JY:45:HIS:CE1 | 2:KA:46:ASN:HD21 | 2.37 | 0.42 |
| 2:LG:133:ILE:HG21 | 2:LG:181:ILE:HD13 | 2.02 | 0.42 |
| 2:BF:92:PRO:HB2 | 2:BF:144:LEU:HD13 | 2.02 | 0.42 |
| 2:BR:133:ILE:HG21 | 2:BR:181:ILE:HD13 | 2.02 | 0.42 |
| 1:BW:11:ALA:HB1 | 1:BW:43:VAL:O | 2.20 | 0.42 |
| 1:CA:77:TYR:N | 1:CA:77:TYR:CD1 | 2.84 | 0.42 |
| 2:CP:92:PRO:HB2 | 2:CP:144:LEU:HD13 | 2.02 | 0.42 |
| 2:DB:133:ILE:HG21 | 2:DB:181:ILE:HD13 | 2.02 | 0.42 |
| 2:DH:133:ILE:HG21 | 2:DH:181:ILE:HD13 | 2.02 | 0.42 |
| 1:FV:11:ALA:HB1 | 1:FV:43:VAL:O | 2.20 | 0.42 |
| 1:GF:21:VAL:HG11 | 1:GF:54:VAL:HG11 | 2.00 | 0.42 |
| 2:HC:149:GLN:HG2 | 2:HC:178:ALA:HB3 | 2.00 | 0.42 |
| 1:HI:21:VAL:HG11 | 1:HI:54:VAL:HG11 | 2.00 | 0.42 |
| 2:IJ:149:GLN:HG2 | 2:IJ:178:ALA:HB3 | 2.00 | 0.42 |
| 2:ZL:133:ILE:HG21 | 2:ZL:181:ILE:HD13 | 2.02 | 0.42 |
| 2:KE:45:HIS:CE1 | 2:KG:46:ASN:HD21 | 2.36 | 0.42 |
| 1:KL:21:VAL:HG11 | 1:KL:54:VAL:HG11 | 2.00 | 0.42 |
| 2:KU:133:ILE:HG21 | 2:KU:181:ILE:HD13 | 2.02 | 0.42 |
| 1:ZQ:81:ARG:NH2 | 2:ZR:281:PHE:O | 2.51 | 0.42 |
| 2:AB:133:ILE:HG21 | 2:AB:181:ILE:HD13 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AO:46:ASN:HD21 | 2:AQ:45:HIS:CE1 | 2.37 | 0.42 |
| 2:AQ:149:GLN:HG2 | 2:AQ:178:ALA:HB3 | 2.00 | 0.42 |
| 2:BL:92:PRO:HB2 | 2:BL:144:LEU:HD13 | 2.02 | 0.42 |
| 2:BN:45:HIS:CE1 | 2:BP:46:ASN:HD21 | 2.37 | 0.42 |
| 1:ZE:11:ALA:HB1 | 1:ZE:43:VAL:O | 2.20 | 0.42 |
| 1:DK:77:TYR:N | 1:DK:77:TYR:CD1 | 2.84 | 0.42 |
| 2:FW:133:ILE:HG21 | 2:FW:181:ILE:HD13 | 2.01 | 0.42 |
| 2:GU:133:ILE:HG21 | 2:GU:181:ILE:HD13 | 2.02 | 0.42 |
| 2:GW:149:GLN:HG2 | 2:GW:178:ALA:HB3 | 2.00 | 0.42 |
| 2:HM:45:HIS:CE1 | 2:HO:46:ASN:HD21 | 2.37 | 0.42 |
| 1:HN:77:TYR:N | 1:HN:77:TYR:CD1 | 2.84 | 0.42 |
| 2:HO:160:ASP:OD1 | 2:HO:168:LYS:NZ | 2.45 | 0.42 |
| 1:IH:11:ALA:HB1 | 1:IH:43:VAL:O | 2.20 | 0.42 |
| 1:IS:11:ALA:HB1 | 1:IS:43:VAL:O | 2.20 | 0.42 |
| 2:IT:160:ASP:OD1 | 2:IT:168:LYS:NZ | 2.36 | 0.42 |
| 1:IW:21:VAL:HG11 | 1:IW:54:VAL:HG11 | 2.00 | 0.42 |
| 1:ZK:11:ALA:HB1 | 1:ZK:43:VAL:O | 2.20 | 0.42 |
| 2:JL:133:ILE:HG21 | 2:JL:181:ILE:HD13 | 2.02 | 0.42 |
| 2:JN:45:HIS:CE1 | 2:JP:46:ASN:HD21 | 2.37 | 0.42 |
| 2:KC:92:PRO:HB2 | 2:KC:144:LEU:HD13 | 2.02 | 0.42 |
| 1:KF:77:TYR:N | 1:KF:77:TYR:CD1 | 2.84 | 0.42 |
| 2:KQ:45:HIS:CE1 | 2:KS:46:ASN:HD21 | 2.36 | 0.42 |
| 2:LO:149:GLN:HG2 | 2:LO:178:ALA:HB3 | 2.00 | 0.42 |
| 1:YC:11:ALA:HB1 | 1:YC:43:VAL:O | 2.20 | 0.42 |
| 2:YD:133:ILE:HG21 | 2:YD:181:ILE:HD13 | 2.02 | 0.42 |
| 2:AD:45:HIS:CE1 | 2:AF:46:ASN:HD21 | 2.37 | 0.42 |
| 1:AG:81:ARG:NH2 | 2:AH:281:PHE:O | 2.51 | 0.42 |
| 2:AH:133:ILE:HG21 | 2:AH:181:ILE:HD13 | 2.02 | 0.42 |
| 2:AJ:149:GLN:HG2 | 2:AJ:178:ALA:HB3 | 2.00 | 0.42 |
| 2:AN:133:ILE:HG21 | 2:AN:181:ILE:HD13 | 2.02 | 0.42 |
| 2:AT:92:PRO:HB2 | 2:AT:144:LEU:HD13 | 2.02 | 0.42 |
| 1:BQ:11:ALA:HB1 | 1:BQ:43:VAL:O | 2.20 | 0.42 |
| 2:CD:92:PRO:HB2 | 2:CD:144:LEU:HD13 | 2.02 | 0.42 |
| 2:CD:133:ILE:HG21 | 2:CD:181:ILE:HD13 | 2.02 | 0.42 |
| 1:CI:81:ARG:NH2 | 2:CJ:281:PHE:O | 2.51 | 0.42 |
| 2:CL:45:HIS:CE1 | 2:CN:46:ASN:HD21 | 2.36 | 0.42 |
| 1:DM:11:ALA:HB1 | 1:DM:43:VAL:O | 2.20 | 0.42 |
| 1:EX:11:ALA:HB1 | 1:EX:43:VAL:O | 2.20 | 0.42 |
| 2:EY:133:ILE:HG21 | 2:EY:181:ILE:HD13 | 2.02 | 0.42 |
| 2:FK:133:ILE:HG21 | 2:FK:181:ILE:HD13 | 2.02 | 0.42 |
| 1:GH:11:ALA:HB1 | 1:GH:43:VAL:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GT:11:ALA:HB1 | 1:GT:43:VAL:O | 2.20 | 0.42 |
| 2:HK:133:ILE:HG21 | 2:HK:181:ILE:HD13 | 2.02 | 0.42 |
| 1:HL:33:ALA:N | 1:HL:34:PRO:CD | 2.83 | 0.42 |
| 2:HW:92:PRO:HB2 | 2:HW:144:LEU:HD13 | 2.02 | 0.42 |
| 2:ID:45:HIS:CE1 | 2:IF:46:ASN:HD21 | 2.37 | 0.42 |
| 2:IN:133:ILE:HG21 | 2:IN:181:ILE:HD13 | 2.02 | 0.42 |
| 2:JT:45:HIS:CE1 | 2:JU:46:ASN:HD21 | 2.37 | 0.42 |
| 2:JW:133:ILE:HG21 | 2:JW:181:ILE:HD13 | 2.02 | 0.42 |
| 2:KO:133:ILE:HG21 | 2:KO:181:ILE:HD13 | 2.02 | 0.42 |
| 2:LS:133:ILE:HG21 | 2:LS:181:ILE:HD13 | 2.02 | 0.42 |
| 2:ZN:149:GLN:HG2 | 2:ZN:178:ALA:HB3 | 2.00 | 0.42 |
| 1:YA:21:VAL:HG11 | 1:YA:54:VAL:HG11 | 2.01 | 0.42 |
| 2:YD:218:ASP:OD1 | 2:YD:219:SER:N | 2.53 | 0.42 |
| 1:AA:11:ALA:HB1 | 1:AA:43:VAL:O | 2.20 | 0.42 |
| 1:AI:33:ALA:N | 1:AI:34:PRO:CD | 2.83 | 0.42 |
| 1:BS:33:ALA:N | 1:BS:34:PRO:CD | 2.83 | 0.42 |
| 1:DA:11:ALA:HB1 | 1:DA:43:VAL:O | 2.20 | 0.42 |
| 1:EV:77:TYR:N | 1:EV:77:TYR:CD1 | 2.84 | 0.42 |
| 2:FE:92:PRO:HB2 | 2:FE:144:LEU:HD13 | 2.02 | 0.42 |
| 2:GI:92:PRO:HB2 | 2:GI:144:LEU:HD13 | 2.02 | 0.42 |
| 1:GP:33:ALA:N | 1:GP:34:PRO:CD | 2.83 | 0.42 |
| 2:HA:133:ILE:HG21 | 2:HA:181:ILE:HD13 | 2.02 | 0.42 |
| 1:WA:11:ALA:HB1 | 1:WA:43:VAL:O | 2.20 | 0.42 |
| 1:WC:11:ALA:HB1 | 1:WC:43:VAL:O | 2.20 | 0.42 |
| 2:IG:133:ILE:HG21 | 2:IG:181:ILE:HD13 | 2.01 | 0.42 |
| 1:IQ:77:TYR:N | 1:IQ:77:TYR:CD1 | 2.84 | 0.42 |
| 1:JX:33:ALA:N | 1:JX:34:PRO:CD | 2.83 | 0.42 |
| 2:KC:218:ASP:OD1 | 2:KC:219:SER:N | 2.53 | 0.42 |
| 2:KI:133:ILE:HG21 | 2:KI:181:ILE:HD13 | 2.02 | 0.42 |
| 2:LG:92:PRO:HB2 | 2:LG:144:LEU:HD13 | 2.02 | 0.42 |
| 1:LH:33:ALA:N | 1:LH:34:PRO:CD | 2.83 | 0.42 |
| 1:ZW:11:ALA:HB1 | 1:ZW:43:VAL:O | 2.20 | 0.42 |
| 2:YP:92:PRO:HB2 | 2:YP:144:LEU:HD13 | 2.02 | 0.42 |
| 2:AB:92:PRO:HB2 | 2:AB:144:LEU:HD13 | 2.02 | 0.42 |
| 1:AR:69:HIS:O | 1:AR:70:ILE:C | 2.63 | 0.42 |
| 1:AY:11:ALA:HB1 | 1:AY:43:VAL:O | 2.20 | 0.42 |
| 1:BK:81:ARG:NH2 | 2:BL:281:PHE:O | 2.51 | 0.42 |
| 1:CE:33:ALA:N | 1:CE:34:PRO:CD | 2.83 | 0.42 |
| 2:CV:133:ILE:HG21 | 2:CV:181:ILE:HD13 | 2.02 | 0.42 |
| 1:DG:11:ALA:HB1 | 1:DG:43:VAL:O | 2.20 | 0.42 |
| 1:EH:33:ALA:N | 1:EH:34:PRO:CD | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EV:98:ASP:OD1 | 1:EV:98:ASP:N | 2.52 | 0.42 |
| 2:EY:218:ASP:OD1 | 2:EY:219:SER:N | 2.53 | 0.42 |
| 1:EZ:33:ALA:N | 1:EZ:34:PRO:CD | 2.83 | 0.42 |
| 1:FP:11:ALA:HB1 | 1:FP:43:VAL:O | 2.20 | 0.42 |
| 1:HD:77:TYR:N | 1:HD:77:TYR:CD1 | 2.84 | 0.42 |
| 1:HN:21:VAL:HG11 | 1:HN:54:VAL:HG11 | 2.00 | 0.42 |
| 2:HY:149:GLN:HG2 | 2:HY:178:ALA:HB3 | 2.00 | 0.42 |
| 2:IG:218:ASP:OD1 | 2:IG:219:SER:N | 2.53 | 0.42 |
| 2:IT:218:ASP:OD1 | 2:IT:219:SER:N | 2.53 | 0.42 |
| 2:JF:218:ASP:OD1 | 2:JF:219:SER:N | 2.53 | 0.42 |
| 2:JL:218:ASP:OD1 | 2:JL:219:SER:N | 2.53 | 0.42 |
| 1:JS:33:ALA:N | 1:JS:34:PRO:CD | 2.83 | 0.42 |
| 1:JV:11:ALA:HB1 | 1:JV:43:VAL:O | 2.20 | 0.42 |
| 1:KN:11:ALA:HB1 | 1:KN:43:VAL:O | 2.20 | 0.42 |
| 2:KW:45:HIS:CE1 | 2:KY:46:ASN:HD21 | 2.37 | 0.42 |
| 1:KZ:11:ALA:HB1 | 1:KZ:43:VAL:O | 2.20 | 0.42 |
| 2:ZR:92:PRO:HB2 | 2:ZR:144:LEU:HD13 | 2.02 | 0.42 |
| 2:YJ:218:ASP:OD1 | 2:YJ:219:SER:N | 2.53 | 0.42 |
| 2:YP:218:ASP:OD1 | 2:YP:219:SER:N | 2.53 | 0.42 |
| 1:YW:33:ALA:N | 1:YW:34:PRO:CD | 2.83 | 0.42 |
| 1:YW:69:HIS:O | 1:YW:70:ILE:C | 2.63 | 0.42 |
| 2:AL:6:LYS:NZ | 2:AL:10:GLU:OE2 | 2.45 | 0.42 |
| 2:AN:218:ASP:OD1 | 2:AN:219:SER:N | 2.53 | 0.42 |
| 1:BI:98:ASP:OD1 | 1:BI:98:ASP:N | 2.52 | 0.42 |
| 2:CD:218:ASP:OD1 | 2:CD:219:SER:N | 2.53 | 0.42 |
| 1:CK:33:ALA:N | 1:CK:34:PRO:CD | 2.83 | 0.42 |
| 1:DC:33:ALA:N | 1:DC:34:PRO:CD | 2.83 | 0.42 |
| 2:DH:92:PRO:HB2 | 2:DH:144:LEU:HD13 | 2.02 | 0.42 |
| 2:EC:149:GLN:HG2 | 2:EC:178:ALA:HB3 | 2.00 | 0.42 |
| 2:FE:218:ASP:OD1 | 2:FE:219:SER:N | 2.53 | 0.42 |
| 2:FK:92:PRO:HB2 | 2:FK:144:LEU:HD13 | 2.02 | 0.42 |
| 2:FQ:92:PRO:HB2 | 2:FQ:144:LEU:HD13 | 2.02 | 0.42 |
| 1:GD:33:ALA:N | 1:GD:34:PRO:CD | 2.83 | 0.42 |
| 1:GP:69:HIS:O | 1:GP:70:ILE:C | 2.63 | 0.42 |
| 1:HR:33:ALA:N | 1:HR:34:PRO:CD | 2.83 | 0.42 |
| 1:HX:33:ALA:N | 1:HX:34:PRO:CD | 2.83 | 0.42 |
| 2:IB:218:ASP:OD1 | 2:IB:219:SER:N | 2.53 | 0.42 |
| 1:JK:11:ALA:HB1 | 1:JK:43:VAL:O | 2.20 | 0.42 |
| 1:JX:69:HIS:O | 1:JX:70:ILE:C | 2.63 | 0.42 |
| 2:KC:133:ILE:HG21 | 2:KC:181:ILE:HD13 | 2.02 | 0.42 |
| 1:KT:11:ALA:HB1 | 1:KT:43:VAL:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZR:218:ASP:OD1 | 2:ZR:219:SER:N | 2.53 | 0.42 |
| 2:ZX:160:ASP:OD1 | 2:ZX:168:LYS:NZ | 2.36 | 0.42 |
| 2:YJ:92:PRO:HB2 | 2:YJ:144:LEU:HD13 | 2.02 | 0.41 |
| 2:AJ:96:LEU:O | 2:AJ:97:GLU:C | 2.63 | 0.41 |
| 1:AM:11:ALA:HB1 | 1:AM:43:VAL:O | 2.20 | 0.41 |
| 1:BG:33:ALA:N | 1:BG:34:PRO:CD | 2.83 | 0.41 |
| 1:BK:11:ALA:HB1 | 1:BK:43:VAL:O | 2.20 | 0.41 |
| 2:BR:92:PRO:HB2 | 2:BR:144:LEU:HD13 | 2.02 | 0.41 |
| 2:BX:133:ILE:HG21 | 2:BX:181:ILE:HD13 | 2.02 | 0.41 |
| 1:BY:69:HIS:O | 1:BY:70:ILE:C | 2.63 | 0.41 |
| 2:CN:160:ASP:OD1 | 2:CN:168:LYS:NZ | 2.45 | 0.41 |
| 2:CP:218:ASP:OD1 | 2:CP:219:SER:N | 2.53 | 0.41 |
| 2:CV:218:ASP:OD1 | 2:CV:219:SER:N | 2.53 | 0.41 |
| 2:EG:133:ILE:HG21 | 2:EG:181:ILE:HD13 | 2.02 | 0.41 |
| 1:EP:21:VAL:HG11 | 1:EP:54:VAL:HG11 | 2.00 | 0.41 |
| 1:ZG:33:ALA:N | 1:ZG:34:PRO:CD | 2.83 | 0.41 |
| 1:ZG:69:HIS:O | 1:ZG:70:ILE:C | 2.63 | 0.41 |
| 1:FN:77:TYR:N | 1:FN:77:TYR:CD1 | 2.84 | 0.41 |
| 1:FX:69:HIS:O | 1:FX:70:ILE:C | 2.63 | 0.41 |
| 1:HB:33:ALA:N | 1:HB:34:PRO:CD | 2.83 | 0.41 |
| 1:HP:11:ALA:HB1 | 1:HP:43:VAL:O | 2.20 | 0.41 |
| 1:IE:21:VAL:HG11 | 1:IE:54:VAL:HG11 | 2.00 | 0.41 |
| 1:JG:33:ALA:N | 1:JG:34:PRO:CD | 2.83 | 0.41 |
| 2:KE:149:GLN:HG2 | 2:KE:178:ALA:HB3 | 2.00 | 0.41 |
| 2:KO:218:ASP:OD1 | 2:KO:219:SER:N | 2.53 | 0.41 |
| 1:KX:21:VAL:HG11 | 1:KX:54:VAL:HG11 | 2.00 | 0.41 |
| 2:LA:133:ILE:HG21 | 2:LA:181:ILE:HD13 | 2.02 | 0.41 |
| 1:YK:33:ALA:N | 1:YK:34:PRO:CD | 2.83 | 0.41 |
| 1:YK:69:HIS:O | 1:YK:70:ILE:C | 2.63 | 0.41 |
| 1:YU:11:ALA:HB1 | 1:YU:43:VAL:O | 2.20 | 0.41 |
| 1:AC:33:ALA:N | 1:AC:34:PRO:CD | 2.83 | 0.41 |
| 1:AG:11:ALA:HB1 | 1:AG:43:VAL:O | 2.20 | 0.41 |
| 1:AU:33:ALA:N | 1:AU:34:PRO:CD | 2.83 | 0.41 |
| 2:BL:133:ILE:HG21 | 2:BL:181:ILE:HD13 | 2.02 | 0.41 |
| 2:BR:218:ASP:OD1 | 2:BR:219:SER:N | 2.53 | 0.41 |
| 1:BS:69:HIS:O | 1:BS:70:ILE:C | 2.63 | 0.41 |
| 1:CK:69:HIS:O | 1:CK:70:ILE:C | 2.63 | 0.41 |
| 2:CR:149:GLN:HG2 | 2:CR:178:ALA:HB3 | 2.00 | 0.41 |
| 1:CS:77:TYR:N | 1:CS:77:TYR:CD1 | 2.84 | 0.41 |
| 2:DN:218:ASP:OD1 | 2:DN:219:SER:N | 2.53 | 0.41 |
| 2:ZF:92:PRO:HB2 | 2:ZF:144:LEU:HD13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EB:33:ALA:N | 1:EB:34:PRO:CD | 2.83 | 0.41 |
| 2:EC:45:HIS:CE1 | 2:EE:46:ASN:HD21 | 2.36 | 0.41 |
| 1:FJ:11:ALA:HB1 | 1:FJ:43:VAL:O | 2.20 | 0.41 |
| 1:GD:69:HIS:O | 1:GD:70:ILE:C | 2.63 | 0.41 |
| 1:GL:21:VAL:HG11 | 1:GL:54:VAL:HG11 | 2.00 | 0.41 |
| 1:GN:81:ARG:NH2 | 2:GO:281:PHE:O | 2.51 | 0.41 |
| 2:GU:92:PRO:HB2 | 2:GU:144:LEU:HD13 | 2.02 | 0.41 |
| 1:GZ:11:ALA:HB1 | 1:GZ:43:VAL:O | 2.20 | 0.41 |
| 1:WB:11:ALA:HB1 | 1:WB:43:VAL:O | 2.20 | 0.41 |
| 1:HG:33:ALA:N | 1:HG:34:PRO:CD | 2.83 | 0.41 |
| 2:HK:92:PRO:HB2 | 2:HK:144:LEU:HD13 | 2.02 | 0.41 |
| 2:HU:160:ASP:OD1 | 2:HU:168:LYS:NZ | 2.45 | 0.41 |
| 1:IO:33:ALA:N | 1:IO:34:PRO:CD | 2.83 | 0.41 |
| 2:IZ:218:ASP:OD1 | 2:IZ:219:SER:N | 2.53 | 0.41 |
| 2:KA:160:ASP:OD1 | 2:KA:168:LYS:NZ | 2.45 | 0.41 |
| 2:KU:92:PRO:HB2 | 2:KU:144:LEU:HD13 | 2.02 | 0.41 |
| 1:ZM:33:ALA:N | 1:ZM:34:PRO:CD | 2.83 | 0.41 |
| 1:LL:11:ALA:HB1 | 1:LL:43:VAL:O | 2.20 | 0.41 |
| 1:ZQ:11:ALA:HB1 | 1:ZQ:43:VAL:O | 2.20 | 0.41 |
| 1:YG:21:VAL:HG11 | 1:YG:54:VAL:HG11 | 2.00 | 0.41 |
| 1:YU:81:ARG:NH2 | 2:YV:281:PHE:O | 2.51 | 0.41 |
| 1:AS:11:ALA:HB1 | 1:AS:43:VAL:O | 2.20 | 0.41 |
| 1:BA:33:ALA:N | 1:BA:34:PRO:CD | 2.83 | 0.41 |
| 2:BV:6:LYS:NZ | 2:BV:10:GLU:OE2 | 2.45 | 0.41 |
| 2:EA:133:ILE:HG21 | 2:EA:181:ILE:HD13 | 2.02 | 0.41 |
| 2:EA:218:ASP:OD1 | 2:EA:219:SER:N | 2.53 | 0.41 |
| 1:ER:11:ALA:HB1 | 1:ER:43:VAL:O | 2.20 | 0.41 |
| 1:ER:81:ARG:NH2 | 2:ES:281:PHE:O | 2.51 | 0.41 |
| 2:FM:96:LEU:O | 2:FM:97:GLU:C | 2.63 | 0.41 |
| 1:FR:33:ALA:N | 1:FR:34:PRO:CD | 2.83 | 0.41 |
| 1:FX:33:ALA:N | 1:FX:34:PRO:CD | 2.83 | 0.41 |
| 1:GB:11:ALA:HB1 | 1:GB:43:VAL:O | 2.20 | 0.41 |
| 1:GN:11:ALA:HB1 | 1:GN:43:VAL:O | 2.20 | 0.41 |
| 2:HF:92:PRO:HB2 | 2:HF:144:LEU:HD13 | 2.02 | 0.41 |
| 1:HG:69:HIS:O | 1:HG:70:ILE:C | 2.63 | 0.41 |
| 1:HV:11:ALA:HB1 | 1:HV:43:VAL:O | 2.20 | 0.41 |
| 1:IM:11:ALA:HB1 | 1:IM:43:VAL:O | 2.20 | 0.41 |
| 1:IU:33:ALA:N | 1:IU:34:PRO:CD | 2.83 | 0.41 |
| 1:JQ:11:ALA:HB1 | 1:JQ:43:VAL:O | 2.20 | 0.41 |
| 2:JW:218:ASP:OD1 | 2:JW:219:SER:N | 2.53 | 0.41 |
| 2:KO:92:PRO:HB2 | 2:KO:144:LEU:HD13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LM:218:ASP:OD1 | 2:LM:219:SER:N | 2.53 | 0.41 |
| 1:LR:11:ALA:HB1 | 1:LR:43:VAL:O | 2.20 | 0.41 |
| 2:ZX:92:PRO:HB2 | 2:ZX:144:LEU:HD13 | 2.02 | 0.41 |
| 1:AK:98:ASP:OD1 | 1:AK:98:ASP:N | 2.52 | 0.41 |
| 1:CW:69:HIS:O | 1:CW:70:ILE:C | 2.63 | 0.41 |
| 2:EA:92:PRO:HB2 | 2:EA:144:LEU:HD13 | 2.02 | 0.41 |
| 2:EG:218:ASP:OD1 | 2:EG:219:SER:N | 2.53 | 0.41 |
| 1:EN:33:ALA:N | 1:EN:34:PRO:CD | 2.83 | 0.41 |
| 2:EO:45:HIS:CE1 | 2:EQ:46:ASN:HD21 | 2.36 | 0.41 |
| 1:ET:33:ALA:N | 1:ET:34:PRO:CD | 2.83 | 0.41 |
| 1:FL:69:HIS:O | 1:FL:70:ILE:C | 2.63 | 0.41 |
| 2:FY:96:LEU:O | 2:FY:97:GLU:C | 2.63 | 0.41 |
| 1:GJ:33:ALA:N | 1:GJ:34:PRO:CD | 2.83 | 0.41 |
| 1:GV:33:ALA:N | 1:GV:34:PRO:CD | 2.83 | 0.41 |
| 2:IJ:96:LEU:O | 2:IJ:97:GLU:C | 2.63 | 0.41 |
| 1:IY:11:ALA:HB1 | 1:IY:43:VAL:O | 2.20 | 0.41 |
| 1:KB:11:ALA:HB1 | 1:KB:43:VAL:O | 2.20 | 0.41 |
| 1:KB:81:ARG:NH2 | 2:KC:281:PHE:O | 2.51 | 0.41 |
| 2:KI:92:PRO:HB2 | 2:KI:144:LEU:HD13 | 2.02 | 0.41 |
| 2:YD:92:PRO:HB2 | 2:YD:144:LEU:HD13 | 2.02 | 0.41 |
| 2:YD:160:ASP:OD1 | 2:YD:168:LYS:NZ | 2.36 | 0.41 |
| 1:YE:69:HIS:O | 1:YE:70:ILE:C | 2.63 | 0.41 |
| 2:AN:92:PRO:HB2 | 2:AN:144:LEU:HD13 | 2.02 | 0.41 |
| 2:BF:133:ILE:HG21 | 2:BF:181:ILE:HD13 | 2.02 | 0.41 |
| 1:BM:33:ALA:N | 1:BM:34:PRO:CD | 2.83 | 0.41 |
| 2:BX:218:ASP:OD1 | 2:BX:219:SER:N | 2.53 | 0.41 |
| 1:CC:81:ARG:NH2 | 2:CD:281:PHE:O | 2.51 | 0.41 |
| 1:CI:11:ALA:HB1 | 1:CI:43:VAL:O | 2.20 | 0.41 |
| 2:CJ:133:ILE:HG21 | 2:CJ:181:ILE:HD13 | 2.02 | 0.41 |
| 2:CN:231:VAL:HG11 | 2:CN:238:MET:HB2 | 2.03 | 0.41 |
| 1:DS:11:ALA:HB1 | 1:DS:43:VAL:O | 2.20 | 0.41 |
| 1:DU:69:HIS:O | 1:DU:70:ILE:C | 2.63 | 0.41 |
| 2:ZF:170:LYS:HG2 | 2:ZF:224:TRP:CH2 | 2.56 | 0.41 |
| 2:ZF:218:ASP:OD1 | 2:ZF:219:SER:N | 2.53 | 0.41 |
| 2:EM:133:ILE:HG21 | 2:EM:181:ILE:HD13 | 2.02 | 0.41 |
| 2:GU:170:LYS:HG2 | 2:GU:224:TRP:CH2 | 2.56 | 0.41 |
| 2:HA:92:PRO:HB2 | 2:HA:144:LEU:HD13 | 2.02 | 0.41 |
| 2:HK:170:LYS:HG2 | 2:HK:224:TRP:CH2 | 2.56 | 0.41 |
| 2:HQ:133:ILE:HG21 | 2:HQ:181:ILE:HD13 | 2.02 | 0.41 |
| 1:IC:33:ALA:N | 1:IC:34:PRO:CD | 2.83 | 0.41 |
| 2:IN:92:PRO:HB2 | 2:IN:144:LEU:HD13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:IZ:92:PRO:HB2 | 2:IZ:144:LEU:HD13 | 2.02 | 0.41 |
| 2:KI:218:ASP:OD1 | 2:KI:219:SER:N | 2.53 | 0.41 |
| 1:KP:33:ALA:N | 1:KP:34:PRO:CD | 2.83 | 0.41 |
| 1:LF:11:ALA:HB1 | 1:LF:43:VAL:O | 2.20 | 0.41 |
| 2:LM:92:PRO:HB2 | 2:LM:144:LEU:HD13 | 2.02 | 0.41 |
| 1:LN:69:HIS:O | 1:LN:70:ILE:C | 2.63 | 0.41 |
| 1:ZS:33:ALA:N | 1:ZS:34:PRO:CD | 2.83 | 0.41 |
| 1:YQ:33:ALA:N | 1:YQ:34:PRO:CD | 2.83 | 0.41 |
| 2:YR:96:LEU:O | 2:YR:97:GLU:C | 2.63 | 0.41 |
| 2:YV:218:ASP:OD1 | 2:YV:219:SER:N | 2.53 | 0.41 |
| 2:AB:218:ASP:OD1 | 2:AB:219:SER:N | 2.53 | 0.41 |
| 2:AF:231:VAL:HG11 | 2:AF:238:MET:HB2 | 2.03 | 0.41 |
| 2:AZ:218:ASP:OD1 | 2:AZ:219:SER:N | 2.53 | 0.41 |
| 2:BD:231:VAL:HG11 | 2:BD:238:MET:HB2 | 2.03 | 0.41 |
| 2:BV:231:VAL:HG11 | 2:BV:238:MET:HB2 | 2.03 | 0.41 |
| 1:CC:11:ALA:HB1 | 1:CC:43:VAL:O | 2.20 | 0.41 |
| 2:CD:170:LYS:HG2 | 2:CD:224:TRP:CH2 | 2.56 | 0.41 |
| 1:CU:11:ALA:HB1 | 1:CU:43:VAL:O | 2.20 | 0.41 |
| 2:CV:170:LYS:HG2 | 2:CV:224:TRP:CH2 | 2.56 | 0.41 |
| 1:DC:69:HIS:O | 1:DC:70:ILE:C | 2.63 | 0.41 |
| 1:DI:69:HIS:O | 1:DI:70:ILE:C | 2.63 | 0.41 |
| 2:DN:170:LYS:HG2 | 2:DN:224:TRP:CH2 | 2.56 | 0.41 |
| 2:EG:170:LYS:HG2 | 2:EG:224:TRP:CH2 | 2.56 | 0.41 |
| 2:ES:92:PRO:HB2 | 2:ES:144:LEU:HD13 | 2.02 | 0.41 |
| 1:EZ:69:HIS:O | 1:EZ:70:ILE:C | 2.63 | 0.41 |
| 2:FO:231:VAL:HG11 | 2:FO:238:MET:HB2 | 2.03 | 0.41 |
| 1:ZI:85:LYS:NZ | 2:ZJ:256:GLU:OE1 | 2.50 | 0.41 |
| 2:HW:218:ASP:OD1 | 2:HW:219:SER:N | 2.53 | 0.41 |
| 2:IL:231:VAL:HG11 | 2:IL:238:MET:HB2 | 2.03 | 0.41 |
| 2:IN:218:ASP:OD1 | 2:IN:219:SER:N | 2.53 | 0.41 |
| 2:IZ:133:ILE:HG21 | 2:IZ:181:ILE:HD13 | 2.02 | 0.41 |
| 1:JA:33:ALA:N | 1:JA:34:PRO:CD | 2.83 | 0.41 |
| 2:JF:92:PRO:HB2 | 2:JF:144:LEU:HD13 | 2.02 | 0.41 |
| 2:JF:133:ILE:HG21 | 2:JF:181:ILE:HD13 | 2.02 | 0.41 |
| 2:JH:149:GLN:HG2 | 2:JH:178:ALA:HB3 | 2.00 | 0.41 |
| 2:JR:92:PRO:HB2 | 2:JR:144:LEU:HD13 | 2.02 | 0.41 |
| 2:LS:92:PRO:HB2 | 2:LS:144:LEU:HD13 | 2.02 | 0.41 |
| 2:ZX:218:ASP:OD1 | 2:ZX:219:SER:N | 2.53 | 0.41 |
| 1:ZY:33:ALA:N | 1:ZY:34:PRO:CD | 2.83 | 0.41 |
| 1:YE:33:ALA:N | 1:YE:34:PRO:CD | 2.83 | 0.41 |
| 1:YI:11:ALA:HB1 | 1:YI:43:VAL:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:YO:11:ALA:HB1 | 1:YO:43:VAL:O | 2.20 | 0.41 |
| 1:AA:81:ARG:NH2 | 2:AB:281:PHE:O | 2.51 | 0.41 |
| 2:AH:92:PRO:HB2 | 2:AH:144:LEU:HD13 | 2.02 | 0.41 |
| 2:AL:231:VAL:HG11 | 2:AL:238:MET:HB2 | 2.03 | 0.41 |
| 1:AM:81:ARG:NH2 | 2:AN:281:PHE:O | 2.51 | 0.41 |
| 2:BF:170:LYS:HG2 | 2:BF:224:TRP:CH2 | 2.56 | 0.41 |
| 2:BL:170:LYS:HG2 | 2:BL:224:TRP:CH2 | 2.56 | 0.41 |
| 1:CY:21:VAL:HG11 | 1:CY:54:VAL:HG11 | 2.01 | 0.41 |
| 2:DW:96:LEU:O | 2:DW:97:GLU:C | 2.63 | 0.41 |
| 2:EG:92:PRO:HB2 | 2:EG:144:LEU:HD13 | 2.02 | 0.41 |
| 1:EJ:77:TYR:CD1 | 1:EJ:77:TYR:N | 2.84 | 0.41 |
| 2:ES:170:LYS:HG2 | 2:ES:224:TRP:CH2 | 2.56 | 0.41 |
| 2:EW:231:VAL:HG11 | 2:EW:238:MET:HB2 | 2.03 | 0.41 |
| 2:FE:133:ILE:HG21 | 2:FE:181:ILE:HD13 | 2.02 | 0.41 |
| 2:GY:231:VAL:HG11 | 2:GY:238:MET:HB2 | 2.03 | 0.41 |
| 2:HM:96:LEU:O | 2:HM:97:GLU:C | 2.63 | 0.41 |
| 2:IA:160:ASP:OD1 | 2:IA:168:LYS:NZ | 2.45 | 0.41 |
| 1:II:33:ALA:N | 1:II:34:PRO:CD | 2.83 | 0.41 |
| 2:IT:170:LYS:HG2 | 2:IT:224:TRP:CH2 | 2.56 | 0.41 |
| 2:IX:160:ASP:OD1 | 2:IX:168:LYS:NZ | 2.45 | 0.41 |
| 1:JA:69:HIS:O | 1:JA:70:ILE:C | 2.63 | 0.41 |
| 2:JD:231:VAL:HG11 | 2:JD:238:MET:HB2 | 2.03 | 0.41 |
| 2:KK:96:LEU:O | 2:KK:97:GLU:C | 2.63 | 0.41 |
| 2:KM:231:VAL:HG11 | 2:KM:238:MET:HB2 | 2.03 | 0.41 |
| 2:LG:218:ASP:OD1 | 2:LG:219:SER:N | 2.53 | 0.41 |
| 2:LS:160:ASP:OD1 | 2:LS:168:LYS:NZ | 2.36 | 0.41 |
| 2:ZX:133:ILE:HG21 | 2:ZX:181:ILE:HD13 | 2.02 | 0.41 |
| 2:ZZ:96:LEU:O | 2:ZZ:97:GLU:C | 2.63 | 0.41 |
| 2:YH:231:VAL:HG11 | 2:YH:238:MET:HB2 | 2.03 | 0.41 |
| 1:YI:81:ARG:NH2 | 2:YJ:281:PHE:O | 2.51 | 0.41 |
| 2:YJ:133:ILE:HG21 | 2:YJ:181:ILE:HD13 | 2.02 | 0.41 |
| 2:YV:92:PRO:HB2 | 2:YV:144:LEU:HD13 | 2.02 | 0.41 |
| 2:AH:218:ASP:OD1 | 2:AH:219:SER:N | 2.53 | 0.41 |
| 2:AZ:92:PRO:HB2 | 2:AZ:144:LEU:HD13 | 2.02 | 0.41 |
| 1:BC:98:ASP:OD1 | 1:BC:98:ASP:N | 2.52 | 0.41 |
| 1:BG:69:HIS:O | 1:BG:70:ILE:C | 2.63 | 0.41 |
| 1:BY:33:ALA:N | 1:BY:34:PRO:CD | 2.83 | 0.41 |
| 2:DB:92:PRO:HB2 | 2:DB:144:LEU:HD13 | 2.02 | 0.41 |
| 2:DH:218:ASP:OD1 | 2:DH:219:SER:N | 2.53 | 0.41 |
| 1:DI:33:ALA:N | 1:DI:34:PRO:CD | 2.83 | 0.41 |
| 2:DT:133:ILE:HG21 | 2:DT:181:ILE:HD13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ZF:133:ILE:HG21 | 2:ZF:181:ILE:HD13 | 2.02 | 0.41 |
| 1:EL:11:ALA:HB1 | 1:EL:43:VAL:O | 2.20 | 0.41 |
| 1:FL:33:ALA:N | 1:FL:34:PRO:CD | 2.83 | 0.41 |
| 2:FW:92:PRO:HB2 | 2:FW:144:LEU:HD13 | 2.02 | 0.41 |
| 2:FW:170:LYS:HG2 | 2:FW:224:TRP:CH2 | 2.56 | 0.41 |
| 1:GL:98:ASP:OD1 | 1:GL:98:ASP:N | 2.52 | 0.41 |
| 2:HF:133:ILE:HG21 | 2:HF:181:ILE:HD13 | 2.02 | 0.41 |
| 2:HQ:218:ASP:OD1 | 2:HQ:219:SER:N | 2.53 | 0.41 |
| 1:HR:69:HIS:O | 1:HR:70:ILE:C | 2.63 | 0.41 |
| 2:IB:281:PHE:O | 1:WC:81:ARG:NH2 | 2.51 | 0.41 |
| 1:IH:98:ASP:OD1 | 1:IH:98:ASP:N | 2.50 | 0.41 |
| 2:IT:92:PRO:HB2 | 2:IT:144:LEU:HD13 | 2.02 | 0.41 |
| 1:IU:69:HIS:O | 1:IU:70:ILE:C | 2.63 | 0.41 |
| 2:ZL:92:PRO:HB2 | 2:ZL:144:LEU:HD13 | 2.02 | 0.41 |
| 2:KI:170:LYS:HG2 | 2:KI:224:TRP:CH2 | 2.56 | 0.41 |
| 2:LA:92:PRO:HB2 | 2:LA:144:LEU:HD13 | 2.02 | 0.41 |
| 1:LB:69:HIS:O | 1:LB:70:ILE:C | 2.63 | 0.41 |
| 1:ZA:69:HIS:O | 1:ZA:70:ILE:C | 2.63 | 0.41 |
| 1:YG:77:TYR:N | 1:YG:77:TYR:CD1 | 2.84 | 0.41 |
| 2:YV:133:ILE:HG21 | 2:YV:181:ILE:HD13 | 2.02 | 0.41 |
| 2:YV:170:LYS:HG2 | 2:YV:224:TRP:CH2 | 2.56 | 0.41 |
| 2:AF:70:ILE:HG23 | 2:AF:74:PHE:CE1 | 2.56 | 0.41 |
| 2:AN:170:LYS:HG2 | 2:AN:224:TRP:CH2 | 2.56 | 0.41 |
| 1:AR:33:ALA:N | 1:AR:34:PRO:CD | 2.83 | 0.41 |
| 2:AT:170:LYS:HG2 | 2:AT:224:TRP:CH2 | 2.56 | 0.41 |
| 2:AT:218:ASP:OD1 | 2:AT:219:SER:N | 2.53 | 0.41 |
| 2:AX:6:LYS:NZ | 2:AX:10:GLU:OE2 | 2.45 | 0.41 |
| 2:AX:231:VAL:HG11 | 2:AX:238:MET:HB2 | 2.03 | 0.41 |
| 1:BE:11:ALA:HB1 | 1:BE:43:VAL:O | 2.20 | 0.41 |
| 2:BJ:160:ASP:OD1 | 2:BJ:168:LYS:NZ | 2.45 | 0.41 |
| 2:BP:160:ASP:OD1 | 2:BP:168:LYS:NZ | 2.45 | 0.41 |
| 2:BP:231:VAL:HG11 | 2:BP:238:MET:HB2 | 2.03 | 0.41 |
| 2:BX:170:LYS:HG2 | 2:BX:224:TRP:CH2 | 2.56 | 0.41 |
| 1:CE:69:HIS:O | 1:CE:70:ILE:C | 2.63 | 0.41 |
| 2:CJ:92:PRO:HB2 | 2:CJ:144:LEU:HD13 | 2.02 | 0.41 |
| 2:CJ:218:ASP:OD1 | 2:CJ:219:SER:N | 2.53 | 0.41 |
| 1:CO:11:ALA:HB1 | 1:CO:43:VAL:O | 2.20 | 0.41 |
| 1:CW:33:ALA:N | 1:CW:34:PRO:CD | 2.83 | 0.41 |
| 2:CZ:70:ILE:HG23 | 2:CZ:74:PHE:CE1 | 2.56 | 0.41 |
| 2:DB:218:ASP:OD1 | 2:DB:219:SER:N | 2.53 | 0.41 |
| 2:DF:231:VAL:HG11 | 2:DF:238:MET:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:DL:70:ILE:HG23 | 2:DL:74:PHE:CE1 | 2.56 | 0.41 |
| 1:DO:33:ALA:N | 1:DO:34:PRO:CD | 2.83 | 0.41 |
| 2:DT:170:LYS:HG2 | 2:DT:224:TRP:CH2 | 2.56 | 0.41 |
| 1:DU:33:ALA:N | 1:DU:34:PRO:CD | 2.83 | 0.41 |
| 2:DY:231:VAL:HG11 | 2:DY:238:MET:HB2 | 2.03 | 0.41 |
| 1:DZ:11:ALA:HB1 | 1:DZ:43:VAL:O | 2.20 | 0.41 |
| 1:EH:69:HIS:O | 1:EH:70:ILE:C | 2.63 | 0.41 |
| 2:EM:92:PRO:HB2 | 2:EM:144:LEU:HD13 | 2.02 | 0.41 |
| 2:EM:170:LYS:HG2 | 2:EM:224:TRP:CH2 | 2.56 | 0.41 |
| 1:EN:69:HIS:O | 1:EN:70:ILE:C | 2.63 | 0.41 |
| 1:FD:11:ALA:HB1 | 1:FD:43:VAL:O | 2.20 | 0.41 |
| 2:FE:170:LYS:HG2 | 2:FE:224:TRP:CH2 | 2.56 | 0.41 |
| 1:FF:33:ALA:N | 1:FF:34:PRO:CD | 2.83 | 0.41 |
| 2:FS:96:LEU:O | 2:FS:97:GLU:C | 2.63 | 0.41 |
| 1:FT:98:ASP:OD1 | 1:FT:98:ASP:N | 2.52 | 0.41 |
| 1:GB:81:ARG:NH2 | 2:GC:281:PHE:O | 2.51 | 0.41 |
| 2:GE:96:LEU:O | 2:GE:97:GLU:C | 2.63 | 0.41 |
| 2:GG:231:VAL:HG11 | 2:GG:238:MET:HB2 | 2.03 | 0.41 |
| 2:GI:170:LYS:HG2 | 2:GI:224:TRP:CH2 | 2.56 | 0.41 |
| 2:GM:70:ILE:HG23 | 2:GM:74:PHE:CE1 | 2.56 | 0.41 |
| 2:GS:160:ASP:OD1 | 2:GS:168:LYS:NZ | 2.45 | 0.41 |
| 2:GS:231:VAL:HG11 | 2:GS:238:MET:HB2 | 2.03 | 0.41 |
| 2:HA:170:LYS:HG2 | 2:HA:224:TRP:CH2 | 2.56 | 0.41 |
| 2:IB:92:PRO:HB2 | 2:IB:144:LEU:HD13 | 2.02 | 0.41 |
| 2:JF:170:LYS:HG2 | 2:JF:224:TRP:CH2 | 2.56 | 0.41 |
| 1:JG:69:HIS:O | 1:JG:70:ILE:C | 2.63 | 0.41 |
| 2:JL:92:PRO:HB2 | 2:JL:144:LEU:HD13 | 2.02 | 0.41 |
| 2:JP:70:ILE:HG23 | 2:JP:74:PHE:CE1 | 2.56 | 0.41 |
| 2:JP:231:VAL:HG11 | 2:JP:238:MET:HB2 | 2.03 | 0.41 |
| 2:JR:218:ASP:OD1 | 2:JR:219:SER:N | 2.53 | 0.41 |
| 2:JU:231:VAL:HG11 | 2:JU:238:MET:HB2 | 2.03 | 0.41 |
| 1:KD:33:ALA:N | 1:KD:34:PRO:CD | 2.83 | 0.41 |
| 1:KH:11:ALA:HB1 | 1:KH:43:VAL:O | 2.20 | 0.41 |
| 1:KL:98:ASP:OD1 | 1:KL:98:ASP:N | 2.52 | 0.41 |
| 1:KV:33:ALA:N | 1:KV:34:PRO:CD | 2.83 | 0.41 |
| 1:ZM:69:HIS:O | 1:ZM:70:ILE:C | 2.63 | 0.41 |
| 1:LH:69:HIS:O | 1:LH:70:ILE:C | 2.63 | 0.41 |
| 2:LM:133:ILE:HG21 | 2:LM:181:ILE:HD13 | 2.02 | 0.41 |
| 2:ZP:231:VAL:HG11 | 2:ZP:238:MET:HB2 | 2.03 | 0.41 |
| 2:YD:170:LYS:HG2 | 2:YD:224:TRP:CH2 | 2.56 | 0.41 |
| 2:YN:70:ILE:HG23 | 2:YN:74:PHE:CE1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:YQ:69:HIS:O | 1:YQ:70:ILE:C | 2.63 | 0.41 |
| 2:AB:170:LYS:HG2 | 2:AB:224:TRP:CH2 | 2.56 | 0.41 |
| 2:YZ:231:VAL:HG11 | 2:YZ:238:MET:HB2 | 2.03 | 0.41 |
| 2:AH:170:LYS:HG2 | 2:AH:224:TRP:CH2 | 2.56 | 0.41 |
| 2:AZ:170:LYS:HG2 | 2:AZ:224:TRP:CH2 | 2.56 | 0.41 |
| 2:BJ:231:VAL:HG11 | 2:BJ:238:MET:HB2 | 2.03 | 0.41 |
| 2:CF:96:LEU:O | 2:CF:97:GLU:C | 2.63 | 0.41 |
| 1:CQ:33:ALA:N | 1:CQ:34:PRO:CD | 2.83 | 0.41 |
| 2:CV:92:PRO:HB2 | 2:CV:144:LEU:HD13 | 2.02 | 0.41 |
| 2:EA:170:LYS:HG2 | 2:EA:224:TRP:CH2 | 2.56 | 0.41 |
| 2:FA:96:LEU:O | 2:FA:97:GLU:C | 2.63 | 0.41 |
| 1:GB:98:ASP:OD1 | 1:GB:98:ASP:N | 2.50 | 0.41 |
| 1:GJ:69:HIS:O | 1:GJ:70:ILE:C | 2.63 | 0.41 |
| 2:HA:218:ASP:OD1 | 2:HA:219:SER:N | 2.53 | 0.41 |
| 2:HF:281:PHE:O | 1:WB:81:ARG:NH2 | 2.51 | 0.41 |
| 2:HH:96:LEU:O | 2:HH:97:GLU:C | 2.63 | 0.41 |
| 2:IF:231:VAL:HG11 | 2:IF:238:MET:HB2 | 2.03 | 0.41 |
| 2:IL:70:ILE:HG23 | 2:IL:74:PHE:CE1 | 2.56 | 0.41 |
| 2:IN:170:LYS:HG2 | 2:IN:224:TRP:CH2 | 2.56 | 0.41 |
| 2:IX:231:VAL:HG11 | 2:IX:238:MET:HB2 | 2.03 | 0.41 |
| 2:JH:96:LEU:O | 2:JH:97:GLU:C | 2.63 | 0.41 |
| 2:JJ:231:VAL:HG11 | 2:JJ:238:MET:HB2 | 2.03 | 0.41 |
| 2:JL:170:LYS:HG2 | 2:JL:224:TRP:CH2 | 2.56 | 0.41 |
| 2:KM:70:ILE:HG23 | 2:KM:74:PHE:CE1 | 2.56 | 0.41 |
| 2:KU:170:LYS:HG2 | 2:KU:224:TRP:CH2 | 2.56 | 0.41 |
| 2:KY:70:ILE:HG23 | 2:KY:74:PHE:CE1 | 2.56 | 0.41 |
| 2:LM:170:LYS:HG2 | 2:LM:224:TRP:CH2 | 2.56 | 0.41 |
| 2:ZX:170:LYS:HG2 | 2:ZX:224:TRP:CH2 | 2.56 | 0.41 |
| 2:YB:160:ASP:OD1 | 2:YB:168:LYS:NZ | 2.45 | 0.41 |
| 2:YF:96:LEU:O | 2:YF:97:GLU:C | 2.63 | 0.40 |
| 2:AO:70:ILE:HG23 | 2:AO:74:PHE:CE1 | 2.56 | 0.40 |
| 2:AZ:133:ILE:HG21 | 2:AZ:181:ILE:HD13 | 2.02 | 0.40 |
| 2:BF:218:ASP:OD1 | 2:BF:219:SER:N | 2.53 | 0.40 |
| 2:BR:170:LYS:HG2 | 2:BR:224:TRP:CH2 | 2.56 | 0.40 |
| 2:CB:70:ILE:HG23 | 2:CB:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CH:70:ILE:HG23 | 2:CH:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CH:222:ILE:O | 2:CH:223:VAL:C | 2.63 | 0.40 |
| 2:DY:222:ILE:O | 2:DY:223:VAL:C | 2.63 | 0.40 |
| 1:EF:11:ALA:HB1 | 1:EF:43:VAL:O | 2.20 | 0.40 |
| 1:EP:77:TYR:N | 1:EP:77:TYR:CD1 | 2.84 | 0.40 |
| 2:EQ:70:ILE:HG23 | 2:EQ:74:PHE:CE1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ES:218:ASP:OD1 | 2:ES:219:SER:N | 2.53 | 0.40 |
| 2:GO:92:PRO:HB2 | 2:GO:144:LEU:HD13 | 2.02 | 0.40 |
| 2:HK:281:PHE:O | 1:WA:81:ARG:NH2 | 2.51 | 0.40 |
| 2:HQ:92:PRO:HB2 | 2:HQ:144:LEU:HD13 | 2.02 | 0.40 |
| 2:HU:70:ILE:HG23 | 2:HU:74:PHE:CE1 | 2.56 | 0.40 |
| 1:HZ:77:TYR:N | 1:HZ:77:TYR:CD1 | 2.84 | 0.40 |
| 2:IG:92:PRO:HB2 | 2:IG:144:LEU:HD13 | 2.02 | 0.40 |
| 1:JE:11:ALA:HB1 | 1:JE:43:VAL:O | 2.20 | 0.40 |
| 2:JW:92:PRO:HB2 | 2:JW:144:LEU:HD13 | 2.02 | 0.40 |
| 2:KM:160:ASP:OD1 | 2:KM:168:LYS:NZ | 2.45 | 0.40 |
| 2:ZV:70:ILE:HG23 | 2:ZV:74:PHE:CE1 | 2.56 | 0.40 |
| 2:YH:70:ILE:HG23 | 2:YH:74:PHE:CE1 | 2.56 | 0.40 |
| 2:YZ:70:ILE:HG23 | 2:YZ:74:PHE:CE1 | 2.56 | 0.40 |
| 2:AF:222:ILE:O | 2:AF:223:VAL:C | 2.63 | 0.40 |
| 2:AL:70:ILE:HG23 | 2:AL:74:PHE:CE1 | 2.56 | 0.40 |
| 2:AO:231:VAL:HG11 | 2:AO:238:MET:HB2 | 2.03 | 0.40 |
| 2:BV:70:ILE:HG23 | 2:BV:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CJ:170:LYS:HG2 | 2:CJ:224:TRP:CH2 | 2.56 | 0.40 |
| 2:CN:70:ILE:HG23 | 2:CN:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CP:133:ILE:HG21 | 2:CP:181:ILE:HD13 | 2.02 | 0.40 |
| 2:CP:170:LYS:HG2 | 2:CP:224:TRP:CH2 | 2.56 | 0.40 |
| 2:DF:70:ILE:HG23 | 2:DF:74:PHE:CE1 | 2.56 | 0.40 |
| 2:DF:160:ASP:OD1 | 2:DF:168:LYS:NZ | 2.45 | 0.40 |
| 1:ED:77:TYR:N | 1:ED:77:TYR:CD1 | 2.84 | 0.40 |
| 2:EI:96:LEU:O | 2:EI:97:GLU:C | 2.63 | 0.40 |
| 2:EQ:231:VAL:HG11 | 2:EQ:238:MET:HB2 | 2.03 | 0.40 |
| 1:EX:81:ARG:NH2 | 2:EY:281:PHE:O | 2.51 | 0.40 |
| 2:EY:92:PRO:HB2 | 2:EY:144:LEU:HD13 | 2.02 | 0.40 |
| 2:EY:170:LYS:HG2 | 2:EY:224:TRP:CH2 | 2.56 | 0.40 |
| 2:HF:218:ASP:OD1 | 2:HF:219:SER:N | 2.53 | 0.40 |
| 1:HV:81:ARG:NH2 | 2:HW:281:PHE:O | 2.51 | 0.40 |
| 2:JJ:70:ILE:HG23 | 2:JJ:74:PHE:CE1 | 2.56 | 0.40 |
| 1:JM:33:ALA:N | 1:JM:34:PRO:CD | 2.83 | 0.40 |
| 2:KA:70:ILE:HG23 | 2:KA:74:PHE:CE1 | 2.56 | 0.40 |
| 2:KQ:96:LEU:O | 2:KQ:97:GLU:C | 2.63 | 0.40 |
| 2:KU:218:ASP:OD1 | 2:KU:219:SER:N | 2.53 | 0.40 |
| 2:LS:218:ASP:OD1 | 2:LS:219:SER:N | 2.53 | 0.40 |
| 2:ZB:96:LEU:O | 2:ZB:97:GLU:C | 2.63 | 0.40 |
| 2:AX:70:ILE:HG23 | 2:AX:74:PHE:CE1 | 2.56 | 0.40 |
| 2:BD:70:ILE:HG23 | 2:BD:74:PHE:CE1 | 2.56 | 0.40 |
| 2:BV:222:ILE:O | 2:BV:223:VAL:C | 2.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:CB:231:VAL:HG11 | 2:CB:238:MET:HB2 | 2.03 | 0.40 |
| 2:DR:70:ILE:HG23 | 2:DR:74:PHE:CE1 | 2.56 | 0.40 |
| 2:DT:218:ASP:OD1 | 2:DT:219:SER:N | 2.53 | 0.40 |
| 2:DY:70:ILE:HG23 | 2:DY:74:PHE:CE1 | 2.56 | 0.40 |
| 2:EW:222:ILE:O | 2:EW:223:VAL:C | 2.63 | 0.40 |
| 2:FC:70:ILE:HG23 | 2:FC:74:PHE:CE1 | 2.56 | 0.40 |
| 1:FD:81:ARG:NH2 | 2:FE:281:PHE:O | 2.51 | 0.40 |
| 2:FK:218:ASP:OD1 | 2:FK:219:SER:N | 2.53 | 0.40 |
| 2:FQ:170:LYS:HG2 | 2:FQ:224:TRP:CH2 | 2.56 | 0.40 |
| 2:FW:218:ASP:OD1 | 2:FW:219:SER:N | 2.53 | 0.40 |
| 2:HC:96:LEU:O | 2:HC:97:GLU:C | 2.63 | 0.40 |
| 2:HE:70:ILE:HG23 | 2:HE:74:PHE:CE1 | 2.56 | 0.40 |
| 2:HF:170:LYS:HG2 | 2:HF:224:TRP:CH2 | 2.56 | 0.40 |
| 2:HO:70:ILE:HG23 | 2:HO:74:PHE:CE1 | 2.56 | 0.40 |
| 2:HO:231:VAL:HG11 | 2:HO:238:MET:HB2 | 2.03 | 0.40 |
| 2:IF:70:ILE:HG23 | 2:IF:74:PHE:CE1 | 2.56 | 0.40 |
| 1:II:69:HIS:O | 1:II:70:ILE:C | 2.63 | 0.40 |
| 1:IO:69:HIS:O | 1:IO:70:ILE:C | 2.63 | 0.40 |
| 2:IZ:170:LYS:HG2 | 2:IZ:224:TRP:CH2 | 2.56 | 0.40 |
| 2:JR:170:LYS:HG2 | 2:JR:224:TRP:CH2 | 2.56 | 0.40 |
| 2:ZL:170:LYS:HG2 | 2:ZL:224:TRP:CH2 | 2.56 | 0.40 |
| 1:KP:69:HIS:O | 1:KP:70:ILE:C | 2.63 | 0.40 |
| 2:LE:70:ILE:HG23 | 2:LE:74:PHE:CE1 | 2.56 | 0.40 |
| 2:AX:222:ILE:O | 2:AX:223:VAL:C | 2.63 | 0.40 |
| 2:ZD:70:ILE:HG23 | 2:ZD:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CZ:222:ILE:O | 2:CZ:223:VAL:C | 2.63 | 0.40 |
| 2:DH:170:LYS:HG2 | 2:DH:224:TRP:CH2 | 2.56 | 0.40 |
| 2:DR:231:VAL:HG11 | 2:DR:238:MET:HB2 | 2.03 | 0.40 |
| 2:EE:231:VAL:HG11 | 2:EE:238:MET:HB2 | 2.03 | 0.40 |
| 2:EK:70:ILE:HG23 | 2:EK:74:PHE:CE1 | 2.56 | 0.40 |
| 1:GV:69:HIS:O | 1:GV:70:ILE:C | 2.63 | 0.40 |
| 2:HW:170:LYS:HG2 | 2:HW:224:TRP:CH2 | 2.56 | 0.40 |
| 2:IB:170:LYS:HG2 | 2:IB:224:TRP:CH2 | 2.56 | 0.40 |
| 2:JW:170:LYS:HG2 | 2:JW:224:TRP:CH2 | 2.56 | 0.40 |
| 2:KA:231:VAL:HG11 | 2:KA:238:MET:HB2 | 2.03 | 0.40 |
| 2:KG:70:ILE:HG23 | 2:KG:74:PHE:CE1 | 2.56 | 0.40 |
| 1:LB:33:ALA:N | 1:LB:34:PRO:CD | 2.83 | 0.40 |
| 2:LK:70:ILE:HG23 | 2:LK:74:PHE:CE1 | 2.56 | 0.40 |
| 1:LN:33:ALA:N | 1:LN:34:PRO:CD | 2.83 | 0.40 |
| 2:LS:170:LYS:HG2 | 2:LS:224:TRP:CH2 | 2.56 | 0.40 |
| 1:ZA:33:ALA:N | 1:ZA:34:PRO:CD | 2.83 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:YJ:170:LYS:HG2 | 2:YJ:224:TRP:CH2 | 2.56 | 0.40 |
| 2:YN:231:VAL:HG11 | 2:YN:238:MET:HB2 | 2.03 | 0.40 |
| 2:YT:70:ILE:HG23 | 2:YT:74:PHE:CE1 | 2.56 | 0.40 |
| 2:CD:133:ILE:HG13 | 2:CD:148:ALA:CB | 2.52 | 0.40 |
| 2:CH:231:VAL:HG11 | 2:CH:238:MET:HB2 | 2.03 | 0.40 |
| 2:DN:92:PRO:HB2 | 2:DN:144:LEU:HD13 | 2.02 | 0.40 |
| 2:EW:70:ILE:HG23 | 2:EW:74:PHE:CE1 | 2.56 | 0.40 |
| 1:FF:69:HIS:O | 1:FF:70:ILE:C | 2.63 | 0.40 |
| 2:FK:170:LYS:HG2 | 2:FK:224:TRP:CH2 | 2.56 | 0.40 |
| 2:FO:70:ILE:HG23 | 2:FO:74:PHE:CE1 | 2.56 | 0.40 |
| 2:FU:70:ILE:HG23 | 2:FU:74:PHE:CE1 | 2.56 | 0.40 |
| 2:GA:70:ILE:HG23 | 2:GA:74:PHE:CE1 | 2.56 | 0.40 |
| 2:GC:170:LYS:HG2 | 2:GC:224:TRP:CH2 | 2.56 | 0.40 |
| 2:HJ:231:VAL:HG11 | 2:HJ:238:MET:HB2 | 2.03 | 0.40 |
| 2:IA:70:ILE:HG23 | 2:IA:74:PHE:CE1 | 2.56 | 0.40 |
| 2:IA:222:ILE:O | 2:IA:223:VAL:C | 2.63 | 0.40 |
| 2:IX:222:ILE:O | 2:IX:223:VAL:C | 2.63 | 0.40 |
| 2:ZL:218:ASP:OD1 | 2:ZL:219:SER:N | 2.53 | 0.40 |
| 1:KJ:33:ALA:N | 1:KJ:34:PRO:CD | 2.83 | 0.40 |
| 1:KR:77:TYR:N | 1:KR:77:TYR:CD1 | 2.84 | 0.40 |
| 2:KS:231:VAL:HG11 | 2:KS:238:MET:HB2 | 2.03 | 0.40 |
| 1:KZ:81:ARG:NH2 | 2:LA:281:PHE:O | 2.51 | 0.40 |
| 2:LC:96:LEU:O | 2:LC:97:GLU:C | 2.63 | 0.40 |
| 2:LG:170:LYS:HG2 | 2:LG:224:TRP:CH2 | 2.56 | 0.40 |
| 2:LQ:70:ILE:HG23 | 2:LQ:74:PHE:CE1 | 2.56 | 0.40 |
| 2:LQ:231:VAL:HG11 | 2:LQ:238:MET:HB2 | 2.03 | 0.40 |
| 2:YB:231:VAL:HG11 | 2:YB:238:MET:HB2 | 2.03 | 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 | AA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | AY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | BY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | CM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | CY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | DZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ED | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EF | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EJ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ER | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ET | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | EX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | EZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FF | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FJ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FT | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | FZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GF | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GJ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GT | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | GZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | HI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HT | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | HZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | II | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | IY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | JV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | JZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KF | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KJ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KT | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KV | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KX | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | KZ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LF | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LH | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LJ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LL | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LN | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LP | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | LR | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | WA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | WB | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | WC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | WD | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | YE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | YY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZA | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZC | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZE | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZG | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZI | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZK | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZM | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZO | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZQ | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZS | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZU | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZW | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 1 | ZY | 104/114 (91%) | 104 (100%) | 0 | 0 | 100 | 100 |
| 2 | AB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | AO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | AZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | BZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | CX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | CZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | DY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EI | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ES | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | EY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FI | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | FK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FS | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | FY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GI | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GS | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | GY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | HS | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | HY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ID | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | IZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | JY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | KA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KI | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KS | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KU | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KW | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | KY | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LA | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LC | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LE | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LG | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LI | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LK | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LM | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LO | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LQ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | LS | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|---------|----------|-------------|-----|
| 2 | YR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | YZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZB | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZD | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZF | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZH | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZJ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZL | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZN | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZP | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZR | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZT | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZV | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZX | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| 2 | ZZ | 290/300 (97%) | 290 (100%) | 0 | 0 | 100 | 100 |
| All | All | 70920/74520 (95%) | 70920 (100%) | 0 | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | AA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | AG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | AY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | BY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | CQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | CY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | DZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ED | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EF | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EJ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ER | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ET | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | EZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | FB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FF | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FJ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FT | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | FZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GF | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GJ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GT | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | GZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | HN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HT | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | HZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | II | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | IY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | JX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | JZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KF | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KJ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KT | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KV | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KX | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | KZ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LF | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LH | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LJ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LL | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LN | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LP | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | LR | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | WA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | WB | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | WC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | WD | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | YI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | YY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZA | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZC | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZE | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZG | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZI | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZK | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZM | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZO | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZQ | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZS | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZU | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZW | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 1 | ZY | 86/94 (92%) | 86 (100%) | 0 | 100 | 100 |
| 2 | AB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | AT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | AZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | BZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | CZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | DD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | DY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EI | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ES | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | EY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FI | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | FO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FS | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | FY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GI | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GS | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | GY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HS | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | HW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | HY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ID | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | IZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | JY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | KE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KI | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KS | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KU | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KW | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | KY | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LA | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LC | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LE | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LG | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LI | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LK | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LM | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LO | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LQ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | LS | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 2 | YV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | YZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZB | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZD | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZF | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZH | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZJ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZL | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZN | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZP | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZR | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZT | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZV | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZX | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| 2 | ZZ | 233/241 (97%) | 233 (100%) | 0 | 100 | 100 |
| All | All | 57420/60300 (95%) | 57420 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | YD | 59 | ASN |
| 2 | ZZ | 259 | GLN |
| 2 | YH | 46 | ASN |
| 1 | YI | 87 | GLN |
| 2 | YJ | 59 | ASN |
| 2 | YN | 46 | ASN |
| 2 | YP | 59 | ASN |
| 2 | YR | 259 | GLN |
| 1 | YU | 87 | GLN |
| 2 | YV | 59 | ASN |
| 2 | YZ | 46 | ASN |
| 2 | AF | 46 | ASN |
| 2 | AL | 46 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AM | 87 | GLN |
| 2 | AN | 59 | ASN |
| 2 | AO | 46 | ASN |
| 2 | AX | 46 | ASN |
| 2 | AZ | 59 | ASN |
| 2 | BN | 259 | GLN |
| 2 | BR | 59 | ASN |
| 2 | BX | 59 | ASN |
| 2 | BZ | 259 | GLN |
| 2 | ZD | 46 | ASN |
| 2 | CB | 46 | ASN |
| 1 | CC | 87 | GLN |
| 2 | CD | 59 | ASN |
| 2 | CH | 46 | ASN |
| 2 | CJ | 59 | ASN |
| 2 | CP | 59 | ASN |
| 2 | CT | 46 | ASN |
| 2 | CV | 59 | ASN |
| 2 | CX | 259 | GLN |
| 2 | DB | 59 | ASN |
| 2 | DF | 46 | ASN |
| 2 | DH | 59 | ASN |
| 2 | DL | 46 | ASN |
| 1 | DM | 87 | GLN |
| 2 | DN | 59 | ASN |
| 2 | DT | 59 | ASN |
| 2 | DY | 46 | ASN |
| 2 | EA | 59 | ASN |
| 2 | ZF | 59 | ASN |
| 2 | EG | 59 | ASN |
| 2 | EI | 259 | GLN |
| 2 | EO | 259 | GLN |
| 2 | EQ | 46 | ASN |
| 2 | ES | 59 | ASN |
| 2 | EW | 46 | ASN |
| 1 | EX | 87 | GLN |
| 2 | FC | 46 | ASN |
| 2 | FE | 59 | ASN |
| 2 | FK | 59 | ASN |
| 2 | FQ | 59 | ASN |
| 2 | FU | 46 | ASN |
| 2 | FW | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | FY | 259 | GLN |
| 2 | GA | 46 | ASN |
| 2 | GG | 46 | ASN |
| 2 | GI | 59 | ASN |
| 1 | GN | 87 | GLN |
| 2 | GO | 59 | ASN |
| 2 | GS | 46 | ASN |
| 2 | GU | 59 | ASN |
| 2 | GY | 46 | ASN |
| 2 | HA | 59 | ASN |
| 2 | HE | 46 | ASN |
| 2 | HF | 59 | ASN |
| 1 | WB | 87 | GLN |
| 2 | HJ | 46 | ASN |
| 2 | HK | 59 | ASN |
| 2 | HS | 259 | GLN |
| 2 | HU | 46 | ASN |
| 2 | HW | 59 | ASN |
| 2 | ZJ | 46 | ASN |
| 2 | IB | 59 | ASN |
| 2 | ID | 259 | GLN |
| 2 | IG | 59 | ASN |
| 2 | IL | 46 | ASN |
| 2 | IN | 59 | ASN |
| 2 | IT | 59 | ASN |
| 2 | IZ | 59 | ASN |
| 2 | JJ | 46 | ASN |
| 2 | JL | 59 | ASN |
| 2 | JW | 59 | ASN |
| 2 | KA | 46 | ASN |
| 2 | ZL | 59 | ASN |
| 2 | KC | 59 | ASN |
| 2 | KG | 46 | ASN |
| 2 | KI | 59 | ASN |
| 2 | KM | 46 | ASN |
| 2 | KO | 59 | ASN |
| 2 | KS | 46 | ASN |
| 2 | KU | 59 | ASN |
| 2 | KY | 46 | ASN |
| 1 | KZ | 87 | GLN |
| 2 | LA | 59 | ASN |
| 2 | LC | 259 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | LE | 46 | ASN |
| 1 | LF | 87 | GLN |
| 2 | LM | 59 | ASN |
| 2 | LQ | 46 | ASN |
| 2 | LS | 59 | ASN |
| 2 | ZN | 259 | GLN |
| 2 | ZP | 46 | ASN |
| 2 | ZR | 59 | ASN |
| 2 | ZV | 46 | ASN |
| 1 | ZW | 87 | GLN |
| 2 | ZX | 59 | ASN |

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-70685. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

6.1.2 Raw 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: 120



Y Index: 120



Z Index: 120

6.2.2 Raw map



X Index: 120



Y Index: 120



Z Index: 120

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: 120



Y Index: 99



Z Index: 75

6.3.2 Raw map



X Index: 120



Y Index: 99



Z Index: 163

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

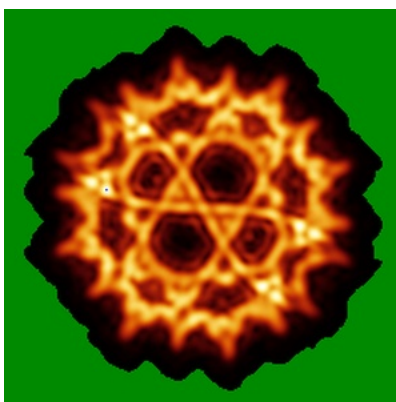


Z

6.4.2 Raw map



X



Y

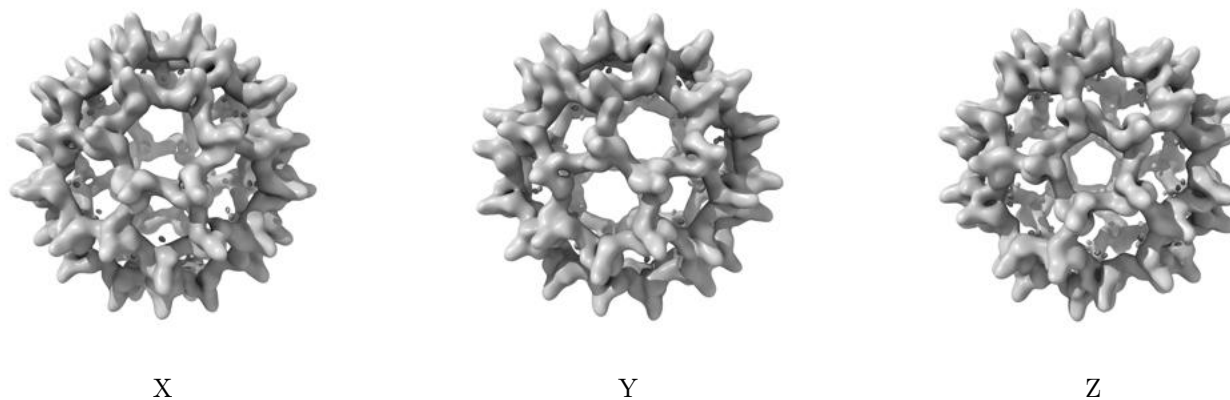


Z

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.

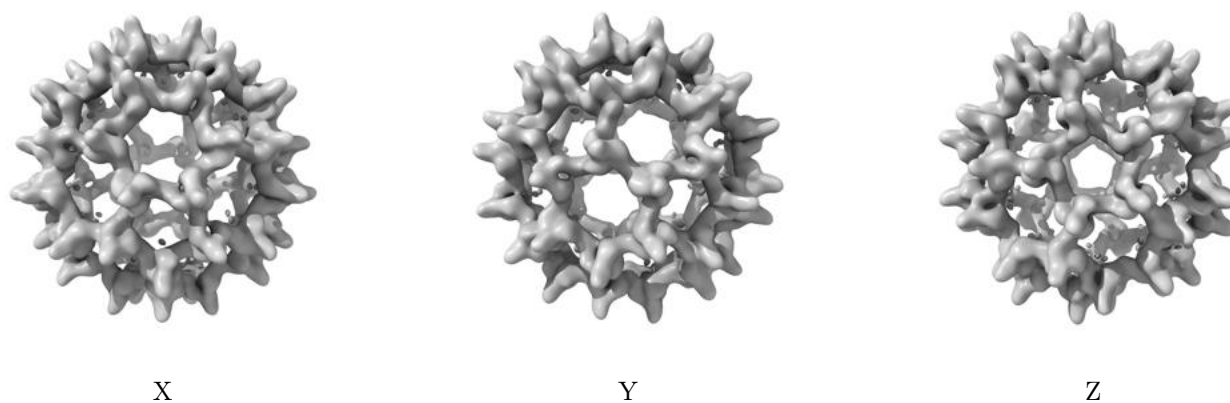
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1854.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

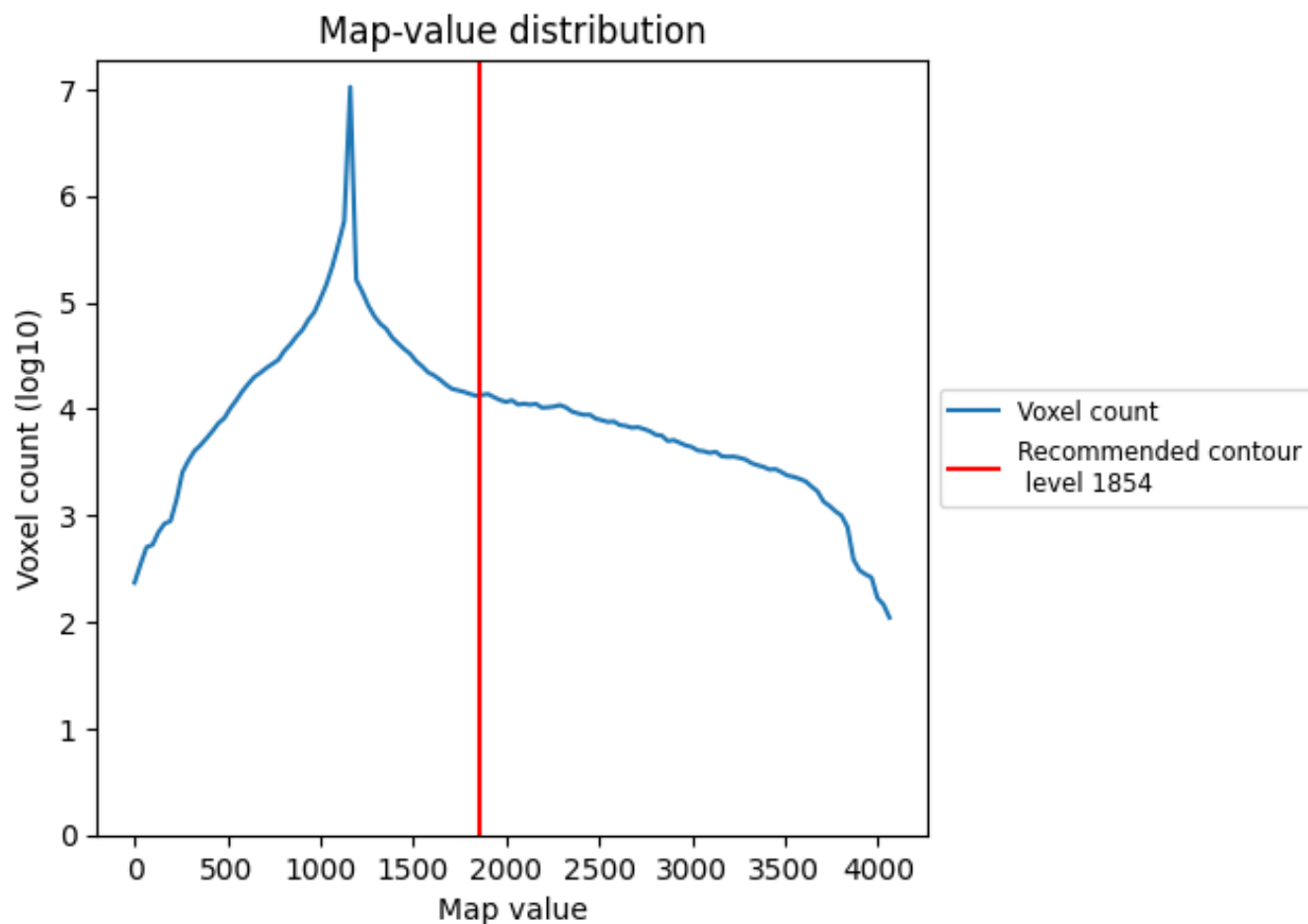
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

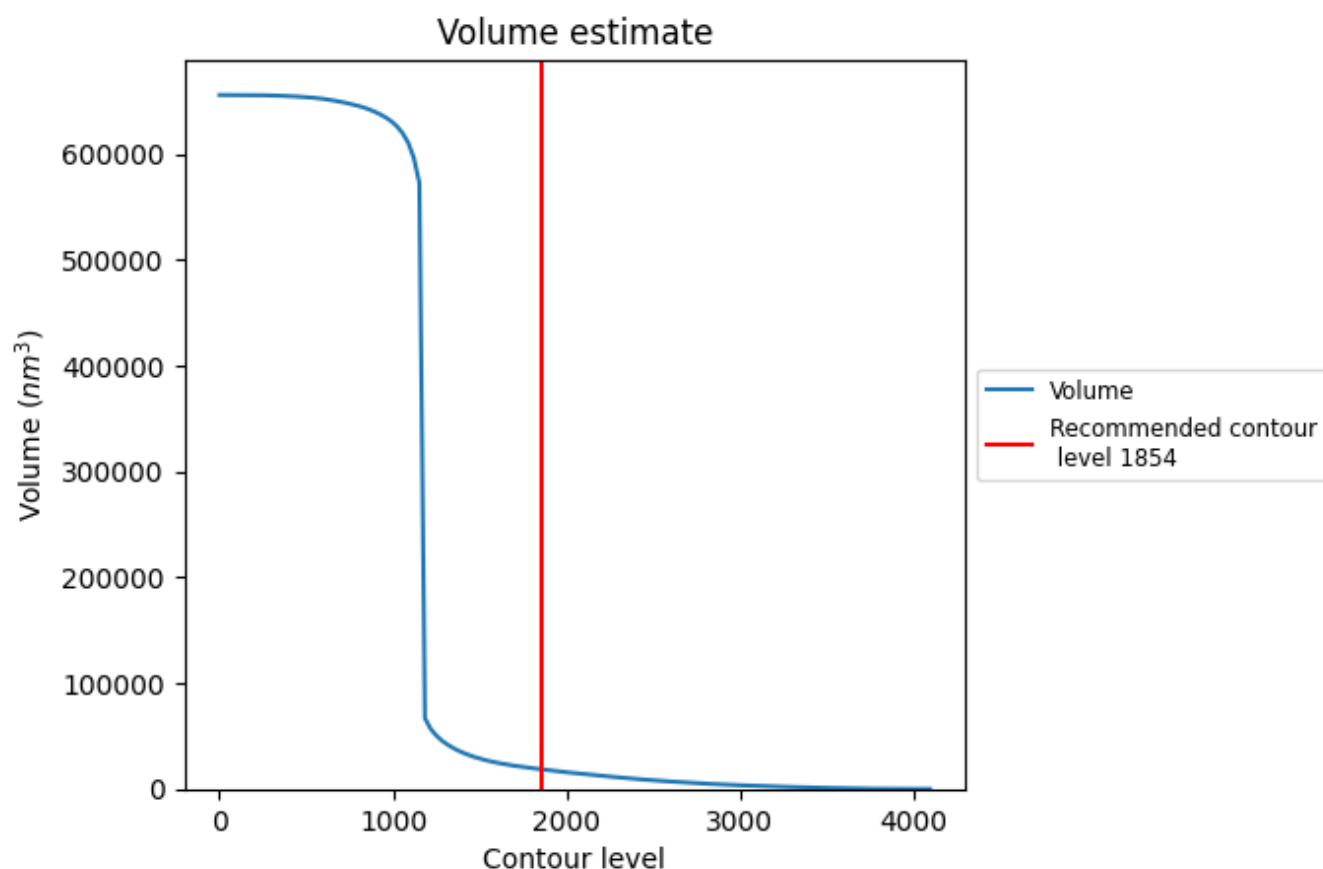
This section contains the results of statistical analysis of the map.

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.

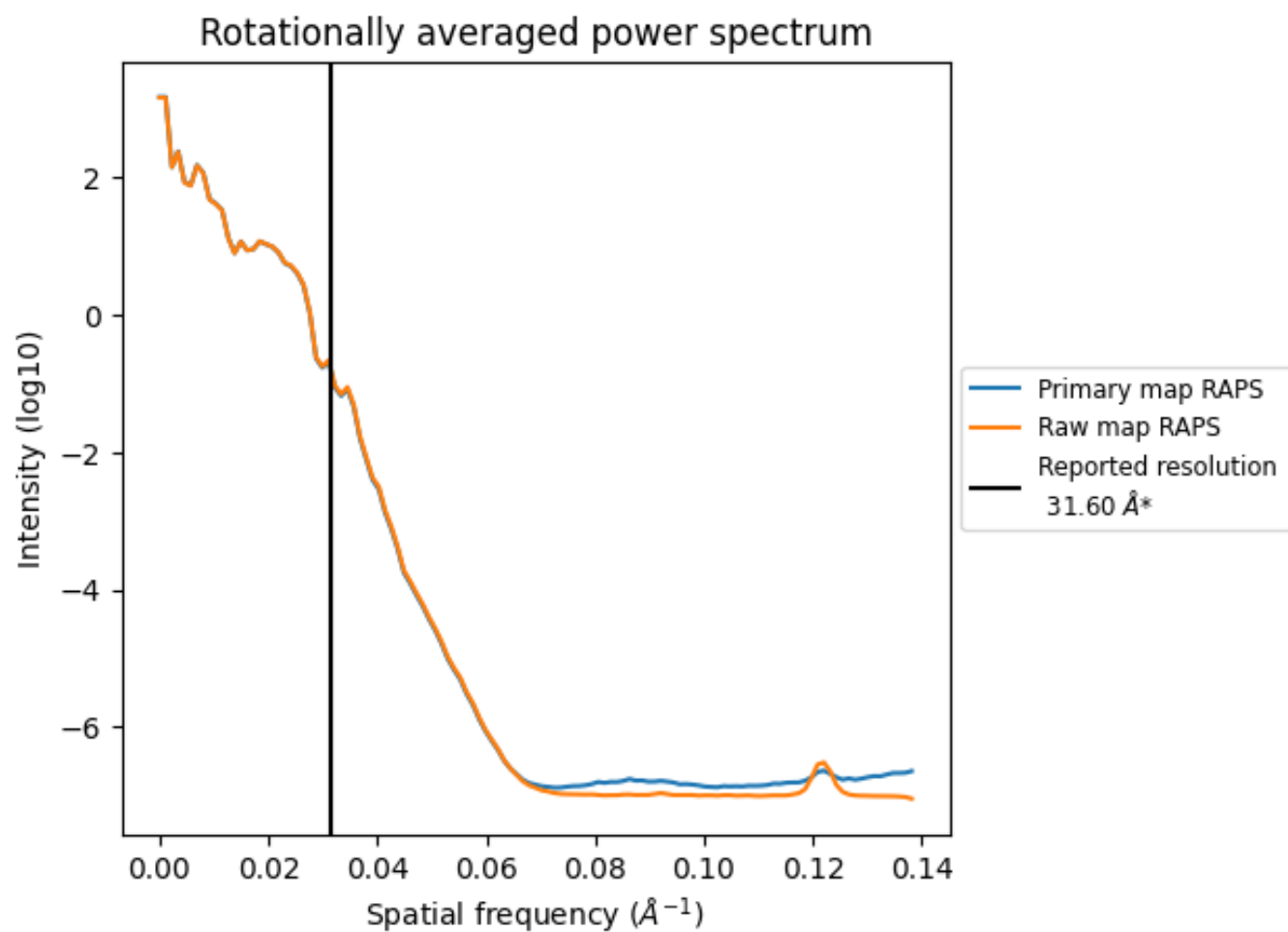
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18602 nm^3 ; this corresponds to an approximate mass of 16804 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 ⓘ

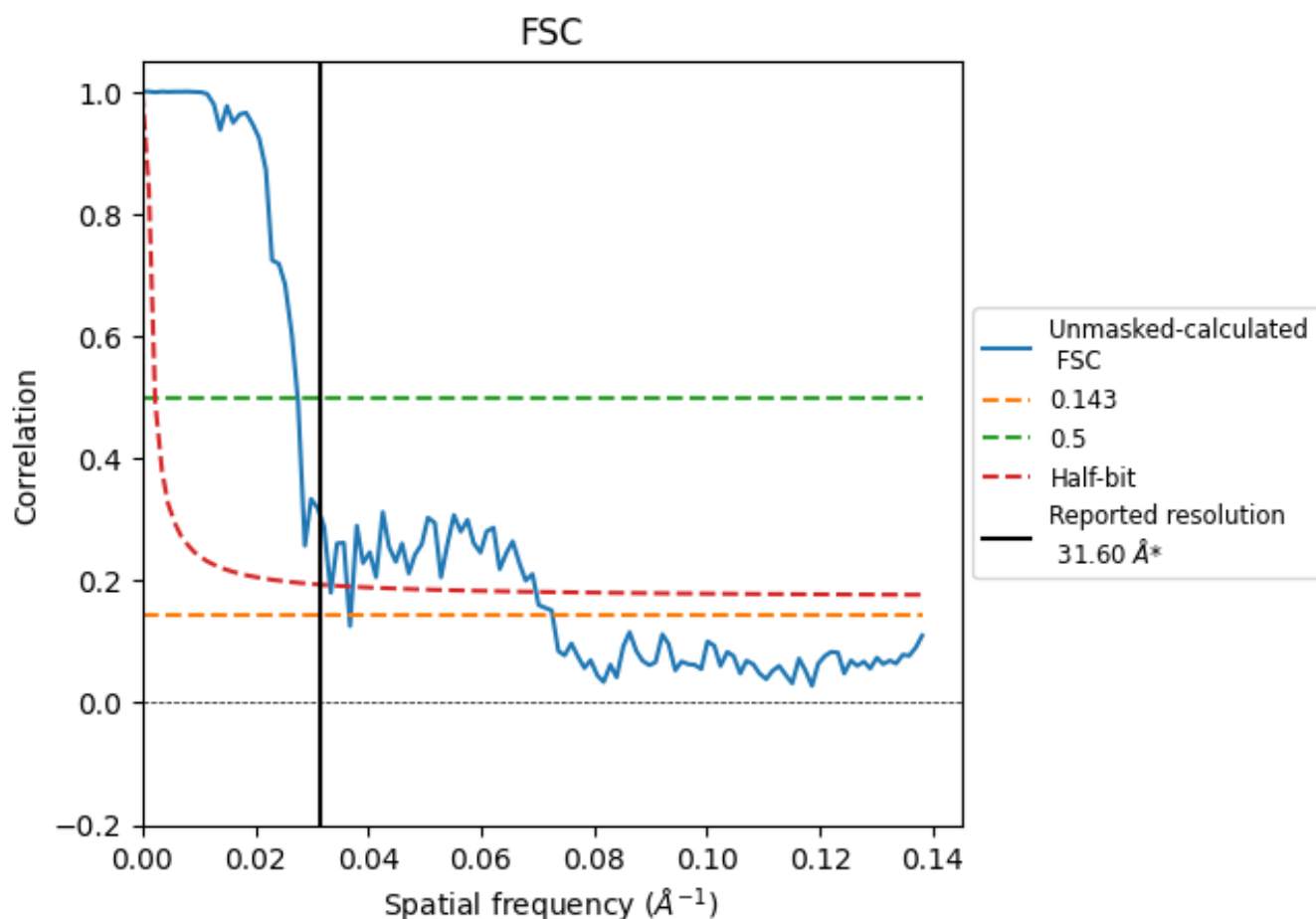


*Reported resolution corresponds to spatial frequency of 0.032 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.032 \AA^{-1}

8.2 Resolution estimates [i](#)

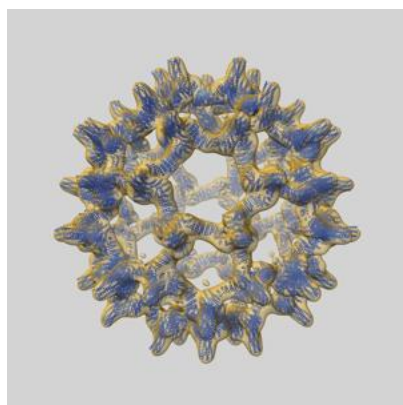
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 31.60 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 27.25 | 36.36 | 30.03 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 27.25 differs from the reported value 31.6 by more than 10 %

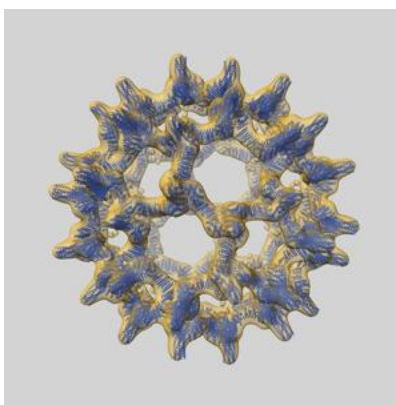
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70685 and PDB model 9OP9. Per-residue inclusion information can be found in section [3](#) on page [36](#).

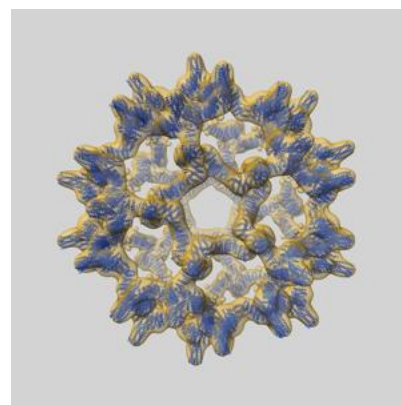
9.1 Map-model overlay [i](#)



X



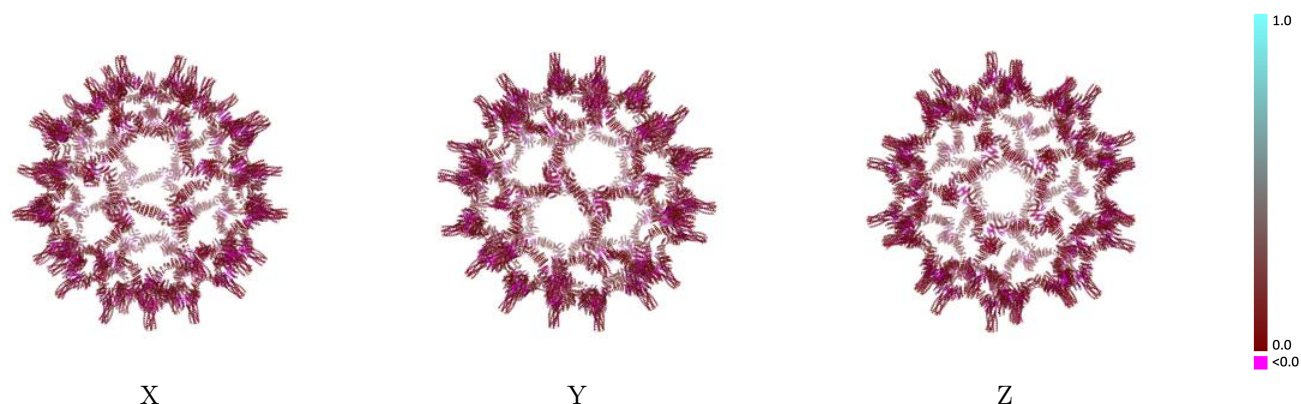
Y



Z

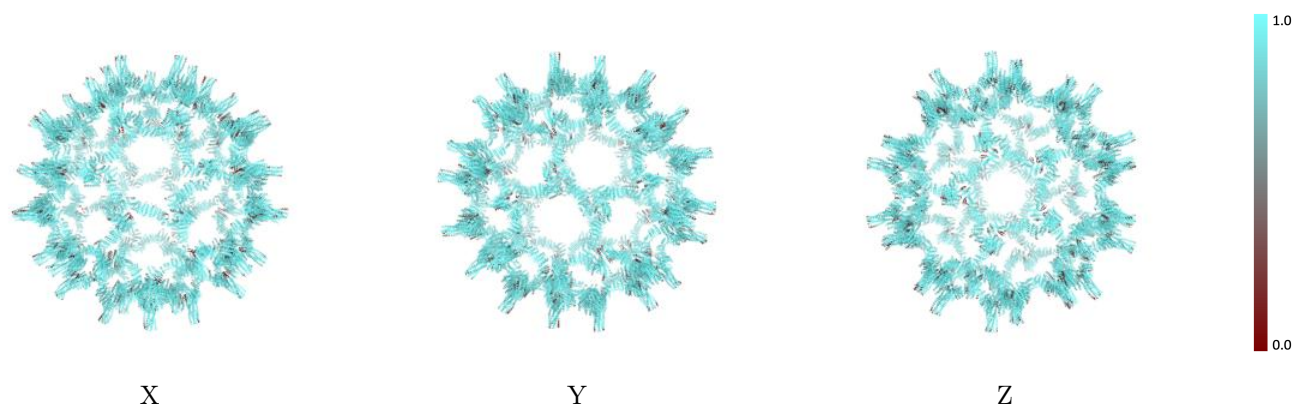
The images above show the 3D surface view of the map at the recommended contour level 1854.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



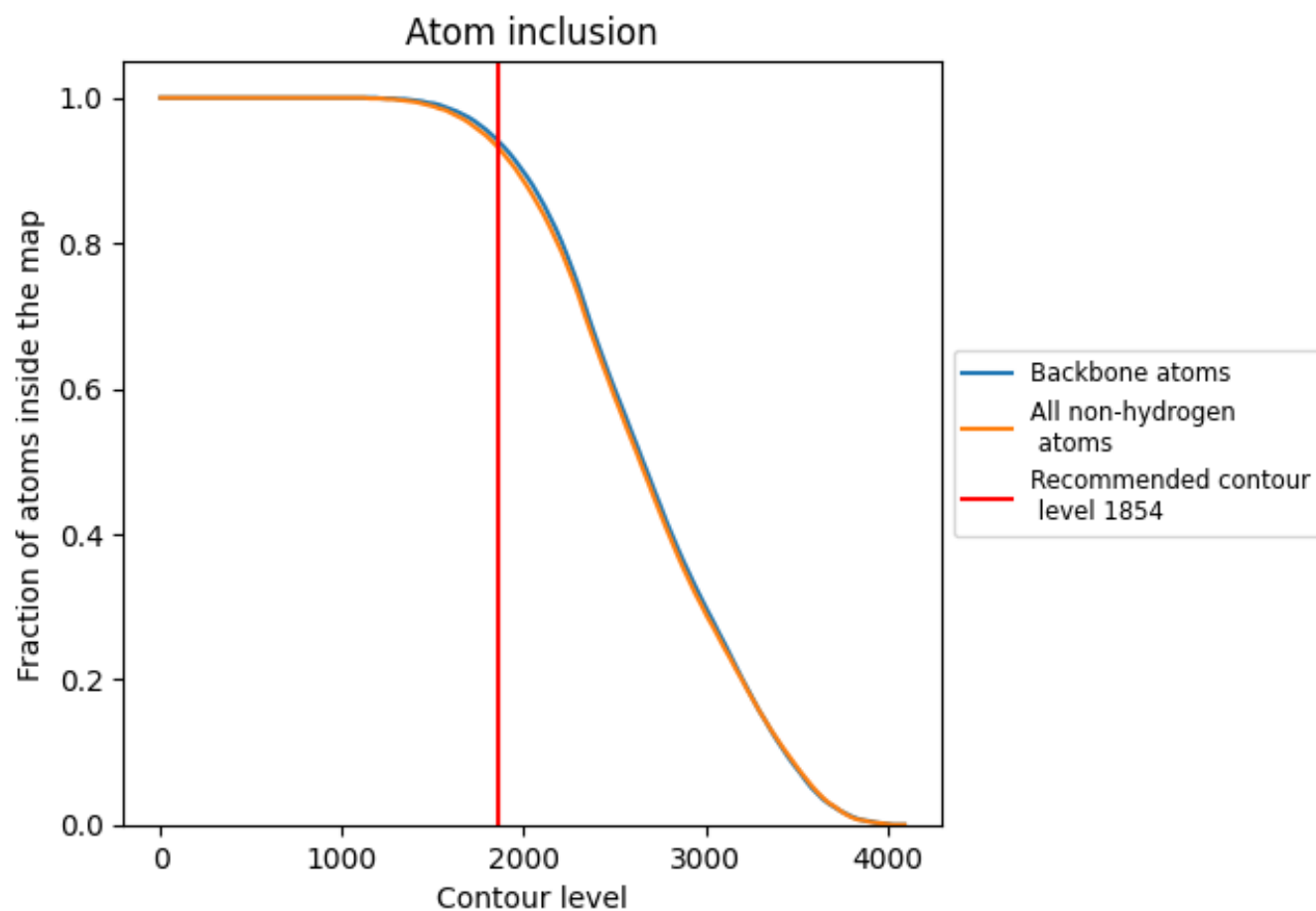
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1854).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (1854) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9330 |  0.0580 |
| AA |  0.9990 |  0.0590 |
| AB |  0.9170 |  0.0550 |
| AC |  0.9860 |  0.0680 |
| AD |  0.9790 |  0.0590 |
| AE |  0.9620 |  0.0870 |
| AF |  0.8180 |  0.0440 |
| AG |  0.9820 |  0.0690 |
| AH |  0.9540 |  0.0560 |
| AI |  0.9630 |  0.0680 |
| AJ |  0.9430 |  0.0570 |
| AK |  0.9890 |  0.0860 |
| AL |  0.8370 |  0.0480 |
| AM |  0.9720 |  0.0680 |
| AN |  0.9330 |  0.0490 |
| AO |  0.7970 |  0.0430 |
| AP |  0.9470 |  0.0860 |
| AQ |  0.9500 |  0.0580 |
| AR |  0.9620 |  0.0690 |
| AS |  0.9950 |  0.0670 |
| AT |  0.9480 |  0.0560 |
| AU |  0.9710 |  0.0670 |
| AV |  0.9370 |  0.0550 |
| AW |  0.9410 |  0.0920 |
| AX |  0.7720 |  0.0380 |
| AY |  0.9980 |  0.0640 |
| AZ |  0.9350 |  0.0520 |
| BA |  0.9780 |  0.0690 |
| BB |  0.9610 |  0.0590 |
| BC |  0.9380 |  0.0840 |
| BD |  0.7820 |  0.0370 |
| BE |  0.9950 |  0.0680 |
| BF |  0.9490 |  0.0530 |
| BG |  0.9920 |  0.0690 |
| BH |  0.9770 |  0.0570 |























































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| BI |  0.9950 |  0.0780 |
| BJ |  0.8770 |  0.0450 |
| BK |  0.9570 |  0.0630 |
| BL |  0.9470 |  0.0580 |
| BM |  0.9730 |  0.0610 |
| BN |  0.9510 |  0.0550 |
| BO |  0.9980 |  0.0770 |
| BP |  0.8820 |  0.0480 |
| BQ |  0.9760 |  0.0680 |
| BR |  0.9200 |  0.0510 |
| BS |  0.9990 |  0.0610 |
| BT |  0.9750 |  0.0600 |
| BU |  0.9720 |  0.0840 |
| BV |  0.8040 |  0.0410 |
| BW |  0.9980 |  0.0630 |
| BX |  0.9330 |  0.0570 |
| BY |  0.9920 |  0.0600 |
| BZ |  0.9660 |  0.0580 |
| CA |  0.9950 |  0.0810 |
| CB |  0.8840 |  0.0470 |
| CC |  0.9950 |  0.0670 |
| CD |  0.9320 |  0.0550 |
| CE |  0.9990 |  0.0690 |
| CF |  0.9800 |  0.0610 |
| CG |  0.9950 |  0.0840 |
| CH |  0.8700 |  0.0460 |
| CI |  0.9940 |  0.0580 |
| CJ |  0.9520 |  0.0600 |
| CK |  0.9980 |  0.0650 |
| CL |  0.9700 |  0.0570 |
| CM |  1.0000 |  0.0750 |
| CN |  0.9180 |  0.0470 |
| CO |  0.9430 |  0.0680 |
| CP |  0.9360 |  0.0530 |
| CQ |  0.9890 |  0.0720 |
| CR |  0.9720 |  0.0580 |
| CS |  0.9890 |  0.0850 |
| CT |  0.8650 |  0.0410 |
| CU |  0.9520 |  0.0730 |
| CV |  0.9490 |  0.0540 |
| CW |  0.9640 |  0.0630 |
| CX |  0.9330 |  0.0580 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| CY |  0.9890 |  0.0910 |
| CZ |  0.8400 |  0.0450 |
| DA |  0.9870 |  0.0740 |
| DB |  0.9150 |  0.0590 |
| DC |  0.9980 |  0.0640 |
| DD |  0.9780 |  0.0600 |
| DE |  0.9640 |  0.0900 |
| DF |  0.7840 |  0.0390 |
| DG |  0.9940 |  0.0640 |
| DH |  0.9350 |  0.0610 |
| DI |  0.9950 |  0.0630 |
| DJ |  0.9670 |  0.0590 |
| DK |  0.9890 |  0.0870 |
| DL |  0.8460 |  0.0490 |
| DM |  0.9990 |  0.0700 |
| DN |  0.9280 |  0.0590 |
| DO |  0.9990 |  0.0690 |
| DP |  0.9800 |  0.0560 |
| DQ |  0.9960 |  0.0870 |
| DR |  0.8710 |  0.0440 |
| DS |  0.9890 |  0.0620 |
| DT |  0.9490 |  0.0590 |
| DU |  0.9890 |  0.0640 |
| DW |  0.9650 |  0.0550 |
| DX |  0.9990 |  0.0810 |
| DY |  0.9120 |  0.0450 |
| DZ |  0.9390 |  0.0710 |
| EA |  0.9260 |  0.0560 |
| EB |  0.9910 |  0.0700 |
| EC |  0.9670 |  0.0560 |
| ED |  0.9950 |  0.0830 |
| EE |  0.8850 |  0.0490 |
| EF |  0.9390 |  0.0680 |
| EG |  0.9440 |  0.0530 |
| EH |  0.9990 |  0.0640 |
| EI |  0.9780 |  0.0570 |
| EJ |  0.9990 |  0.0910 |
| EK |  0.8860 |  0.0470 |
| EL |  0.9960 |  0.0580 |
| EM |  0.9480 |  0.0590 |
| EN |  0.9770 |  0.0690 |
| EO |  0.9450 |  0.0590 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| EP |  0.9870 |  0.0880 |
| EQ |  0.8340 |  0.0490 |
| ER |  0.9920 |  0.0670 |
| ES |  0.9150 |  0.0560 |
| ET |  1.0000 |  0.0670 |
| EU |  0.9820 |  0.0560 |
| EV |  0.9810 |  0.0870 |
| EW |  0.8130 |  0.0440 |
| EX |  0.9910 |  0.0620 |
| EY |  0.9490 |  0.0570 |
| EZ |  0.9990 |  0.0620 |
| FA |  0.9780 |  0.0600 |
| FB |  0.9890 |  0.0870 |
| FC |  0.8430 |  0.0450 |
| FD |  0.9990 |  0.0630 |
| FE |  0.9440 |  0.0580 |
| FF |  0.9990 |  0.0660 |
| FG |  0.9760 |  0.0570 |
| FH |  0.9990 |  0.0780 |
| FI |  0.8980 |  0.0460 |
| FJ |  0.9670 |  0.0710 |
| FK |  0.9440 |  0.0540 |
| FL |  0.9870 |  0.0590 |
| FM |  0.9660 |  0.0570 |
| FN |  0.9990 |  0.0820 |
| FO |  0.9090 |  0.0470 |
| FP |  0.9660 |  0.0700 |
| FQ |  0.9270 |  0.0560 |
| FR |  0.9960 |  0.0590 |
| FS |  0.9700 |  0.0560 |
| FT |  0.9990 |  0.0800 |
| FU |  0.9100 |  0.0460 |
| FV |  0.9400 |  0.0640 |
| FW |  0.9390 |  0.0570 |
| FX |  0.9850 |  0.0580 |
| FY |  0.9590 |  0.0620 |
| FZ |  0.9920 |  0.0880 |
| GA |  0.8730 |  0.0460 |
| GB |  0.9920 |  0.0670 |
| GC |  0.9240 |  0.0550 |
| GD |  0.9990 |  0.0690 |
| GE |  0.9820 |  0.0570 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| GF |  0.9900 |  0.0820 |
| GG |  0.8450 |  0.0420 |
| GH |  0.9920 |  0.0660 |
| GI |  0.9500 |  0.0570 |
| GJ |  0.9990 |  0.0680 |
| GK |  0.9740 |  0.0570 |
| GL |  1.0000 |  0.0780 |
| GM |  0.9110 |  0.0420 |
| GN |  0.9690 |  0.0700 |
| GO |  0.9450 |  0.0580 |
| GP |  0.9980 |  0.0620 |
| GQ |  0.9740 |  0.0590 |
| GR |  0.9990 |  0.0780 |
| GS |  0.9120 |  0.0480 |
| GT |  0.9850 |  0.0640 |
| GU |  0.9360 |  0.0570 |
| GV |  1.0000 |  0.0600 |
| GW |  0.9730 |  0.0550 |
| GX |  0.9990 |  0.0790 |
| GY |  0.9030 |  0.0450 |
| GZ |  0.9500 |  0.0690 |
| HA |  0.9440 |  0.0580 |
| HB |  0.9850 |  0.0620 |
| HC |  0.9620 |  0.0570 |
| HD |  0.9990 |  0.0850 |
| HE |  0.8960 |  0.0470 |
| HF |  0.9240 |  0.0560 |
| HG |  0.9990 |  0.0660 |
| HH |  0.9810 |  0.0570 |
| HI |  0.9890 |  0.0810 |
| HJ |  0.8390 |  0.0430 |
| HK |  0.9410 |  0.0580 |
| HL |  0.9990 |  0.0670 |
| HM |  0.9750 |  0.0580 |
| HN |  0.9990 |  0.0780 |
| HO |  0.9050 |  0.0460 |
| HP |  0.9910 |  0.0630 |
| HQ |  0.9400 |  0.0540 |
| HR |  0.9990 |  0.0600 |
| HS |  0.9770 |  0.0590 |
| HT |  0.9990 |  0.0880 |
| HU |  0.8950 |  0.0470 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| HV |  0.9940 |  0.0660 |
| HW |  0.9470 |  0.0630 |
| HX |  0.9780 |  0.0640 |
| HY |  0.9330 |  0.0610 |
| HZ |  0.9710 |  0.0870 |
| IA |  0.7880 |  0.0400 |
| IB |  0.9130 |  0.0580 |
| IC |  0.9960 |  0.0650 |
| ID |  0.9810 |  0.0570 |
| IE |  0.9690 |  0.0870 |
| IF |  0.8060 |  0.0420 |
| IG |  0.9560 |  0.0580 |
| IH |  0.9910 |  0.0650 |
| II |  0.9670 |  0.0670 |
| IJ |  0.9580 |  0.0560 |
| IK |  0.9870 |  0.0900 |
| IL |  0.8550 |  0.0400 |
| IM |  0.9540 |  0.0740 |
| IN |  0.9400 |  0.0530 |
| IO |  0.9730 |  0.0730 |
| IP |  0.9630 |  0.0570 |
| IQ |  0.9400 |  0.0820 |
| IR |  0.7910 |  0.0400 |
| IS |  0.9940 |  0.0680 |
| IT |  0.9530 |  0.0550 |
| IU |  0.9610 |  0.0660 |
| IV |  0.9420 |  0.0550 |
| IW |  0.9540 |  0.0880 |
| IX |  0.7990 |  0.0390 |
| IY |  0.9950 |  0.0680 |
| IZ |  0.9410 |  0.0540 |
| JA |  0.9770 |  0.0610 |
| JB |  0.9460 |  0.0620 |
| JC |  0.9380 |  0.0900 |
| JD |  0.7650 |  0.0370 |
| JE |  0.9980 |  0.0660 |
| JF |  0.9330 |  0.0590 |
| JG |  0.9800 |  0.0620 |
| JH |  0.9480 |  0.0580 |
| JI |  0.9820 |  0.0830 |
| JJ |  0.8200 |  0.0410 |
| JK |  0.9980 |  0.0670 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| JL |  0.9140 |  0.0570 |
| JM |  1.0000 |  0.0730 |
| JN |  0.9820 |  0.0590 |
| JO |  0.9850 |  0.0820 |
| JP |  0.8320 |  0.0390 |
| JQ |  0.9900 |  0.0620 |
| JR |  0.9550 |  0.0590 |
| JS |  0.9800 |  0.0610 |
| JT |  0.9630 |  0.0550 |
| JU |  0.8910 |  0.0460 |
| JV |  0.9380 |  0.0710 |
| JW |  0.9360 |  0.0520 |
| JX |  0.9820 |  0.0670 |
| JY |  0.9720 |  0.0560 |
| JZ |  0.9620 |  0.0880 |
| KA |  0.8220 |  0.0350 |
| KB |  0.9720 |  0.0730 |
| KC |  0.9560 |  0.0530 |
| KD |  0.9580 |  0.0640 |
| KE |  0.9350 |  0.0600 |
| KF |  0.9820 |  0.0840 |
| KG |  0.8220 |  0.0370 |
| KH |  0.9860 |  0.0720 |
| KI |  0.9270 |  0.0560 |
| KJ |  0.9910 |  0.0570 |
| KK |  0.9570 |  0.0570 |
| KL |  0.9470 |  0.0830 |
| KM |  0.7630 |  0.0390 |
| KN |  0.9980 |  0.0650 |
| KO |  0.9270 |  0.0590 |
| KP |  0.9920 |  0.0570 |
| KQ |  0.9620 |  0.0600 |
| KR |  0.9800 |  0.0870 |
| KS |  0.8200 |  0.0440 |
| KT |  1.0000 |  0.0620 |
| KU |  0.9240 |  0.0580 |
| KV |  0.9960 |  0.0680 |
| KW |  0.9800 |  0.0580 |
| KX |  0.9920 |  0.0830 |
| KY |  0.8620 |  0.0360 |
| KZ |  0.9810 |  0.0710 |
| LA |  0.9520 |  0.0550 |

































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| LB |  0.9810 |  0.0610 |
| LC |  0.9620 |  0.0570 |
| LD |  0.9990 |  0.0720 |
| LE |  0.9020 |  0.0450 |
| LF |  0.9400 |  0.0650 |
| LG |  0.9280 |  0.0580 |
| LH |  0.9800 |  0.0660 |
| LI |  0.9670 |  0.0540 |
| LJ |  0.9750 |  0.0810 |
| LK |  0.8530 |  0.0410 |
| LL |  0.9580 |  0.0690 |
| LM |  0.9530 |  0.0510 |
| LN |  0.9660 |  0.0580 |
| LO |  0.9310 |  0.0590 |
| LP |  0.9830 |  0.0870 |
| LQ |  0.8130 |  0.0420 |
| LR |  0.9920 |  0.0670 |
| LS |  0.9160 |  0.0560 |
| WA |  0.9960 |  0.0600 |
| WB |  0.9820 |  0.0680 |
| WC |  0.9990 |  0.0720 |
| WD |  0.9980 |  0.0770 |
| YA |  0.9950 |  0.0860 |
| YB |  0.8720 |  0.0520 |
| YC |  0.9680 |  0.0610 |
| YD |  0.9210 |  0.0550 |
| YE |  0.9660 |  0.0690 |
| YF |  0.9550 |  0.0610 |
| YG |  0.9660 |  0.0840 |
| YH |  0.8280 |  0.0430 |
| YI |  0.9660 |  0.0670 |
| YJ |  0.9490 |  0.0540 |
| YK |  0.9720 |  0.0630 |
| YL |  0.9300 |  0.0610 |
| YM |  0.9660 |  0.0880 |
| YN |  0.7820 |  0.0410 |
| YO |  0.9990 |  0.0650 |
| YP |  0.9170 |  0.0570 |
| YQ |  0.9920 |  0.0720 |
| YR |  0.9740 |  0.0570 |
| YS |  0.9480 |  0.0850 |
| YT |  0.7870 |  0.0360 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| YU |  0.9910 |  0.0700 |
| YV |  0.9480 |  0.0530 |
| YW |  0.9860 |  0.0640 |
| YX |  0.9490 |  0.0600 |
| YY |  0.9530 |  0.0870 |
| YZ |  0.7670 |  0.0400 |
| ZA |  0.9990 |  0.0630 |
| ZB |  0.9740 |  0.0580 |
| ZC |  1.0000 |  0.0790 |
| ZD |  0.9170 |  0.0490 |
| ZE |  0.9710 |  0.0650 |
| ZF |  0.9390 |  0.0560 |
| ZG |  0.9980 |  0.0680 |
| ZH |  0.9730 |  0.0580 |
| ZI |  0.9610 |  0.0880 |
| ZJ |  0.7760 |  0.0360 |
| ZK |  0.9940 |  0.0660 |
| ZL |  0.9370 |  0.0600 |
| ZM |  0.9980 |  0.0630 |
| ZN |  0.9660 |  0.0570 |
| ZO |  0.9620 |  0.0900 |
| ZP |  0.7920 |  0.0460 |
| ZQ |  0.9980 |  0.0610 |
| ZR |  0.9260 |  0.0590 |
| ZS |  0.9910 |  0.0720 |
| ZT |  0.9810 |  0.0560 |
| ZU |  0.9900 |  0.0850 |
| ZV |  0.8570 |  0.0400 |
| ZW |  0.9670 |  0.0720 |
| ZX |  0.9510 |  0.0530 |
| ZY |  0.9680 |  0.0690 |
| ZZ |  0.9470 |  0.0590 |