



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 10:30 AM UTC

PDB ID : 9ON9 / pdb_00009on9
BMRB ID : 31246
Title : Immature HIV-1 CACTD-SP1 lattice with Maturation inhibitor PF-46396 (R) and Inositol hexakisphosphate (IP6)
Authors : Zadorozhnyi, R.; Quinn, C.M.; Zadrozny, K.K.; Ablan, S.D.; Kennedy, B.J.; Yap, G.P.A.; Sanner, D.; Kraml, C.; Freed, E.O.; Ganser-Pornillos, B.K.; Pornillos, O.; Gronenborn, A.M.; Polenova, T.
Deposited on : 2025-05-14

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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](#) ①) were used in the production of this report:

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

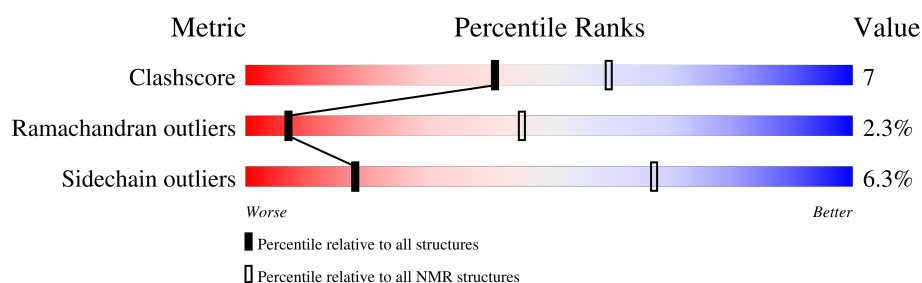
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 6%.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 102 | |
| 1 | H | 102 | |
| 1 | I | 102 | |
| 1 | J | 102 | |
| 1 | K | 102 | |
| 1 | L | 102 | |

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|--|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | G:148-G:239, H:148-H:238, I:148-I:221, I:227-I:238, J:147-J:239, K:147-K:238, L:148-L:238 (545) | 0.78 | 7 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

| Cluster number | Models |
|----------------|------------------|
| 1 | 1, 3, 4, 6, 7, 8 |
| 2 | 2, 9 |
| 3 | 5, 10 |

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9410 atoms, of which 4703 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

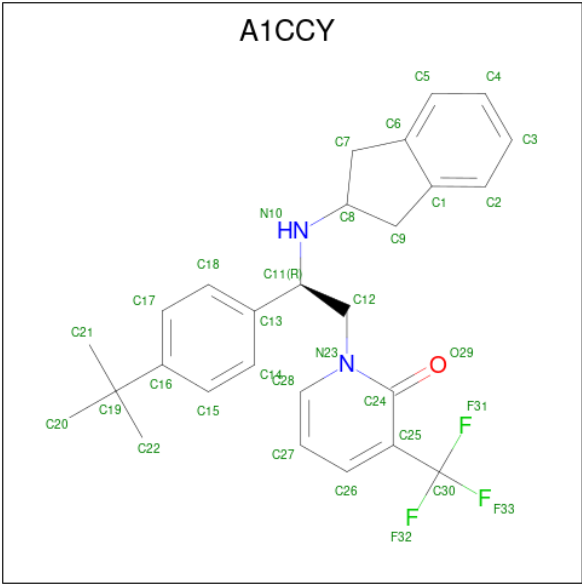
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | G | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | H | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | I | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | J | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | K | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | L | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 144 | GLY | - | expression tag | UNP P12497 |
| G | 145 | GLY | - | expression tag | UNP P12497 |
| G | 241 | THR | PRO | conflict | UNP P12497 |
| H | 144 | GLY | - | expression tag | UNP P12497 |
| H | 145 | GLY | - | expression tag | UNP P12497 |
| H | 241 | THR | PRO | conflict | UNP P12497 |
| I | 144 | GLY | - | expression tag | UNP P12497 |
| I | 145 | GLY | - | expression tag | UNP P12497 |
| I | 241 | THR | PRO | conflict | UNP P12497 |
| J | 144 | GLY | - | expression tag | UNP P12497 |
| J | 145 | GLY | - | expression tag | UNP P12497 |
| J | 241 | THR | PRO | conflict | UNP P12497 |
| K | 144 | GLY | - | expression tag | UNP P12497 |
| K | 145 | GLY | - | expression tag | UNP P12497 |
| K | 241 | THR | PRO | conflict | UNP P12497 |
| L | 144 | GLY | - | expression tag | UNP P12497 |
| L | 145 | GLY | - | expression tag | UNP P12497 |
| L | 241 | THR | PRO | conflict | UNP P12497 |

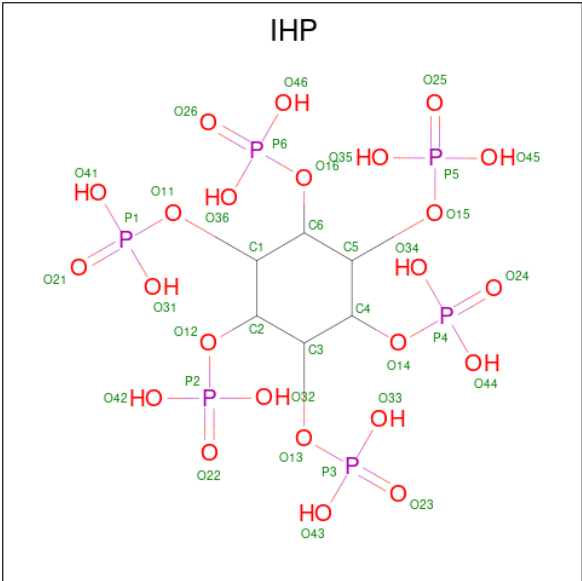
- Molecule 2 is 1-{(2R)-2-(4-tert-butylphenyl)-2-[(2,3-dihydro-1H-inden-2-yl)amino]ethyl}-3-(trifluoromethyl)pyridin-2(1H)-one (CCD ID: A1CCY) (formula: C₂₇H₂₉F₃N₂O) (labeled as

"Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | |
|-----|-------|----------|-------|----|---|----|---|---|
| | | | Total | C | F | H | N | O |
| 2 | H | 1 | 62 | 27 | 3 | 29 | 2 | 1 |

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



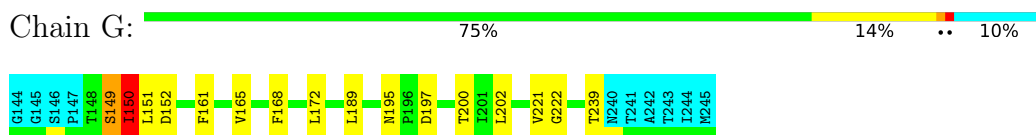
| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|---|---|----|---|
| | | | Total | C | H | O | P |
| 3 | I | 1 | 42 | 6 | 6 | 24 | 6 |

4 Residue-property plots [i](#)

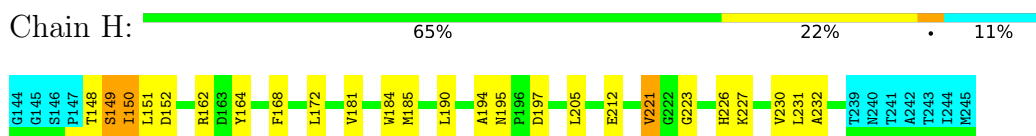
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

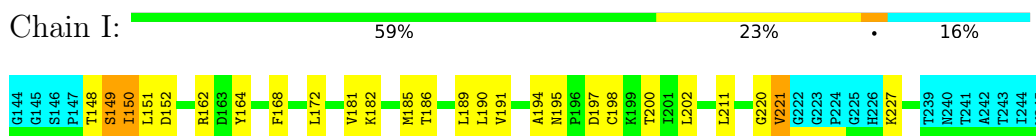
- Molecule 1: Capsid protein p24



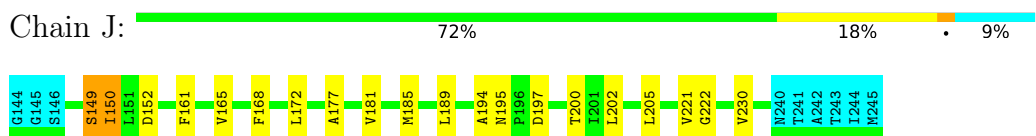
- Molecule 1: Capsid protein p24



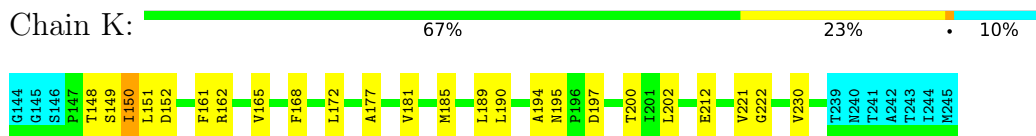
- Molecule 1: Capsid protein p24



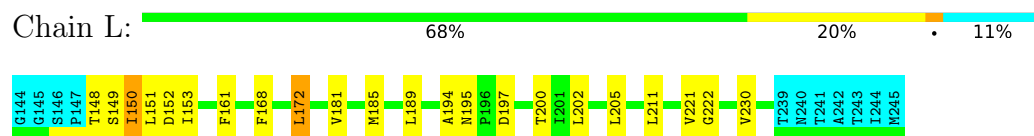
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

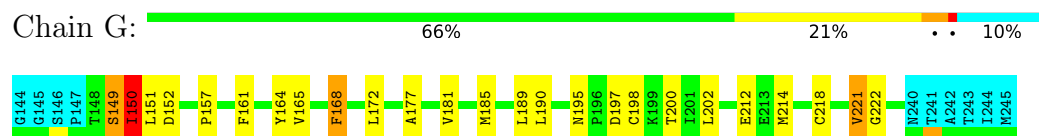


4.2 Scores per residue for each member of the ensemble

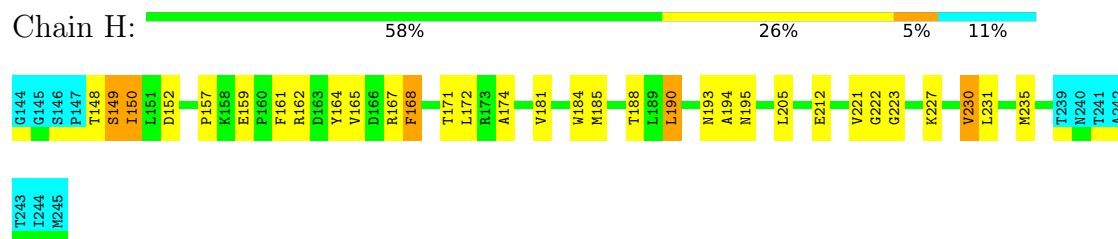
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

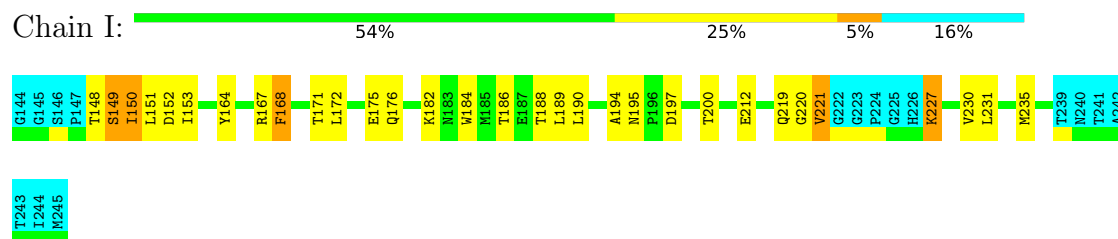
- Molecule 1: Capsid protein p24



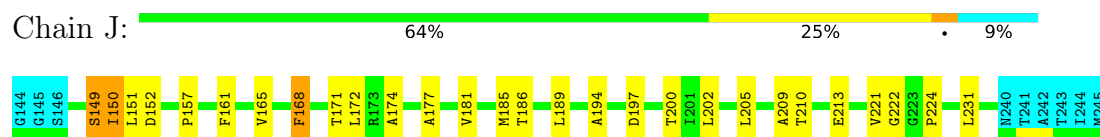
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

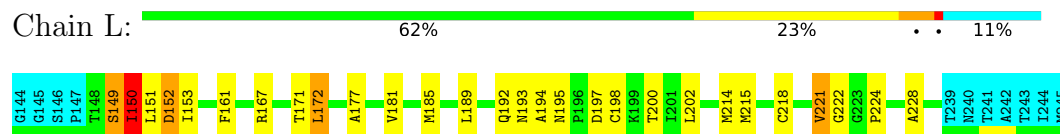


- Molecule 1: Capsid protein p24



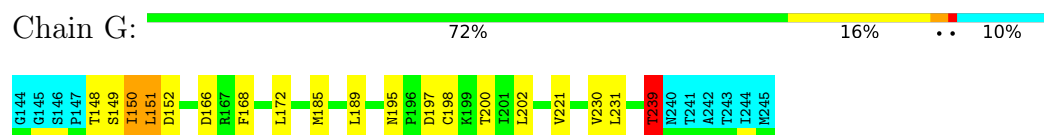


- Molecule 1: Capsid protein p24

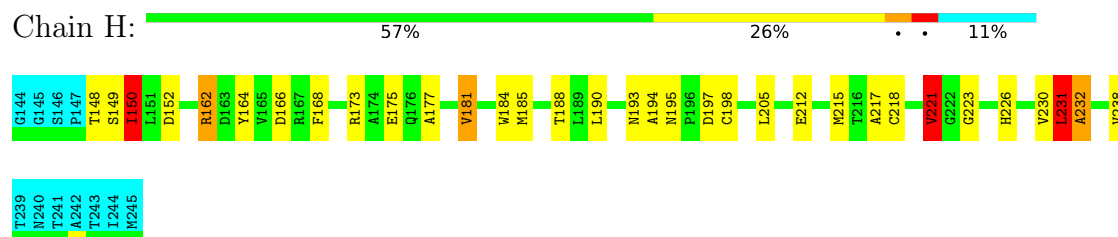


4.2.2 Score per residue for model 2

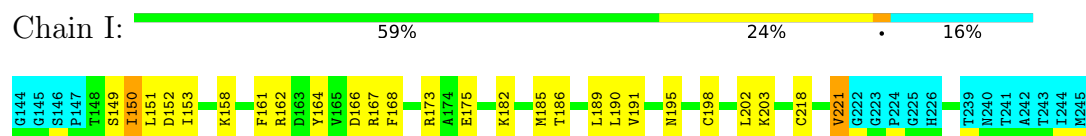
- Molecule 1: Capsid protein p24



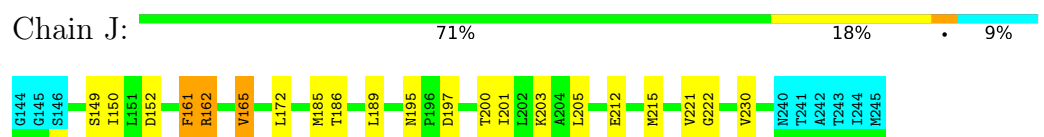
- Molecule 1: Capsid protein p24



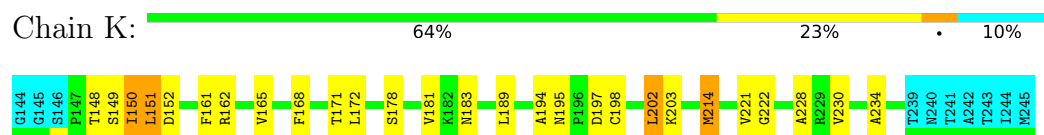
- Molecule 1: Capsid protein p24



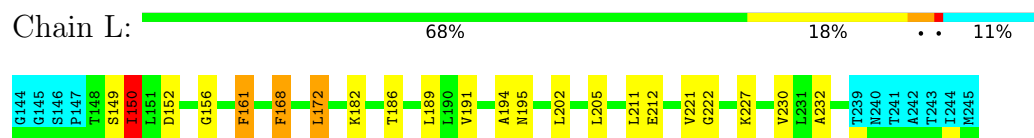
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

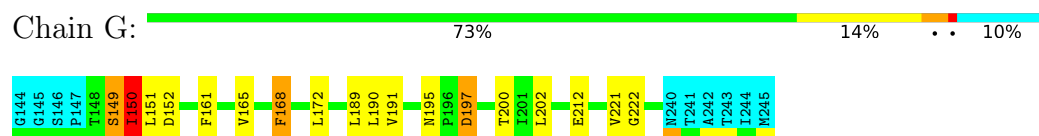


- Molecule 1: Capsid protein p24

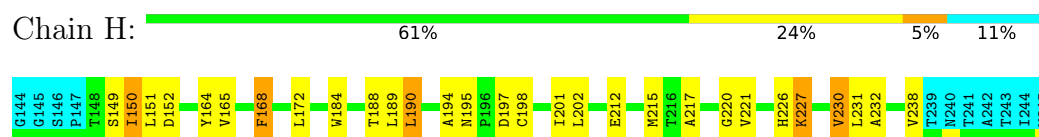


4.2.3 Score per residue for model 3

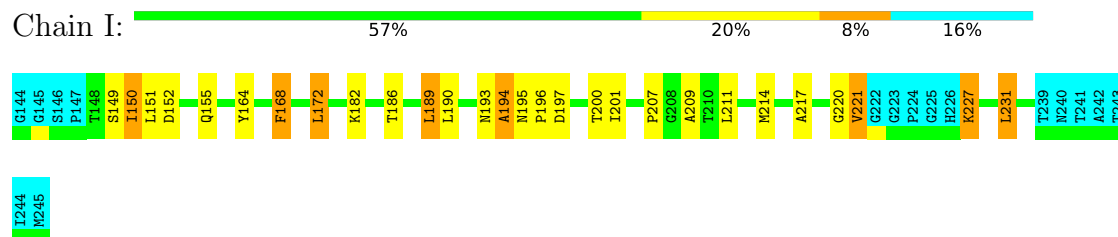
- Molecule 1: Capsid protein p24



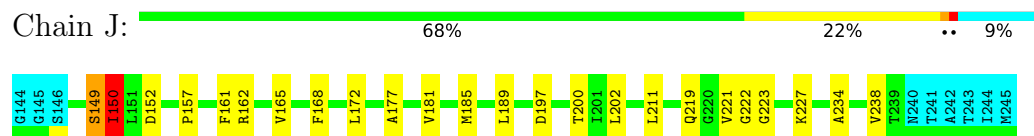
- Molecule 1: Capsid protein p24



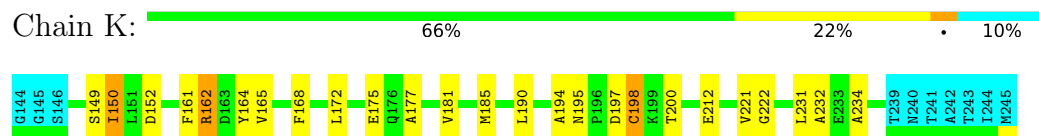
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

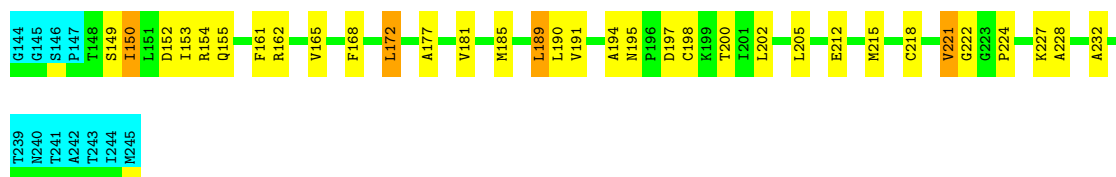


- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24





4.2.4 Score per residue for model 4

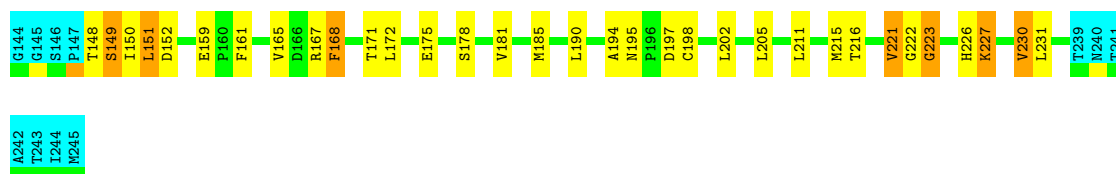
- Molecule 1: Capsid protein p24

Chain G: 71% 16% 10%



- Molecule 1: Capsid protein p24

Chain H: 57% 25% 7% 11%



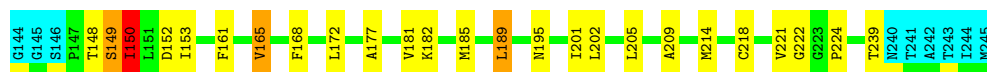
- Molecule 1: Capsid protein p24

Chain I: 62% 19% 16%



- Molecule 1: Capsid protein p24

Chain J: 67% 21% 9%



- Molecule 1: Capsid protein p24

Chain K: 75% 13% 10%



- Molecule 1: Capsid protein p24

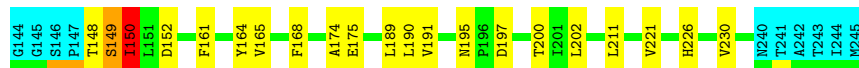
Chain L: 66% 22% 11%



4.2.5 Score per residue for model 5

- Molecule 1: Capsid protein p24

Chain G: 70% 19% 10%



- Molecule 1: Capsid protein p24

Chain H: 64% 18% 8% 11%



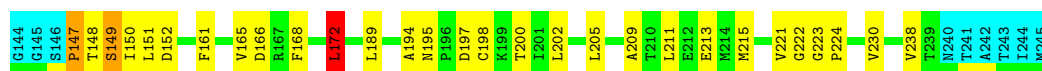
- Molecule 1: Capsid protein p24

Chain I: 52% 26% 6% 16%



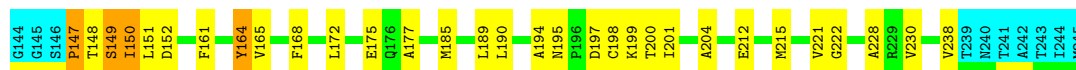
- Molecule 1: Capsid protein p24

Chain J: 63% 25% 9%



- Molecule 1: Capsid protein p24

Chain K: 60% 26% 10%



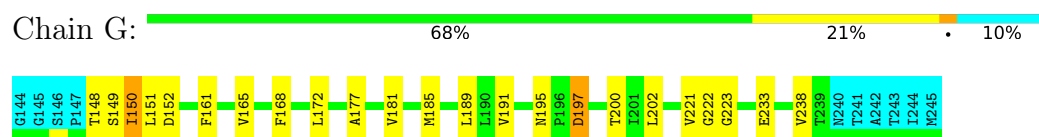
- Molecule 1: Capsid protein p24

Chain L: 64% 21% 11%

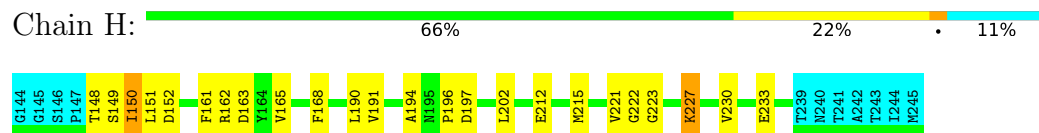


4.2.6 Score per residue for model 6

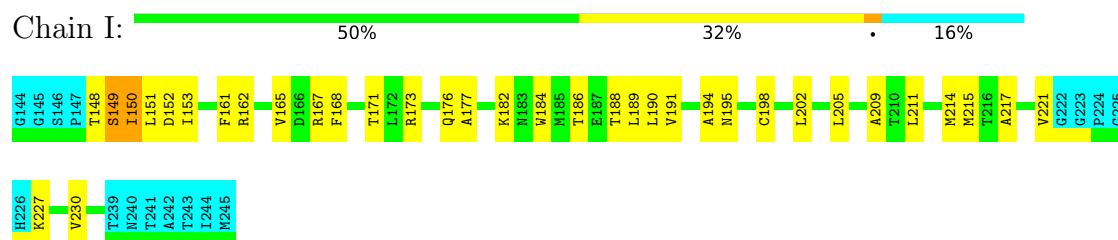
- Molecule 1: Capsid protein p24



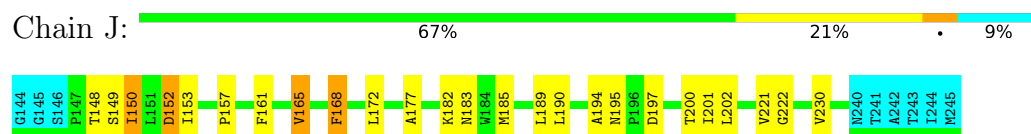
- Molecule 1: Capsid protein p24



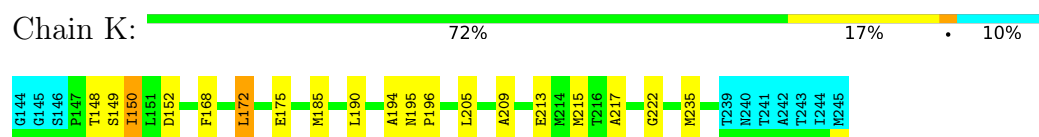
- Molecule 1: Capsid protein p24



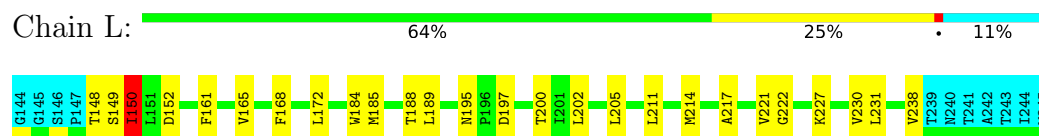
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



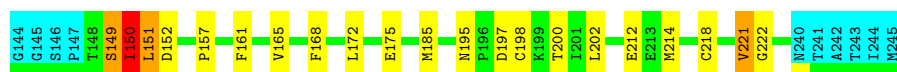
- Molecule 1: Capsid protein p24



4.2.7 Score per residue for model 7 (medoid)

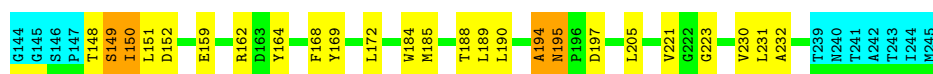
- Molecule 1: Capsid protein p24

Chain G:  70% 17% • • 10%



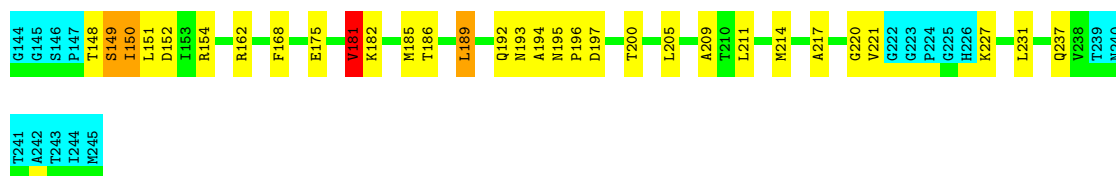
- Molecule 1: Capsid protein p24

Chain H:  65% 21% • 11%



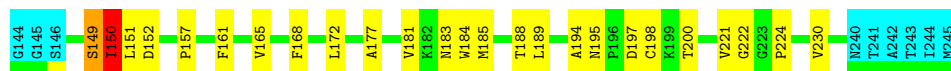
- Molecule 1: Capsid protein p24

Chain I:  54% 26% • • 16%



- Molecule 1: Capsid protein p24

Chain J:  67% 23% • • 9%



- Molecule 1: Capsid protein p24

Chain K:  62% 26% • • 10%



- Molecule 1: Capsid protein p24

Chain L:  63% 20% 7% 11%



4.2.8 Score per residue for model 8

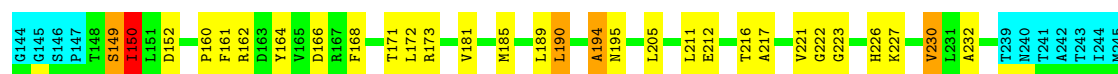
- Molecule 1: Capsid protein p24

Chain G: 



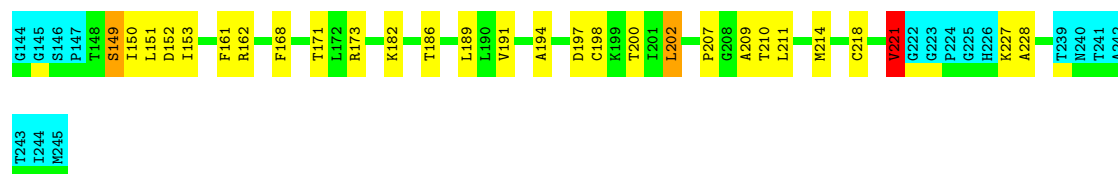
- Molecule 1: Capsid protein p24

Chain H: 



- Molecule 1: Capsid protein p24

Chain I: 



- Molecule 1: Capsid protein p24

Chain J: 



- Molecule 1: Capsid protein p24

Chain K: 



- Molecule 1: Capsid protein p24

Chain L: 



4.2.9 Score per residue for model 9

- Molecule 1: Capsid protein p24

Chain G: 



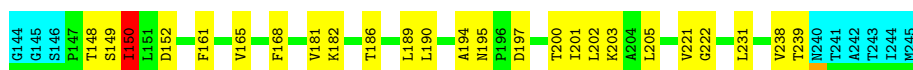
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



4.2.10 Score per residue for model 10

- Molecule 1: Capsid protein p24





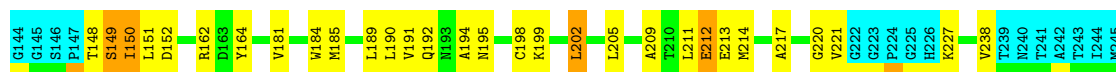
- Molecule 1: Capsid protein p24

Chain H: 61% 24% 5% 11%



- Molecule 1: Capsid protein p24

Chain I: 55% 25% 16%



- Molecule 1: Capsid protein p24

Chain J: 63% 25% 9%



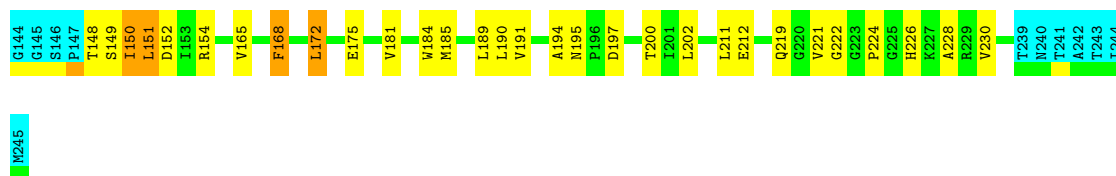
- Molecule 1: Capsid protein p24

Chain K: 67% 21% 10%



- Molecule 1: Capsid protein p24

Chain L: 60% 25% 11%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH | structure calculation | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 516 |
| Number of shifts mapped to atoms | 516 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 6% |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, A1CCY

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 (average) 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 | G | 1.29±0.05 | 3±1/720 (0.4± 0.2%) | 1.49±0.03 | 9±2/974 (0.9± 0.2%) |
| 1 | H | 1.39±0.04 | 6±2/713 (0.8± 0.3%) | 1.58±0.07 | 13±3/964 (1.4± 0.3%) |
| 1 | I | 1.34±0.07 | 4±2/682 (0.7± 0.3%) | 1.51±0.04 | 11±2/922 (1.2± 0.2%) |
| 1 | J | 1.19±0.05 | 2±2/728 (0.3± 0.3%) | 1.52±0.03 | 13±2/985 (1.3± 0.2%) |
| 1 | K | 1.24±0.06 | 2±2/721 (0.3± 0.2%) | 1.48±0.06 | 10±3/975 (1.0± 0.3%) |
| 1 | L | 1.27±0.06 | 4±1/713 (0.5± 0.2%) | 1.52±0.06 | 11±2/964 (1.1± 0.3%) |
| All | All | 1.29 | 216/42770 (0.5%) | 1.52 | 663/57840 (1.1%) |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | H | 0.0±0.0 | 0.3±0.5 |
| 1 | I | 0.0±0.0 | 0.6±0.7 |
| 1 | K | 0.0±0.0 | 0.4±0.5 |
| 1 | L | 0.0±0.0 | 0.2±0.4 |
| All | All | 0 | 15 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | L | 152 | ASP | C-N | 12.06 | 1.45 | 1.33 | 9 | 6 |
| 1 | L | 221 | VAL | C-N | 10.29 | 1.41 | 1.33 | 4 | 6 |
| 1 | H | 221 | VAL | N-CA | 10.10 | 1.58 | 1.46 | 9 | 9 |
| 1 | I | 151 | LEU | N-CA | -9.92 | 1.34 | 1.46 | 5 | 2 |
| 1 | I | 152 | ASP | C-N | 9.68 | 1.46 | 1.33 | 2 | 3 |
| 1 | I | 221 | VAL | CA-C | -9.68 | 1.40 | 1.52 | 4 | 7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | H | 232 | ALA | N-CA | -9.61 | 1.34 | 1.46 | 2 | 4 |
| 1 | H | 223 | GLY | C-N | -9.12 | 1.23 | 1.34 | 6 | 5 |
| 1 | I | 221 | VAL | N-CA | 8.56 | 1.57 | 1.46 | 7 | 6 |
| 1 | H | 221 | VAL | C-N | 8.23 | 1.42 | 1.32 | 8 | 6 |
| 1 | G | 150 | ILE | C-N | -8.15 | 1.22 | 1.33 | 7 | 4 |
| 1 | K | 150 | ILE | C-N | -8.12 | 1.22 | 1.33 | 7 | 2 |
| 1 | H | 149 | SER | C-O | -7.94 | 1.14 | 1.24 | 4 | 2 |
| 1 | L | 151 | LEU | C-N | 7.86 | 1.44 | 1.33 | 10 | 1 |
| 1 | J | 152 | ASP | N-CA | -7.85 | 1.38 | 1.46 | 3 | 2 |
| 1 | I | 149 | SER | C-N | -7.74 | 1.24 | 1.33 | 5 | 2 |
| 1 | I | 150 | ILE | N-CA | 7.73 | 1.53 | 1.46 | 10 | 1 |
| 1 | K | 152 | ASP | N-CA | -7.71 | 1.37 | 1.46 | 1 | 5 |
| 1 | J | 150 | ILE | C-N | -7.51 | 1.23 | 1.33 | 3 | 1 |
| 1 | L | 152 | ASP | N-CA | -7.36 | 1.38 | 1.46 | 8 | 2 |
| 1 | I | 227 | LYS | N-CA | -7.29 | 1.36 | 1.46 | 3 | 2 |
| 1 | J | 151 | LEU | CA-C | -7.18 | 1.43 | 1.52 | 7 | 1 |
| 1 | G | 151 | LEU | CA-CB | -7.04 | 1.42 | 1.53 | 2 | 5 |
| 1 | I | 220 | GLY | C-N | 7.03 | 1.42 | 1.33 | 10 | 5 |
| 1 | H | 231 | LEU | CA-C | -7.00 | 1.44 | 1.52 | 2 | 5 |
| 1 | J | 223 | GLY | CA-C | 6.97 | 1.56 | 1.51 | 5 | 2 |
| 1 | K | 221 | VAL | C-N | 6.94 | 1.38 | 1.33 | 5 | 1 |
| 1 | L | 151 | LEU | N-CA | -6.94 | 1.37 | 1.46 | 5 | 2 |
| 1 | K | 223 | GLY | CA-C | 6.92 | 1.61 | 1.51 | 9 | 1 |
| 1 | H | 220 | GLY | C-N | 6.81 | 1.43 | 1.33 | 9 | 3 |
| 1 | H | 221 | VAL | CA-C | -6.73 | 1.44 | 1.52 | 9 | 3 |
| 1 | J | 150 | ILE | N-CA | 6.67 | 1.52 | 1.46 | 7 | 1 |
| 1 | G | 150 | ILE | CA-C | -6.64 | 1.44 | 1.52 | 10 | 2 |
| 1 | G | 152 | ASP | N-CA | -6.63 | 1.38 | 1.46 | 6 | 3 |
| 1 | K | 151 | LEU | CA-C | -6.63 | 1.44 | 1.52 | 1 | 2 |
| 1 | J | 221 | VAL | C-N | 6.58 | 1.38 | 1.33 | 9 | 5 |
| 1 | G | 239 | THR | N-CA | -6.58 | 1.38 | 1.46 | 2 | 1 |
| 1 | I | 149 | SER | N-CA | -6.57 | 1.38 | 1.46 | 6 | 2 |
| 1 | H | 150 | ILE | N-CA | 6.54 | 1.52 | 1.46 | 8 | 1 |
| 1 | J | 152 | ASP | C-N | 6.54 | 1.42 | 1.33 | 6 | 5 |
| 1 | G | 223 | GLY | C-N | -6.52 | 1.26 | 1.34 | 6 | 2 |
| 1 | K | 195 | ASN | N-CA | 6.47 | 1.55 | 1.46 | 7 | 2 |
| 1 | H | 152 | ASP | C-N | 6.39 | 1.40 | 1.33 | 5 | 1 |
| 1 | L | 153 | ILE | CA-CB | 6.38 | 1.61 | 1.53 | 9 | 2 |
| 1 | L | 221 | VAL | N-CA | 6.23 | 1.54 | 1.46 | 4 | 2 |
| 1 | G | 149 | SER | CA-CB | -6.20 | 1.43 | 1.53 | 5 | 1 |
| 1 | H | 152 | ASP | N-CA | -6.17 | 1.38 | 1.46 | 7 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | G | 151 | LEU | N-CA | -6.15 | 1.38 | 1.46 | 7 | 5 |
| 1 | G | 221 | VAL | C-N | 6.14 | 1.42 | 1.33 | 6 | 2 |
| 1 | G | 151 | LEU | CA-C | -6.11 | 1.44 | 1.52 | 6 | 2 |
| 1 | G | 221 | VAL | N-CA | 6.04 | 1.53 | 1.46 | 8 | 2 |
| 1 | I | 152 | ASP | N-CA | -6.01 | 1.38 | 1.46 | 7 | 3 |
| 1 | I | 227 | LYS | CA-CB | -5.93 | 1.43 | 1.53 | 1 | 1 |
| 1 | L | 149 | SER | C-O | -5.87 | 1.16 | 1.23 | 7 | 2 |
| 1 | L | 150 | ILE | C-N | -5.75 | 1.26 | 1.33 | 3 | 3 |
| 1 | I | 149 | SER | C-O | -5.75 | 1.16 | 1.24 | 5 | 3 |
| 1 | L | 154 | ARG | N-CA | 5.74 | 1.53 | 1.45 | 3 | 1 |
| 1 | H | 221 | VAL | C-O | -5.72 | 1.17 | 1.24 | 9 | 1 |
| 1 | I | 202 | LEU | CB-CG | 5.67 | 1.64 | 1.53 | 9 | 1 |
| 1 | L | 174 | ALA | N-CA | 5.67 | 1.53 | 1.45 | 5 | 1 |
| 1 | K | 214 | MET | C-O | -5.63 | 1.17 | 1.24 | 2 | 1 |
| 1 | J | 161 | PHE | C-N | 5.63 | 1.40 | 1.33 | 2 | 1 |
| 1 | H | 194 | ALA | CA-C | 5.60 | 1.59 | 1.53 | 4 | 2 |
| 1 | I | 198 | CYS | C-O | -5.58 | 1.17 | 1.24 | 6 | 1 |
| 1 | K | 198 | CYS | C-O | -5.58 | 1.17 | 1.24 | 5 | 1 |
| 1 | H | 151 | LEU | N-CA | -5.53 | 1.39 | 1.46 | 10 | 2 |
| 1 | J | 151 | LEU | C-N | 5.53 | 1.41 | 1.33 | 5 | 1 |
| 1 | L | 151 | LEU | CA-C | -5.53 | 1.45 | 1.52 | 1 | 1 |
| 1 | J | 149 | SER | C-O | -5.52 | 1.17 | 1.24 | 7 | 1 |
| 1 | L | 149 | SER | C-N | 5.52 | 1.40 | 1.33 | 9 | 1 |
| 1 | K | 152 | ASP | C-N | 5.50 | 1.39 | 1.33 | 4 | 2 |
| 1 | L | 151 | LEU | CA-CB | -5.50 | 1.44 | 1.53 | 1 | 2 |
| 1 | K | 148 | THR | N-CA | 5.48 | 1.53 | 1.46 | 1 | 1 |
| 1 | K | 149 | SER | C-N | -5.47 | 1.28 | 1.33 | 1 | 1 |
| 1 | H | 232 | ALA | CA-C | 5.41 | 1.60 | 1.52 | 2 | 2 |
| 1 | L | 175 | GLU | CA-CB | 5.36 | 1.61 | 1.53 | 5 | 1 |
| 1 | G | 239 | THR | CA-C | 5.36 | 1.59 | 1.52 | 4 | 1 |
| 1 | K | 194 | ALA | CA-C | 5.35 | 1.59 | 1.52 | 9 | 1 |
| 1 | J | 198 | CYS | C-O | -5.34 | 1.17 | 1.24 | 7 | 2 |
| 1 | I | 176 | GLN | N-CA | 5.30 | 1.53 | 1.46 | 6 | 1 |
| 1 | K | 151 | LEU | N-CA | -5.28 | 1.39 | 1.46 | 4 | 1 |
| 1 | H | 151 | LEU | CA-C | -5.27 | 1.46 | 1.52 | 7 | 1 |
| 1 | K | 223 | GLY | C-N | -5.25 | 1.27 | 1.34 | 8 | 1 |
| 1 | I | 190 | LEU | N-CA | 5.20 | 1.52 | 1.46 | 9 | 1 |
| 1 | H | 151 | LEU | C-N | 5.17 | 1.40 | 1.33 | 3 | 1 |
| 1 | L | 153 | ILE | C-N | 5.16 | 1.40 | 1.33 | 3 | 2 |
| 1 | L | 155 | GLN | N-CA | 5.16 | 1.52 | 1.46 | 3 | 1 |
| 1 | I | 181 | VAL | C-O | -5.14 | 1.18 | 1.24 | 7 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | H | 193 | ASN | C-N | 5.11 | 1.40 | 1.33 | 2 | 2 |
| 1 | G | 149 | SER | C-O | -5.09 | 1.18 | 1.24 | 8 | 1 |
| 1 | H | 150 | ILE | C-N | -5.09 | 1.27 | 1.33 | 10 | 1 |
| 1 | H | 162 | ARG | CZ-NH2 | -5.06 | 1.26 | 1.33 | 7 | 1 |
| 1 | I | 150 | ILE | CA-CB | 5.06 | 1.60 | 1.54 | 10 | 1 |
| 1 | H | 195 | ASN | N-CA | 5.06 | 1.53 | 1.46 | 7 | 1 |
| 1 | L | 181 | VAL | C-O | -5.05 | 1.18 | 1.24 | 8 | 1 |
| 1 | H | 222 | GLY | CA-C | -5.03 | 1.44 | 1.51 | 6 | 1 |
| 1 | J | 149 | SER | N-CA | -5.03 | 1.40 | 1.46 | 8 | 1 |
| 1 | K | 214 | MET | C-N | -5.03 | 1.27 | 1.33 | 7 | 1 |
| 1 | L | 162 | ARG | C-N | 5.02 | 1.39 | 1.33 | 5 | 1 |
| 1 | I | 162 | ARG | CZ-NH2 | -5.01 | 1.26 | 1.33 | 10 | 1 |
| 1 | I | 151 | LEU | C-N | 5.00 | 1.43 | 1.34 | 5 | 1 |
| 1 | H | 160 | PRO | N-CA | 5.00 | 1.51 | 1.46 | 8 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | H | 230 | VAL | N-CA-C | 12.95 | 122.86 | 110.30 | 1 | 8 |
| 1 | L | 222 | GLY | N-CA-C | 12.36 | 127.31 | 111.37 | 3 | 1 |
| 1 | K | 222 | GLY | CA-C-N | 9.92 | 137.44 | 121.87 | 9 | 10 |
| 1 | K | 222 | GLY | C-N-CA | 9.92 | 137.44 | 121.87 | 9 | 10 |
| 1 | H | 222 | GLY | CA-C-O | -9.78 | 114.41 | 122.33 | 5 | 3 |
| 1 | L | 149 | SER | N-CA-C | 9.17 | 120.88 | 111.07 | 1 | 1 |
| 1 | L | 221 | VAL | CA-C-O | -9.05 | 112.08 | 122.13 | 1 | 7 |
| 1 | I | 221 | VAL | N-CA-C | -8.92 | 97.33 | 109.37 | 6 | 4 |
| 1 | I | 152 | ASP | CA-C-N | -8.84 | 111.33 | 122.37 | 2 | 8 |
| 1 | I | 152 | ASP | C-N-CA | -8.84 | 111.33 | 122.37 | 2 | 8 |
| 1 | I | 152 | ASP | CA-C-O | -8.75 | 111.74 | 119.97 | 3 | 6 |
| 1 | I | 150 | ILE | CB-CA-C | 8.74 | 122.31 | 111.65 | 3 | 3 |
| 1 | L | 222 | GLY | CA-C-O | -8.64 | 115.07 | 122.16 | 10 | 4 |
| 1 | J | 222 | GLY | CA-C-O | -8.56 | 116.12 | 122.37 | 6 | 2 |
| 1 | J | 152 | ASP | CA-C-O | -8.34 | 112.13 | 119.97 | 7 | 2 |
| 1 | H | 222 | GLY | CA-C-N | -8.29 | 108.85 | 121.87 | 4 | 1 |
| 1 | H | 222 | GLY | C-N-CA | -8.29 | 108.85 | 121.87 | 4 | 1 |
| 1 | I | 221 | VAL | CA-C-N | -8.28 | 107.45 | 120.86 | 4 | 9 |
| 1 | I | 221 | VAL | C-N-CA | -8.28 | 107.45 | 120.86 | 4 | 9 |
| 1 | K | 222 | GLY | CA-C-O | -8.21 | 115.68 | 122.33 | 5 | 2 |
| 1 | G | 152 | ASP | CA-C-N | -8.16 | 109.88 | 120.98 | 9 | 10 |
| 1 | G | 152 | ASP | C-N-CA | -8.16 | 109.88 | 120.98 | 9 | 10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | G | 222 | GLY | CA-C-O | -8.08 | 115.78 | 122.33 | 4 | 2 |
| 1 | H | 151 | LEU | N-CA-C | -8.02 | 102.54 | 111.28 | 9 | 2 |
| 1 | G | 149 | SER | N-CA-C | 8.00 | 119.78 | 111.14 | 3 | 8 |
| 1 | H | 152 | ASP | CA-C-O | -8.00 | 113.82 | 121.02 | 6 | 4 |
| 1 | H | 152 | ASP | CA-C-N | -7.96 | 110.16 | 120.98 | 1 | 7 |
| 1 | H | 152 | ASP | C-N-CA | -7.96 | 110.16 | 120.98 | 1 | 7 |
| 1 | L | 151 | LEU | N-CA-C | -7.91 | 102.66 | 111.28 | 9 | 3 |
| 1 | K | 152 | ASP | CA-C-N | -7.90 | 110.23 | 120.98 | 7 | 10 |
| 1 | K | 152 | ASP | C-N-CA | -7.90 | 110.23 | 120.98 | 7 | 10 |
| 1 | H | 221 | VAL | CA-C-O | -7.84 | 112.10 | 121.28 | 7 | 8 |
| 1 | I | 221 | VAL | CA-C-O | -7.83 | 112.05 | 121.13 | 6 | 2 |
| 1 | L | 152 | ASP | CA-C-N | -7.82 | 110.86 | 121.80 | 2 | 8 |
| 1 | L | 152 | ASP | C-N-CA | -7.82 | 110.86 | 121.80 | 2 | 8 |
| 1 | H | 197 | ASP | CA-CB-CG | -7.80 | 104.80 | 112.60 | 10 | 6 |
| 1 | I | 151 | LEU | N-CA-C | -7.77 | 102.81 | 111.28 | 5 | 6 |
| 1 | J | 147 | PRO | N-CA-C | -7.72 | 99.06 | 111.19 | 5 | 2 |
| 1 | H | 184 | TRP | CB-CG-CD2 | 7.71 | 137.59 | 126.80 | 5 | 1 |
| 1 | G | 212 | GLU | N-CA-C | -7.69 | 102.98 | 111.36 | 3 | 4 |
| 1 | G | 221 | VAL | CA-C-O | -7.69 | 112.90 | 121.36 | 9 | 7 |
| 1 | L | 152 | ASP | N-CA-CB | -7.68 | 97.51 | 110.49 | 1 | 4 |
| 1 | J | 152 | ASP | CA-C-N | -7.64 | 111.12 | 121.66 | 5 | 7 |
| 1 | J | 152 | ASP | C-N-CA | -7.64 | 111.12 | 121.66 | 5 | 7 |
| 1 | J | 152 | ASP | N-CA-CB | -7.60 | 97.65 | 110.49 | 6 | 5 |
| 1 | H | 152 | ASP | N-CA-CB | -7.58 | 97.67 | 110.49 | 9 | 2 |
| 1 | I | 220 | GLY | N-CA-C | -7.46 | 105.13 | 114.16 | 5 | 7 |
| 1 | H | 162 | ARG | N-CA-C | 7.46 | 119.20 | 111.14 | 2 | 3 |
| 1 | J | 223 | GLY | O-C-N | -7.43 | 118.39 | 121.07 | 5 | 1 |
| 1 | H | 150 | ILE | N-CA-C | 7.38 | 120.29 | 113.20 | 2 | 2 |
| 1 | L | 161 | PHE | CA-CB-CG | -7.28 | 106.53 | 113.80 | 2 | 2 |
| 1 | I | 221 | VAL | N-CA-CB | 7.27 | 119.64 | 110.05 | 1 | 3 |
| 1 | I | 194 | ALA | N-CA-C | 7.24 | 120.20 | 107.61 | 5 | 8 |
| 1 | K | 194 | ALA | N-CA-C | 7.20 | 119.33 | 109.11 | 8 | 5 |
| 1 | J | 194 | ALA | N-CA-C | 7.17 | 120.43 | 108.73 | 9 | 7 |
| 1 | I | 150 | ILE | N-CA-C | 7.16 | 118.97 | 112.17 | 6 | 4 |
| 1 | K | 223 | GLY | N-CA-C | 7.16 | 126.95 | 112.34 | 9 | 1 |
| 1 | J | 162 | ARG | N-CA-C | 7.13 | 118.74 | 110.97 | 2 | 2 |
| 1 | J | 205 | LEU | N-CA-C | -7.12 | 103.52 | 111.28 | 2 | 7 |
| 1 | H | 149 | SER | N-CA-C | 7.11 | 122.14 | 112.68 | 10 | 4 |
| 1 | H | 194 | ALA | N-CA-C | 7.11 | 120.07 | 108.26 | 1 | 10 |
| 1 | H | 159 | GLU | N-CA-C | 7.09 | 118.72 | 109.93 | 4 | 4 |
| 1 | K | 149 | SER | N-CA-C | 7.08 | 122.10 | 112.68 | 5 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | L | 221 | VAL | N-CA-C | -7.06 | 102.23 | 110.21 | 1 | 2 |
| 1 | J | 152 | ASP | CA-CB-CG | -7.04 | 105.56 | 112.60 | 7 | 2 |
| 1 | L | 194 | ALA | N-CA-C | 6.96 | 120.93 | 107.71 | 5 | 7 |
| 1 | L | 222 | GLY | CA-C-N | -6.94 | 110.98 | 121.87 | 1 | 9 |
| 1 | L | 222 | GLY | C-N-CA | -6.94 | 110.98 | 121.87 | 1 | 9 |
| 1 | J | 221 | VAL | CA-C-O | -6.91 | 113.76 | 121.36 | 3 | 8 |
| 1 | J | 150 | ILE | N-CA-C | 6.90 | 118.77 | 112.43 | 3 | 2 |
| 1 | L | 174 | ALA | N-CA-C | 6.89 | 122.79 | 113.97 | 5 | 1 |
| 1 | J | 222 | GLY | N-CA-C | -6.87 | 105.15 | 112.08 | 6 | 2 |
| 1 | J | 149 | SER | N-CA-C | 6.80 | 118.77 | 111.36 | 1 | 6 |
| 1 | K | 150 | ILE | N-CA-C | 6.76 | 119.69 | 113.20 | 7 | 1 |
| 1 | H | 223 | GLY | N-CA-C | 6.75 | 126.10 | 112.34 | 1 | 5 |
| 1 | H | 153 | ILE | N-CA-CB | -6.74 | 103.40 | 110.95 | 5 | 1 |
| 1 | L | 150 | ILE | CB-CA-C | 6.74 | 117.90 | 110.62 | 1 | 2 |
| 1 | G | 152 | ASP | CA-C-O | -6.72 | 113.47 | 120.32 | 6 | 2 |
| 1 | H | 151 | LEU | CB-CA-C | -6.72 | 99.64 | 110.79 | 7 | 2 |
| 1 | K | 223 | GLY | O-C-N | -6.65 | 115.12 | 121.77 | 9 | 1 |
| 1 | J | 222 | GLY | CA-C-N | -6.63 | 111.45 | 121.87 | 7 | 9 |
| 1 | J | 222 | GLY | C-N-CA | -6.63 | 111.45 | 121.87 | 7 | 9 |
| 1 | H | 230 | VAL | N-CA-CB | -6.59 | 103.44 | 110.62 | 6 | 2 |
| 1 | G | 150 | ILE | CB-CA-C | 6.58 | 117.22 | 110.70 | 1 | 1 |
| 1 | H | 212 | GLU | N-CA-C | -6.58 | 104.11 | 111.28 | 3 | 6 |
| 1 | H | 184 | TRP | CA-CB-CG | 6.58 | 126.10 | 113.60 | 5 | 1 |
| 1 | J | 149 | SER | CA-C-O | -6.57 | 113.87 | 120.90 | 7 | 1 |
| 1 | J | 221 | VAL | CA-C-N | -6.56 | 113.21 | 122.85 | 10 | 9 |
| 1 | J | 221 | VAL | C-N-CA | -6.56 | 113.21 | 122.85 | 10 | 9 |
| 1 | K | 197 | ASP | CA-CB-CG | -6.54 | 106.06 | 112.60 | 2 | 1 |
| 1 | I | 151 | LEU | CB-CA-C | -6.51 | 99.98 | 110.79 | 7 | 3 |
| 1 | L | 150 | ILE | N-CA-CB | -6.50 | 104.59 | 112.33 | 1 | 2 |
| 1 | J | 221 | VAL | N-CA-C | -6.49 | 100.61 | 109.37 | 2 | 5 |
| 1 | G | 221 | VAL | CA-C-N | -6.46 | 113.22 | 122.64 | 8 | 4 |
| 1 | G | 221 | VAL | C-N-CA | -6.46 | 113.22 | 122.64 | 8 | 4 |
| 1 | J | 161 | PHE | CA-CB-CG | -6.44 | 107.36 | 113.80 | 2 | 1 |
| 1 | J | 201 | ILE | CB-CA-C | -6.37 | 102.67 | 111.65 | 8 | 4 |
| 1 | H | 222 | GLY | N-CA-C | -6.36 | 103.27 | 112.17 | 4 | 2 |
| 1 | H | 231 | LEU | O-C-N | 6.36 | 128.62 | 122.07 | 2 | 1 |
| 1 | G | 197 | ASP | CA-CB-CG | -6.34 | 106.26 | 112.60 | 6 | 3 |
| 1 | H | 221 | VAL | CA-C-N | -6.31 | 113.80 | 122.57 | 5 | 4 |
| 1 | H | 221 | VAL | C-N-CA | -6.31 | 113.80 | 122.57 | 5 | 4 |
| 1 | L | 221 | VAL | CA-C-N | -6.29 | 110.28 | 121.67 | 3 | 6 |
| 1 | L | 221 | VAL | C-N-CA | -6.29 | 110.28 | 121.67 | 3 | 6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | H | 220 | GLY | N-CA-C | -6.22 | 106.64 | 114.16 | 3 | 1 |
| 1 | L | 192 | GLN | N-CA-C | 6.21 | 118.13 | 111.36 | 1 | 2 |
| 1 | H | 184 | TRP | CB-CG-CD1 | -6.16 | 117.66 | 126.90 | 5 | 1 |
| 1 | K | 221 | VAL | CA-C-O | -6.14 | 114.10 | 121.28 | 5 | 4 |
| 1 | J | 172 | LEU | CB-CA-C | -6.13 | 101.00 | 110.81 | 5 | 1 |
| 1 | L | 205 | LEU | N-CA-C | -6.13 | 104.60 | 111.28 | 8 | 5 |
| 1 | I | 149 | SER | N-CA-C | 6.10 | 122.40 | 110.56 | 10 | 4 |
| 1 | L | 150 | ILE | CA-CB-CG2 | 6.10 | 120.88 | 110.50 | 8 | 1 |
| 1 | L | 212 | GLU | N-CA-C | -6.10 | 104.71 | 111.36 | 3 | 3 |
| 1 | K | 221 | VAL | CA-C-N | -6.08 | 114.11 | 122.57 | 5 | 4 |
| 1 | K | 221 | VAL | C-N-CA | -6.08 | 114.11 | 122.57 | 5 | 4 |
| 1 | J | 165 | VAL | CB-CA-C | -6.07 | 104.11 | 111.88 | 4 | 3 |
| 1 | K | 152 | ASP | CA-C-O | -6.07 | 114.26 | 119.97 | 7 | 1 |
| 1 | K | 212 | GLU | N-CA-C | -6.07 | 104.67 | 111.28 | 4 | 6 |
| 1 | H | 150 | ILE | CB-CA-C | 6.06 | 118.41 | 110.84 | 7 | 2 |
| 1 | L | 152 | ASP | CA-C-O | -6.04 | 113.40 | 120.53 | 9 | 6 |
| 1 | I | 187 | GLU | N-CA-C | 6.04 | 117.53 | 111.07 | 5 | 1 |
| 1 | L | 149 | SER | CA-C-N | 6.03 | 130.12 | 121.02 | 9 | 1 |
| 1 | L | 149 | SER | C-N-CA | 6.03 | 130.12 | 121.02 | 9 | 1 |
| 1 | L | 151 | LEU | CA-C-O | -6.02 | 114.17 | 120.55 | 4 | 1 |
| 1 | G | 150 | ILE | CA-CB-CG2 | 5.97 | 120.65 | 110.50 | 5 | 5 |
| 1 | J | 151 | LEU | CA-C-O | -5.95 | 114.21 | 120.63 | 10 | 2 |
| 1 | H | 168 | PHE | CA-CB-CG | -5.94 | 107.86 | 113.80 | 4 | 3 |
| 1 | K | 155 | GLN | N-CA-C | -5.94 | 101.16 | 110.36 | 7 | 1 |
| 1 | H | 205 | LEU | N-CA-C | -5.93 | 104.81 | 111.28 | 10 | 4 |
| 1 | G | 239 | THR | CA-C-N | 5.90 | 132.81 | 121.54 | 4 | 1 |
| 1 | G | 239 | THR | C-N-CA | 5.90 | 132.81 | 121.54 | 4 | 1 |
| 1 | H | 227 | LYS | CB-CG-CD | -5.89 | 97.74 | 111.30 | 6 | 1 |
| 1 | H | 161 | PHE | CA-CB-CG | -5.88 | 107.92 | 113.80 | 4 | 1 |
| 1 | G | 222 | GLY | CA-C-N | -5.86 | 112.66 | 121.87 | 3 | 8 |
| 1 | G | 222 | GLY | C-N-CA | -5.86 | 112.66 | 121.87 | 3 | 8 |
| 1 | H | 152 | ASP | N-CA-C | 5.84 | 117.30 | 110.41 | 6 | 1 |
| 1 | J | 238 | VAL | CA-C-N | 5.82 | 132.66 | 121.54 | 9 | 1 |
| 1 | J | 238 | VAL | C-N-CA | 5.82 | 132.66 | 121.54 | 9 | 1 |
| 1 | J | 151 | LEU | CB-CA-C | -5.81 | 101.15 | 110.79 | 1 | 1 |
| 1 | K | 147 | PRO | N-CA-C | -5.78 | 102.13 | 111.03 | 5 | 2 |
| 1 | I | 212 | GLU | N-CA-C | -5.77 | 104.99 | 111.28 | 9 | 3 |
| 1 | K | 221 | VAL | N-CA-C | -5.75 | 101.35 | 109.63 | 3 | 4 |
| 1 | K | 222 | GLY | N-CA-C | -5.72 | 105.78 | 111.85 | 7 | 1 |
| 1 | K | 151 | LEU | CB-CA-C | -5.72 | 101.30 | 110.79 | 9 | 1 |
| 1 | I | 181 | VAL | N-CA-C | -5.71 | 104.80 | 110.62 | 9 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | I | 162 | ARG | N-CA-C | 5.70 | 117.17 | 111.07 | 7 | 1 |
| 1 | H | 150 | ILE | N-CA-CB | -5.67 | 105.97 | 112.21 | 7 | 1 |
| 1 | L | 184 | TRP | N-CA-CB | -5.65 | 101.59 | 110.06 | 10 | 1 |
| 1 | I | 227 | LYS | CB-CA-C | 5.64 | 120.55 | 109.72 | 9 | 1 |
| 1 | I | 192 | GLN | N-CA-C | 5.63 | 117.22 | 111.14 | 10 | 3 |
| 1 | I | 151 | LEU | CA-C-N | -5.62 | 113.65 | 122.65 | 2 | 1 |
| 1 | I | 151 | LEU | C-N-CA | -5.62 | 113.65 | 122.65 | 2 | 1 |
| 1 | G | 152 | ASP | N-CA-CB | -5.62 | 101.93 | 111.20 | 1 | 2 |
| 1 | I | 152 | ASP | N-CA-CB | -5.60 | 101.03 | 110.49 | 7 | 2 |
| 1 | G | 222 | GLY | N-CA-C | -5.59 | 105.92 | 111.85 | 4 | 1 |
| 1 | J | 166 | ASP | N-CA-C | -5.58 | 105.20 | 111.28 | 5 | 1 |
| 1 | H | 153 | ILE | N-CA-C | 5.54 | 120.86 | 109.34 | 9 | 1 |
| 1 | J | 150 | ILE | CA-CB-CG2 | 5.51 | 119.87 | 110.50 | 7 | 1 |
| 1 | L | 195 | ASN | CA-CB-CG | -5.50 | 107.11 | 112.60 | 9 | 1 |
| 1 | G | 221 | VAL | N-CA-C | -5.49 | 101.72 | 109.63 | 9 | 4 |
| 1 | L | 182 | LYS | CB-CA-C | -5.49 | 102.44 | 110.95 | 5 | 1 |
| 1 | I | 219 | GLN | N-CA-CB | 5.48 | 118.43 | 110.26 | 1 | 1 |
| 1 | K | 162 | ARG | N-CA-C | 5.48 | 116.93 | 111.07 | 3 | 1 |
| 1 | H | 181 | VAL | CB-CA-C | -5.47 | 104.97 | 111.97 | 1 | 1 |
| 1 | K | 198 | CYS | N-CA-C | -5.46 | 105.75 | 112.90 | 3 | 1 |
| 1 | K | 172 | LEU | N-CA-C | -5.46 | 105.75 | 112.90 | 4 | 1 |
| 1 | K | 193 | ASN | CA-CB-CG | -5.46 | 107.14 | 112.60 | 8 | 1 |
| 1 | H | 151 | LEU | CA-C-O | -5.44 | 114.79 | 120.55 | 3 | 1 |
| 1 | H | 201 | ILE | CB-CA-C | -5.44 | 104.92 | 112.04 | 10 | 1 |
| 1 | L | 197 | ASP | CB-CA-C | -5.43 | 101.66 | 110.79 | 6 | 1 |
| 1 | L | 166 | ASP | N-CA-C | -5.43 | 105.52 | 111.82 | 5 | 1 |
| 1 | K | 168 | PHE | N-CA-CB | -5.42 | 102.20 | 110.33 | 5 | 1 |
| 1 | J | 210 | THR | N-CA-C | -5.41 | 103.76 | 110.41 | 1 | 1 |
| 1 | J | 226 | HIS | CA-CB-CG | -5.39 | 108.41 | 113.80 | 10 | 1 |
| 1 | I | 158 | LYS | N-CA-C | -5.39 | 107.08 | 113.97 | 5 | 2 |
| 1 | K | 150 | ILE | N-CA-CB | -5.36 | 104.47 | 112.67 | 7 | 2 |
| 1 | H | 227 | LYS | CG-CD-CE | 5.36 | 123.63 | 111.30 | 8 | 1 |
| 1 | I | 150 | ILE | N-CA-CB | -5.35 | 103.94 | 112.07 | 1 | 1 |
| 1 | H | 154 | ARG | CA-CB-CG | -5.33 | 103.43 | 114.10 | 9 | 1 |
| 1 | K | 208 | GLY | N-CA-C | -5.31 | 108.76 | 115.08 | 10 | 1 |
| 1 | L | 149 | SER | CB-CA-C | -5.29 | 102.34 | 110.81 | 5 | 1 |
| 1 | K | 168 | PHE | CA-CB-CG | -5.29 | 108.51 | 113.80 | 1 | 1 |
| 1 | G | 239 | THR | N-CA-C | -5.28 | 105.43 | 111.07 | 2 | 2 |
| 1 | G | 151 | LEU | CB-CA-C | -5.28 | 102.56 | 110.90 | 9 | 1 |
| 1 | K | 154 | ARG | N-CA-C | 5.25 | 116.96 | 108.34 | 10 | 1 |
| 1 | I | 230 | VAL | N-CA-C | 5.25 | 115.47 | 110.53 | 1 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | I | 149 | SER | CA-C-O | -5.24 | 115.30 | 121.07 | 6 | 1 |
| 1 | H | 162 | ARG | CB-CA-C | -5.24 | 102.89 | 110.96 | 10 | 1 |
| 1 | J | 212 | GLU | N-CA-C | -5.21 | 105.60 | 111.28 | 2 | 2 |
| 1 | H | 197 | ASP | CB-CA-C | -5.21 | 101.99 | 110.85 | 9 | 1 |
| 1 | H | 150 | ILE | CA-CB-CG2 | 5.21 | 119.35 | 110.50 | 2 | 3 |
| 1 | J | 150 | ILE | CB-CA-C | 5.20 | 115.84 | 110.70 | 4 | 1 |
| 1 | G | 195 | ASN | CA-CB-CG | -5.19 | 107.41 | 112.60 | 8 | 1 |
| 1 | J | 151 | LEU | N-CA-C | -5.17 | 105.64 | 111.28 | 1 | 1 |
| 1 | I | 175 | GLU | CB-CG-CD | -5.16 | 103.84 | 112.60 | 2 | 1 |
| 1 | H | 159 | GLU | N-CA-CB | -5.15 | 103.33 | 110.29 | 1 | 1 |
| 1 | I | 184 | TRP | N-CA-CB | -5.15 | 102.55 | 110.12 | 10 | 1 |
| 1 | K | 152 | ASP | N-CA-CB | -5.14 | 102.42 | 111.42 | 1 | 1 |
| 1 | K | 161 | PHE | CA-CB-CG | -5.13 | 108.67 | 113.80 | 9 | 1 |
| 1 | G | 168 | PHE | CA-CB-CG | -5.13 | 108.67 | 113.80 | 3 | 1 |
| 1 | K | 150 | ILE | CB-CA-C | 5.12 | 115.77 | 110.70 | 9 | 1 |
| 1 | I | 189 | LEU | N-CA-C | 5.11 | 117.97 | 111.69 | 3 | 1 |
| 1 | K | 202 | LEU | N-CA-C | -5.09 | 105.86 | 111.71 | 10 | 1 |
| 1 | H | 202 | LEU | N-CA-C | -5.08 | 105.87 | 111.71 | 4 | 1 |
| 1 | J | 152 | ASP | O-C-N | 5.08 | 129.34 | 122.59 | 4 | 1 |
| 1 | G | 194 | ALA | N-CA-C | 5.05 | 118.40 | 107.49 | 9 | 1 |
| 1 | H | 223 | GLY | O-C-N | -5.05 | 116.72 | 121.77 | 2 | 1 |
| 1 | K | 172 | LEU | N-CA-CB | 5.03 | 117.52 | 110.12 | 6 | 1 |
| 1 | H | 231 | LEU | CB-CA-C | -5.02 | 102.31 | 110.85 | 1 | 1 |
| 1 | I | 154 | ARG | N-CA-C | 5.02 | 118.40 | 109.96 | 7 | 1 |
| 1 | L | 172 | LEU | N-CA-C | -5.02 | 105.81 | 111.28 | 10 | 1 |
| 1 | K | 164 | TYR | CA-CB-CG | -5.02 | 104.87 | 113.90 | 5 | 1 |
| 1 | J | 150 | ILE | N-CA-CB | -5.00 | 105.86 | 112.36 | 9 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | I | 221 | VAL | Mainchain | 5 |
| 1 | H | 162 | ARG | Sidechain | 2 |
| 1 | K | 162 | ARG | Sidechain | 2 |
| 1 | K | 154 | ARG | Sidechain | 2 |
| 1 | L | 152 | ASP | Mainchain | 1 |
| 1 | I | 162 | ARG | Sidechain | 1 |
| 1 | L | 173 | ARG | Sidechain | 1 |
| 1 | H | 154 | ARG | Sidechain | 1 |

6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | G | 708 | 713 | 713 | 8±2 |
| 1 | H | 701 | 706 | 706 | 10±4 |
| 1 | I | 672 | 683 | 683 | 12±3 |
| 1 | J | 715 | 720 | 720 | 10±2 |
| 1 | K | 708 | 713 | 713 | 10±3 |
| 1 | L | 701 | 706 | 706 | 11±4 |
| 2 | H | 33 | 29 | 0 | 0±0 |
| All | All | 42740 | 42760 | 42470 | 591 |

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 7.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:K:234:ALA:HB1 | 1:L:232:ALA:HB2 | 1.07 | 1.26 | 3 | 2 |
| 1:J:150:ILE:HD11 | 1:J:172:LEU:HD22 | 1.04 | 1.28 | 5 | 2 |
| 1:G:150:ILE:HD13 | 1:G:172:LEU:HD21 | 0.74 | 1.57 | 1 | 4 |
| 1:J:150:ILE:HD13 | 1:J:172:LEU:HD21 | 0.73 | 1.60 | 1 | 5 |
| 1:K:181:VAL:HG12 | 1:K:185:MET:HE2 | 0.73 | 1.60 | 1 | 1 |
| 1:H:150:ILE:HG21 | 1:H:185:MET:SD | 0.70 | 2.26 | 5 | 1 |
| 1:I:218:CYS:O | 1:I:221:VAL:HG23 | 0.70 | 1.87 | 8 | 2 |
| 1:H:149:SER:O | 1:H:150:ILE:HD12 | 0.70 | 1.87 | 2 | 7 |
| 1:G:149:SER:O | 1:G:150:ILE:HD12 | 0.69 | 1.87 | 8 | 10 |
| 1:J:149:SER:O | 1:J:150:ILE:HD12 | 0.69 | 1.87 | 7 | 9 |
| 1:L:161:PHE:O | 1:L:165:VAL:HG23 | 0.69 | 1.88 | 5 | 4 |
| 1:L:149:SER:O | 1:L:150:ILE:HD12 | 0.69 | 1.87 | 5 | 6 |
| 1:K:190:LEU:O | 1:K:194:ALA:HB2 | 0.69 | 1.87 | 9 | 2 |
| 1:G:150:ILE:HG23 | 1:G:189:LEU:HG | 0.69 | 1.65 | 8 | 6 |
| 1:H:184:TRP:CH2 | 1:H:188:THR:HG21 | 0.69 | 2.23 | 3 | 3 |
| 1:J:161:PHE:O | 1:J:165:VAL:HG23 | 0.69 | 1.87 | 1 | 10 |
| 1:K:149:SER:O | 1:K:150:ILE:HD12 | 0.69 | 1.88 | 1 | 10 |
| 1:I:149:SER:O | 1:I:150:ILE:HD12 | 0.68 | 1.88 | 9 | 7 |
| 1:K:165:VAL:HG22 | 1:K:190:LEU:HD11 | 0.68 | 1.65 | 5 | 2 |
| 1:K:161:PHE:O | 1:K:165:VAL:HG23 | 0.68 | 1.88 | 7 | 6 |
| 1:I:191:VAL:HG22 | 1:I:202:LEU:HD23 | 0.68 | 1.64 | 6 | 3 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:J:197:ASP:O | 1:J:200:THR:HG22 | 0.68 | 1.88 | 9 | 9 |
| 1:I:167:ARG:O | 1:I:171:THR:HG22 | 0.67 | 1.89 | 6 | 2 |
| 1:L:226:HIS:O | 1:L:230:VAL:HG23 | 0.67 | 1.89 | 4 | 4 |
| 1:G:150:ILE:HD13 | 1:G:172:LEU:CD2 | 0.67 | 2.20 | 8 | 4 |
| 1:L:198:CYS:O | 1:L:202:LEU:HD12 | 0.66 | 1.89 | 1 | 1 |
| 1:I:197:ASP:O | 1:I:200:THR:HG22 | 0.66 | 1.90 | 8 | 6 |
| 1:L:197:ASP:O | 1:L:200:THR:HG22 | 0.66 | 1.89 | 5 | 8 |
| 1:L:150:ILE:HG23 | 1:L:189:LEU:HG | 0.66 | 1.67 | 8 | 2 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:CE | 0.66 | 2.21 | 10 | 2 |
| 1:J:181:VAL:CG1 | 1:J:185:MET:HE3 | 0.65 | 2.21 | 8 | 2 |
| 1:K:226:HIS:O | 1:K:230:VAL:HG23 | 0.65 | 1.91 | 4 | 2 |
| 1:L:150:ILE:CD1 | 1:L:172:LEU:HD21 | 0.65 | 2.21 | 2 | 4 |
| 1:J:150:ILE:HD11 | 1:J:168:PHE:CE2 | 0.65 | 2.27 | 4 | 1 |
| 1:J:209:ALA:O | 1:J:214:MET:HE2 | 0.65 | 1.91 | 4 | 1 |
| 1:J:150:ILE:HD13 | 1:J:172:LEU:CD2 | 0.65 | 2.21 | 1 | 5 |
| 1:J:150:ILE:HD11 | 1:J:172:LEU:CD2 | 0.65 | 2.21 | 2 | 1 |
| 1:L:205:LEU:HD11 | 1:L:217:ALA:HB3 | 0.64 | 1.68 | 6 | 1 |
| 1:I:181:VAL:HG12 | 1:I:185:MET:HE3 | 0.64 | 1.68 | 7 | 1 |
| 1:L:162:ARG:NH2 | 1:L:165:VAL:HG11 | 0.64 | 2.08 | 7 | 2 |
| 1:L:201:ILE:HD13 | 1:L:217:ALA:O | 0.64 | 1.92 | 4 | 1 |
| 1:K:172:LEU:CD2 | 1:K:185:MET:HE2 | 0.64 | 2.23 | 8 | 1 |
| 1:G:198:CYS:O | 1:G:202:LEU:HD12 | 0.63 | 1.93 | 1 | 4 |
| 1:I:205:LEU:HD21 | 1:I:217:ALA:HB2 | 0.63 | 1.70 | 7 | 2 |
| 1:H:150:ILE:HG23 | 1:H:189:LEU:HG | 0.63 | 1.70 | 8 | 4 |
| 1:J:181:VAL:HG12 | 1:J:185:MET:HE3 | 0.63 | 1.71 | 8 | 2 |
| 1:H:164:TYR:CE2 | 1:H:190:LEU:HD12 | 0.63 | 2.29 | 1 | 8 |
| 1:L:205:LEU:HD11 | 1:L:217:ALA:CB | 0.63 | 2.23 | 6 | 1 |
| 1:I:150:ILE:HD11 | 1:I:168:PHE:CE2 | 0.63 | 2.29 | 5 | 1 |
| 1:I:161:PHE:CE1 | 1:I:202:LEU:HD11 | 0.62 | 2.28 | 8 | 2 |
| 1:G:226:HIS:O | 1:G:230:VAL:HG23 | 0.62 | 1.94 | 5 | 1 |
| 1:I:150:ILE:HD13 | 1:I:185:MET:HE3 | 0.62 | 1.70 | 9 | 1 |
| 1:K:175:GLU:OE2 | 1:K:185:MET:HE1 | 0.62 | 1.94 | 1 | 1 |
| 1:I:209:ALA:O | 1:I:214:MET:HE3 | 0.62 | 1.94 | 3 | 5 |
| 1:I:182:LYS:O | 1:I:186:THR:HG23 | 0.62 | 1.94 | 1 | 7 |
| 1:I:155:GLN:HB2 | 1:I:194:ALA:HB1 | 0.62 | 1.72 | 3 | 1 |
| 1:H:235:MET:HE1 | 1:I:235:MET:HE3 | 0.61 | 1.69 | 1 | 1 |
| 1:K:150:ILE:HD13 | 1:K:172:LEU:CD2 | 0.61 | 2.25 | 2 | 3 |
| 1:L:150:ILE:HD11 | 1:L:168:PHE:CD1 | 0.61 | 2.30 | 10 | 1 |
| 1:I:153:ILE:HD11 | 1:I:167:ARG:HB3 | 0.61 | 1.73 | 4 | 3 |
| 1:H:161:PHE:O | 1:H:165:VAL:HG23 | 0.61 | 1.96 | 6 | 2 |
| 1:H:191:VAL:HG22 | 1:H:202:LEU:CD2 | 0.60 | 2.26 | 9 | 2 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:G:165:VAL:HG22 | 1:G:190:LEU:HD11 | 0.60 | 1.72 | 1 | 3 |
| 1:L:150:ILE:HG21 | 1:L:185:MET:SD | 0.60 | 2.35 | 1 | 1 |
| 1:L:167:ARG:O | 1:L:171:THR:HG22 | 0.59 | 1.97 | 9 | 2 |
| 1:J:168:PHE:O | 1:J:172:LEU:HD23 | 0.59 | 1.96 | 5 | 1 |
| 1:K:162:ARG:NH2 | 1:K:165:VAL:HG11 | 0.59 | 2.12 | 7 | 1 |
| 1:K:197:ASP:O | 1:K:200:THR:HG22 | 0.59 | 1.97 | 5 | 6 |
| 1:H:154:ARG:HD3 | 1:I:215:MET:HE3 | 0.59 | 1.74 | 5 | 1 |
| 1:J:150:ILE:HG23 | 1:J:189:LEU:HG | 0.59 | 1.75 | 7 | 2 |
| 1:I:175:GLU:OE2 | 1:I:185:MET:HE1 | 0.59 | 1.97 | 5 | 1 |
| 1:I:205:LEU:HD11 | 1:I:217:ALA:HB3 | 0.59 | 1.75 | 6 | 1 |
| 1:I:149:SER:C | 1:I:150:ILE:HD12 | 0.59 | 2.22 | 3 | 5 |
| 1:H:226:HIS:O | 1:H:230:VAL:HG23 | 0.59 | 1.97 | 2 | 5 |
| 1:H:231:LEU:HD23 | 1:H:232:ALA:HA | 0.58 | 1.73 | 2 | 1 |
| 1:K:184:TRP:CH2 | 1:K:188:THR:HG21 | 0.58 | 2.33 | 9 | 1 |
| 1:G:197:ASP:O | 1:G:200:THR:HG22 | 0.58 | 1.98 | 5 | 10 |
| 1:H:198:CYS:HB3 | 1:H:221:VAL:HG21 | 0.58 | 1.75 | 9 | 3 |
| 1:K:150:ILE:HD13 | 1:K:172:LEU:HD21 | 0.58 | 1.75 | 1 | 3 |
| 1:J:150:ILE:CD1 | 1:J:172:LEU:HD22 | 0.58 | 2.19 | 5 | 1 |
| 1:L:150:ILE:HD11 | 1:L:168:PHE:CZ | 0.58 | 2.34 | 5 | 2 |
| 1:G:161:PHE:O | 1:G:165:VAL:HG23 | 0.58 | 1.98 | 6 | 7 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:CG1 | 0.58 | 2.29 | 3 | 2 |
| 1:J:150:ILE:HD11 | 1:J:168:PHE:CZ | 0.58 | 2.33 | 3 | 2 |
| 1:L:191:VAL:HG22 | 1:L:202:LEU:CD2 | 0.58 | 2.29 | 3 | 1 |
| 1:L:150:ILE:HD13 | 1:L:172:LEU:HD21 | 0.57 | 1.74 | 6 | 1 |
| 1:L:150:ILE:HG21 | 1:L:185:MET:HB3 | 0.57 | 1.75 | 7 | 1 |
| 1:I:153:ILE:HD13 | 1:I:171:THR:HG21 | 0.57 | 1.76 | 1 | 3 |
| 1:I:162:ARG:NH2 | 1:I:165:VAL:HG11 | 0.57 | 2.14 | 6 | 1 |
| 1:I:150:ILE:HG23 | 1:I:189:LEU:HG | 0.57 | 1.75 | 10 | 2 |
| 1:L:165:VAL:HG22 | 1:L:190:LEU:HD11 | 0.57 | 1.75 | 3 | 3 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:HE2 | 0.57 | 1.77 | 10 | 1 |
| 1:H:198:CYS:CB | 1:H:221:VAL:HG21 | 0.56 | 2.29 | 4 | 3 |
| 1:K:181:VAL:CG1 | 1:K:185:MET:HE2 | 0.56 | 2.29 | 1 | 1 |
| 1:J:177:ALA:HB1 | 1:J:181:VAL:CG1 | 0.56 | 2.30 | 4 | 4 |
| 1:J:149:SER:CB | 1:J:150:ILE:HD12 | 0.56 | 2.31 | 2 | 1 |
| 1:L:161:PHE:CE1 | 1:L:202:LEU:HD11 | 0.56 | 2.36 | 2 | 1 |
| 1:G:191:VAL:HG22 | 1:G:202:LEU:HD23 | 0.56 | 1.78 | 4 | 4 |
| 1:L:191:VAL:HG22 | 1:L:202:LEU:HD23 | 0.56 | 1.78 | 3 | 2 |
| 1:H:218:CYS:O | 1:H:221:VAL:HG23 | 0.56 | 2.00 | 2 | 1 |
| 1:I:172:LEU:HD21 | 1:I:185:MET:SD | 0.56 | 2.41 | 4 | 1 |
| 1:K:209:ALA:HB1 | 1:K:213:GLU:CB | 0.56 | 2.30 | 8 | 1 |
| 1:J:150:ILE:HG21 | 1:J:185:MET:HB3 | 0.56 | 1.77 | 6 | 2 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:150:ILE:HD13 | 1:L:172:LEU:HD11 | 0.56 | 1.76 | 8 | 1 |
| 1:J:226:HIS:O | 1:J:230:VAL:HG23 | 0.55 | 2.01 | 8 | 2 |
| 1:I:181:VAL:CG1 | 1:I:185:MET:HE3 | 0.55 | 2.32 | 7 | 1 |
| 1:J:224:PRO:O | 1:J:228:ALA:HB3 | 0.55 | 2.02 | 10 | 1 |
| 1:H:205:LEU:HD11 | 1:H:217:ALA:HB3 | 0.54 | 1.79 | 2 | 2 |
| 1:L:218:CYS:O | 1:L:221:VAL:HG23 | 0.54 | 2.02 | 3 | 2 |
| 1:I:175:GLU:OE1 | 1:I:185:MET:HE1 | 0.54 | 2.02 | 7 | 1 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:CG | 0.54 | 2.32 | 7 | 1 |
| 1:H:226:HIS:CE1 | 1:H:230:VAL:HG21 | 0.54 | 2.38 | 10 | 1 |
| 1:H:184:TRP:CD1 | 1:H:188:THR:HG1 | 0.54 | 2.21 | 2 | 1 |
| 1:I:153:ILE:HD13 | 1:I:171:THR:CG2 | 0.54 | 2.32 | 1 | 1 |
| 1:K:164:TYR:CE2 | 1:K:190:LEU:HD12 | 0.54 | 2.36 | 9 | 2 |
| 1:L:150:ILE:HD13 | 1:L:172:LEU:CD2 | 0.54 | 2.32 | 10 | 1 |
| 1:H:184:TRP:CZ2 | 1:H:188:THR:HG21 | 0.54 | 2.37 | 1 | 1 |
| 1:J:149:SER:C | 1:J:150:ILE:HD12 | 0.54 | 2.27 | 5 | 4 |
| 1:K:185:MET:HA | 1:K:189:LEU:HD23 | 0.54 | 1.79 | 5 | 1 |
| 1:L:182:LYS:O | 1:L:186:THR:HG23 | 0.54 | 2.03 | 2 | 1 |
| 1:K:172:LEU:HD21 | 1:K:185:MET:HE2 | 0.54 | 1.80 | 8 | 1 |
| 1:L:177:ALA:HB1 | 1:L:181:VAL:CG1 | 0.53 | 2.34 | 1 | 5 |
| 1:H:150:ILE:HG22 | 1:H:151:LEU:HD13 | 0.53 | 1.78 | 5 | 1 |
| 1:K:234:ALA:HB1 | 1:L:232:ALA:CB | 0.53 | 2.19 | 3 | 1 |
| 1:I:198:CYS:O | 1:I:202:LEU:HD22 | 0.53 | 2.03 | 4 | 1 |
| 1:L:198:CYS:HB3 | 1:L:221:VAL:HG21 | 0.53 | 1.79 | 3 | 2 |
| 1:L:224:PRO:O | 1:L:228:ALA:HB2 | 0.53 | 2.03 | 3 | 4 |
| 1:H:150:ILE:HG22 | 1:H:151:LEU:CD1 | 0.53 | 2.34 | 5 | 1 |
| 1:I:150:ILE:HD13 | 1:I:172:LEU:CD1 | 0.53 | 2.32 | 3 | 1 |
| 1:H:150:ILE:HD13 | 1:H:172:LEU:CD2 | 0.53 | 2.34 | 5 | 2 |
| 1:I:177:ALA:HB1 | 1:I:181:VAL:HG12 | 0.53 | 1.79 | 4 | 1 |
| 1:I:184:TRP:CD1 | 1:I:188:THR:HG1 | 0.53 | 2.22 | 9 | 1 |
| 1:I:205:LEU:HD11 | 1:I:217:ALA:CB | 0.53 | 2.33 | 6 | 1 |
| 1:H:150:ILE:HD11 | 1:H:168:PHE:CE1 | 0.52 | 2.39 | 1 | 1 |
| 1:J:168:PHE:CE1 | 1:J:186:THR:HG22 | 0.52 | 2.39 | 1 | 1 |
| 1:H:164:TYR:CE2 | 1:H:194:ALA:HB2 | 0.52 | 2.40 | 8 | 3 |
| 1:H:198:CYS:CA | 1:H:221:VAL:HG21 | 0.52 | 2.35 | 4 | 1 |
| 1:H:165:VAL:HG22 | 1:H:190:LEU:HD11 | 0.52 | 1.81 | 6 | 3 |
| 1:H:231:LEU:HD23 | 1:H:232:ALA:CA | 0.51 | 2.35 | 2 | 1 |
| 1:L:201:ILE:CG2 | 1:L:217:ALA:HB1 | 0.51 | 2.35 | 4 | 1 |
| 1:H:191:VAL:HG22 | 1:H:202:LEU:HD22 | 0.51 | 1.81 | 9 | 1 |
| 1:I:161:PHE:O | 1:I:165:VAL:HG23 | 0.51 | 2.05 | 6 | 2 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:HE3 | 0.51 | 1.83 | 1 | 2 |
| 1:K:235:MET:HE1 | 1:L:231:LEU:O | 0.51 | 2.05 | 6 | 1 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:H:164:TYR:HE2 | 1:H:190:LEU:HD12 | 0.51 | 1.66 | 1 | 2 |
| 1:H:181:VAL:O | 1:H:185:MET:HE3 | 0.51 | 2.06 | 5 | 1 |
| 1:J:182:LYS:O | 1:J:186:THR:HG23 | 0.51 | 2.05 | 9 | 1 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:HB | 0.51 | 1.83 | 9 | 1 |
| 1:H:209:ALA:O | 1:H:214:MET:HE3 | 0.51 | 2.06 | 9 | 1 |
| 1:I:164:TYR:CE2 | 1:I:190:LEU:HD12 | 0.50 | 2.41 | 3 | 6 |
| 1:K:172:LEU:HD23 | 1:K:175:GLU:OE1 | 0.50 | 2.06 | 1 | 1 |
| 1:G:177:ALA:HB1 | 1:G:181:VAL:CG1 | 0.50 | 2.36 | 1 | 4 |
| 1:G:202:LEU:HD23 | 1:G:214:MET:SD | 0.50 | 2.46 | 7 | 2 |
| 1:J:150:ILE:O | 1:J:189:LEU:HD12 | 0.50 | 2.05 | 4 | 1 |
| 1:H:177:ALA:HB1 | 1:H:181:VAL:CG1 | 0.50 | 2.36 | 2 | 1 |
| 1:K:202:LEU:HD23 | 1:K:214:MET:SD | 0.50 | 2.46 | 2 | 2 |
| 1:H:171:THR:O | 1:H:174:ALA:HB3 | 0.50 | 2.06 | 1 | 1 |
| 1:J:234:ALA:HB1 | 1:K:232:ALA:HB2 | 0.50 | 1.84 | 3 | 1 |
| 1:I:155:GLN:CB | 1:I:194:ALA:HB1 | 0.50 | 2.37 | 3 | 1 |
| 1:I:189:LEU:HD12 | 1:I:193:ASN:ND2 | 0.50 | 2.22 | 3 | 1 |
| 1:K:175:GLU:OE1 | 1:K:185:MET:HE1 | 0.50 | 2.06 | 3 | 3 |
| 1:L:198:CYS:CB | 1:L:221:VAL:HG21 | 0.50 | 2.37 | 3 | 1 |
| 1:J:168:PHE:CD2 | 1:J:190:LEU:HD13 | 0.49 | 2.42 | 6 | 3 |
| 1:H:172:LEU:HD22 | 1:H:185:MET:SD | 0.49 | 2.47 | 4 | 1 |
| 1:H:150:ILE:CG1 | 1:H:185:MET:HE2 | 0.49 | 2.37 | 1 | 2 |
| 1:K:150:ILE:HD11 | 1:K:168:PHE:CE2 | 0.49 | 2.43 | 3 | 1 |
| 1:L:161:PHE:CZ | 1:L:165:VAL:HG21 | 0.49 | 2.43 | 3 | 1 |
| 1:K:209:ALA:HB1 | 1:K:213:GLU:HB2 | 0.49 | 1.83 | 8 | 3 |
| 1:I:177:ALA:HB1 | 1:I:181:VAL:CG1 | 0.49 | 2.38 | 4 | 1 |
| 1:L:201:ILE:HG21 | 1:L:217:ALA:HB1 | 0.49 | 1.85 | 4 | 1 |
| 1:L:161:PHE:HE1 | 1:L:202:LEU:HD11 | 0.49 | 1.67 | 2 | 1 |
| 1:L:178:SER:HB2 | 1:L:181:VAL:HG23 | 0.48 | 1.85 | 7 | 1 |
| 1:K:168:PHE:CD2 | 1:K:190:LEU:HD13 | 0.48 | 2.43 | 8 | 1 |
| 1:I:189:LEU:HD13 | 1:I:193:ASN:ND2 | 0.48 | 2.22 | 7 | 1 |
| 1:G:215:MET:HE3 | 1:L:154:ARG:HH11 | 0.48 | 1.68 | 8 | 2 |
| 1:H:150:ILE:HD11 | 1:H:168:PHE:HE1 | 0.48 | 1.68 | 1 | 1 |
| 1:K:178:SER:HB2 | 1:K:181:VAL:HG23 | 0.48 | 1.84 | 2 | 1 |
| 1:I:150:ILE:HD13 | 1:I:172:LEU:HD11 | 0.48 | 1.85 | 3 | 1 |
| 1:K:191:VAL:HG22 | 1:K:202:LEU:CD2 | 0.48 | 2.38 | 7 | 1 |
| 1:L:149:SER:CB | 1:L:171:THR:HG21 | 0.48 | 2.38 | 7 | 1 |
| 1:I:209:ALA:HB1 | 1:I:213:GLU:HB2 | 0.48 | 1.85 | 10 | 1 |
| 1:J:209:ALA:HB1 | 1:J:213:GLU:HB2 | 0.48 | 1.85 | 5 | 2 |
| 1:I:189:LEU:HD12 | 1:I:193:ASN:HD22 | 0.48 | 1.69 | 3 | 1 |
| 1:G:238:VAL:HG21 | 1:H:233:GLU:OE2 | 0.48 | 2.08 | 6 | 1 |
| 1:K:201:ILE:CG2 | 1:K:217:ALA:HB1 | 0.47 | 2.39 | 1 | 1 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:161:PHE:CE1 | 1:L:165:VAL:HG21 | 0.47 | 2.44 | 3 | 1 |
| 1:H:149:SER:C | 1:H:150:ILE:HD12 | 0.47 | 2.34 | 2 | 2 |
| 1:J:184:TRP:CH2 | 1:J:188:THR:HG21 | 0.47 | 2.45 | 7 | 2 |
| 1:H:231:LEU:HD23 | 1:H:232:ALA:N | 0.47 | 2.23 | 2 | 1 |
| 1:J:172:LEU:HD11 | 1:J:186:THR:HG23 | 0.47 | 1.85 | 2 | 1 |
| 1:L:153:ILE:HD11 | 1:L:167:ARG:HB3 | 0.47 | 1.84 | 4 | 1 |
| 1:K:201:ILE:O | 1:K:204:ALA:HB3 | 0.47 | 2.10 | 5 | 1 |
| 1:L:184:TRP:CH2 | 1:L:188:THR:HG21 | 0.47 | 2.44 | 6 | 1 |
| 1:K:150:ILE:HG21 | 1:K:185:MET:SD | 0.47 | 2.50 | 10 | 1 |
| 1:J:230:VAL:HG12 | 1:K:228:ALA:HB1 | 0.47 | 1.86 | 2 | 3 |
| 1:I:191:VAL:HG22 | 1:I:202:LEU:CD2 | 0.47 | 2.37 | 6 | 1 |
| 1:L:153:ILE:HG21 | 1:L:168:PHE:HB2 | 0.47 | 1.86 | 7 | 1 |
| 2:H:301:A1CCY:C9 | 1:I:231:LEU:HD22 | 0.47 | 2.40 | 1 | 2 |
| 1:L:150:ILE:HD12 | 1:L:172:LEU:HD21 | 0.47 | 1.87 | 8 | 1 |
| 1:G:150:ILE:CD1 | 1:G:172:LEU:HD21 | 0.47 | 2.38 | 9 | 1 |
| 1:L:168:PHE:O | 1:L:172:LEU:HD23 | 0.47 | 2.08 | 2 | 2 |
| 1:H:201:ILE:CG2 | 1:H:217:ALA:HB1 | 0.47 | 2.39 | 3 | 1 |
| 1:I:198:CYS:O | 1:I:202:LEU:HD13 | 0.47 | 2.10 | 2 | 3 |
| 1:K:198:CYS:O | 1:K:202:LEU:HD12 | 0.47 | 2.10 | 2 | 2 |
| 1:I:150:ILE:HG23 | 1:I:189:LEU:CD2 | 0.46 | 2.41 | 1 | 1 |
| 1:H:151:LEU:HD12 | 1:H:151:LEU:H | 0.46 | 1.69 | 4 | 1 |
| 1:K:182:LYS:O | 1:K:186:THR:HG23 | 0.46 | 2.10 | 1 | 1 |
| 1:G:150:ILE:HD11 | 1:G:168:PHE:CZ | 0.46 | 2.45 | 3 | 1 |
| 1:H:148:THR:O | 1:H:151:LEU:HD12 | 0.46 | 2.10 | 4 | 1 |
| 1:H:168:PHE:CE2 | 1:H:172:LEU:HD11 | 0.46 | 2.46 | 4 | 1 |
| 1:H:177:ALA:HB3 | 1:H:182:LYS:HE2 | 0.46 | 1.88 | 10 | 1 |
| 1:J:209:ALA:HB1 | 1:J:213:GLU:CB | 0.46 | 2.41 | 1 | 1 |
| 1:J:150:ILE:HD13 | 1:J:172:LEU:CG | 0.46 | 2.41 | 6 | 2 |
| 1:K:153:ILE:HD11 | 1:K:167:ARG:HB3 | 0.46 | 1.88 | 10 | 1 |
| 1:I:201:ILE:CG2 | 1:I:217:ALA:HB1 | 0.45 | 2.41 | 3 | 1 |
| 1:L:177:ALA:HB1 | 1:L:181:VAL:HG12 | 0.45 | 1.88 | 4 | 1 |
| 1:H:178:SER:HB2 | 1:H:181:VAL:HG23 | 0.45 | 1.87 | 4 | 1 |
| 1:K:226:HIS:O | 1:K:230:VAL:HG22 | 0.45 | 2.10 | 9 | 1 |
| 1:K:164:TYR:CE2 | 1:K:194:ALA:HB2 | 0.45 | 2.46 | 3 | 1 |
| 1:L:161:PHE:CE2 | 1:L:165:VAL:HG21 | 0.45 | 2.46 | 5 | 1 |
| 1:G:218:CYS:O | 1:G:221:VAL:HG23 | 0.45 | 2.11 | 7 | 2 |
| 1:L:149:SER:HB3 | 1:L:172:LEU:HD22 | 0.45 | 1.87 | 8 | 1 |
| 1:G:164:TYR:CE2 | 1:G:190:LEU:HD12 | 0.45 | 2.47 | 5 | 3 |
| 1:I:215:MET:HE2 | 1:I:216:THR:HA | 0.45 | 1.89 | 5 | 1 |
| 1:L:162:ARG:CZ | 1:L:165:VAL:HG11 | 0.45 | 2.41 | 7 | 1 |
| 1:K:224:PRO:O | 1:K:228:ALA:HB3 | 0.45 | 2.11 | 10 | 1 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:150:ILE:HG23 | 1:L:189:LEU:CD2 | 0.45 | 2.41 | 1 | 1 |
| 1:K:175:GLU:OE2 | 1:K:177:ALA:HB2 | 0.45 | 2.11 | 5 | 1 |
| 1:J:230:VAL:HG12 | 1:K:228:ALA:CB | 0.45 | 2.42 | 8 | 1 |
| 1:L:150:ILE:N | 1:L:150:ILE:HD12 | 0.45 | 2.26 | 9 | 1 |
| 1:H:150:ILE:HD11 | 1:H:168:PHE:CZ | 0.45 | 2.45 | 3 | 1 |
| 1:I:199:LYS:HA | 1:I:202:LEU:HD22 | 0.45 | 1.87 | 10 | 1 |
| 1:G:154:ARG:CD | 1:H:215:MET:HE3 | 0.45 | 2.41 | 10 | 1 |
| 1:I:153:ILE:HD11 | 1:I:167:ARG:CB | 0.45 | 2.42 | 2 | 1 |
| 1:J:238:VAL:CG1 | 1:K:232:ALA:HB1 | 0.44 | 2.41 | 3 | 1 |
| 1:H:197:ASP:HB2 | 1:H:221:VAL:HG13 | 0.44 | 1.89 | 10 | 2 |
| 1:L:150:ILE:CD1 | 1:L:172:LEU:HD11 | 0.44 | 2.41 | 8 | 1 |
| 1:L:181:VAL:HG12 | 1:L:185:MET:HE3 | 0.44 | 1.88 | 10 | 1 |
| 1:K:161:PHE:CE2 | 1:K:165:VAL:HG21 | 0.44 | 2.47 | 7 | 2 |
| 1:I:191:VAL:HA | 1:I:202:LEU:HD23 | 0.44 | 1.88 | 4 | 2 |
| 1:I:162:ARG:HH22 | 1:I:165:VAL:HG11 | 0.44 | 1.72 | 6 | 1 |
| 1:G:150:ILE:HG21 | 1:G:185:MET:HG2 | 0.44 | 1.90 | 1 | 1 |
| 1:I:231:LEU:C | 1:I:231:LEU:HD13 | 0.44 | 2.38 | 7 | 1 |
| 1:H:227:LYS:HB3 | 2:H:301:A1CCY:C27 | 0.44 | 2.43 | 3 | 1 |
| 1:J:153:ILE:HG21 | 1:J:168:PHE:HB2 | 0.44 | 1.90 | 8 | 1 |
| 1:H:175:GLU:OE1 | 1:H:185:MET:HE1 | 0.44 | 2.13 | 2 | 1 |
| 1:H:172:LEU:HD23 | 1:H:175:GLU:CD | 0.44 | 2.38 | 4 | 1 |
| 1:J:177:ALA:HB3 | 1:J:182:LYS:HE3 | 0.44 | 1.90 | 6 | 1 |
| 1:G:150:ILE:O | 1:G:189:LEU:HD12 | 0.44 | 2.13 | 10 | 1 |
| 1:I:165:VAL:HG13 | 1:I:168:PHE:HE2 | 0.44 | 1.72 | 6 | 1 |
| 1:K:167:ARG:O | 1:K:171:THR:HG22 | 0.44 | 2.13 | 9 | 1 |
| 1:I:178:SER:HB2 | 1:I:181:VAL:HG23 | 0.43 | 1.89 | 9 | 1 |
| 1:K:149:SER:O | 1:K:171:THR:HG21 | 0.43 | 2.13 | 2 | 1 |
| 1:H:150:ILE:HD13 | 1:H:172:LEU:HD21 | 0.43 | 1.89 | 5 | 1 |
| 1:H:150:ILE:HG12 | 1:H:185:MET:HE2 | 0.43 | 1.90 | 7 | 1 |
| 1:I:168:PHE:O | 1:I:172:LEU:HD23 | 0.43 | 2.13 | 5 | 1 |
| 1:I:191:VAL:HG22 | 1:I:202:LEU:HD22 | 0.43 | 1.88 | 8 | 1 |
| 1:J:201:ILE:HG21 | 1:J:218:CYS:SG | 0.43 | 2.52 | 4 | 1 |
| 1:I:168:PHE:CE1 | 1:I:186:THR:HG22 | 0.43 | 2.48 | 9 | 2 |
| 1:J:147:PRO:C | 1:J:148:THR:HG23 | 0.43 | 2.39 | 10 | 2 |
| 1:I:149:SER:HB3 | 1:I:171:THR:HG23 | 0.43 | 1.90 | 6 | 1 |
| 1:L:202:LEU:HD23 | 1:L:214:MET:SD | 0.43 | 2.54 | 1 | 2 |
| 1:L:150:ILE:HD11 | 1:L:168:PHE:CE1 | 0.43 | 2.47 | 5 | 1 |
| 1:J:231:LEU:HD13 | 1:K:231:LEU:HD23 | 0.43 | 1.89 | 1 | 1 |
| 1:K:147:PRO:C | 1:K:148:THR:HG23 | 0.42 | 2.39 | 10 | 2 |
| 1:I:177:ALA:HB3 | 1:I:182:LYS:HE3 | 0.42 | 1.91 | 6 | 1 |
| 1:I:184:TRP:CH2 | 1:I:188:THR:HG21 | 0.42 | 2.49 | 6 | 2 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:I:168:PHE:O | 1:I:172:LEU:HD22 | 0.42 | 2.15 | 3 | 1 |
| 1:L:164:TYR:CE2 | 1:L:194:ALA:HB2 | 0.42 | 2.49 | 4 | 1 |
| 1:H:150:ILE:CB | 1:H:185:MET:HE2 | 0.42 | 2.44 | 1 | 1 |
| 1:J:149:SER:HB2 | 1:J:150:ILE:HD12 | 0.42 | 1.90 | 2 | 1 |
| 1:J:230:VAL:CG1 | 1:K:228:ALA:HB1 | 0.42 | 2.44 | 5 | 1 |
| 1:L:175:GLU:CD | 1:L:185:MET:HE1 | 0.42 | 2.40 | 9 | 1 |
| 1:H:167:ARG:O | 1:H:171:THR:HG22 | 0.42 | 2.15 | 4 | 2 |
| 1:I:198:CYS:O | 1:I:202:LEU:HD12 | 0.42 | 2.14 | 8 | 1 |
| 1:J:149:SER:O | 1:J:171:THR:HG21 | 0.42 | 2.14 | 8 | 1 |
| 1:G:151:LEU:H | 1:G:151:LEU:HD12 | 0.42 | 1.74 | 10 | 1 |
| 1:J:150:ILE:HD12 | 1:J:150:ILE:N | 0.42 | 2.30 | 2 | 1 |
| 1:K:205:LEU:HD11 | 1:K:217:ALA:HB3 | 0.42 | 1.92 | 6 | 1 |
| 1:H:149:SER:O | 1:H:171:THR:HG21 | 0.42 | 2.15 | 8 | 1 |
| 1:J:230:VAL:HG11 | 1:K:224:PRO:O | 0.42 | 2.15 | 8 | 1 |
| 1:G:168:PHE:CD2 | 1:G:190:LEU:HD13 | 0.42 | 2.49 | 10 | 1 |
| 1:G:177:ALA:HB3 | 1:G:182:LYS:HE2 | 0.42 | 1.92 | 10 | 1 |
| 1:J:177:ALA:HB3 | 1:J:182:LYS:CG | 0.42 | 2.45 | 4 | 1 |
| 1:G:150:ILE:HD11 | 1:G:168:PHE:HD1 | 0.41 | 1.74 | 1 | 1 |
| 1:G:231:LEU:HD13 | 2:H:301:A1CCY:C21 | 0.41 | 2.45 | 10 | 1 |
| 1:I:209:ALA:HB1 | 1:I:213:GLU:CB | 0.41 | 2.44 | 10 | 1 |
| 1:I:172:LEU:HD23 | 1:I:175:GLU:OE2 | 0.41 | 2.16 | 1 | 1 |
| 1:H:198:CYS:HA | 1:H:221:VAL:HG21 | 0.41 | 1.92 | 4 | 1 |
| 1:H:215:MET:HE2 | 1:H:216:THR:CA | 0.41 | 2.45 | 4 | 1 |
| 1:K:172:LEU:HD13 | 1:K:185:MET:SD | 0.41 | 2.55 | 4 | 1 |
| 1:L:149:SER:C | 1:L:150:ILE:HD12 | 0.41 | 2.39 | 5 | 1 |
| 1:J:165:VAL:HG13 | 1:J:168:PHE:CD2 | 0.41 | 2.49 | 1 | 1 |
| 1:L:198:CYS:HA | 1:L:201:ILE:HD12 | 0.41 | 1.92 | 4 | 1 |
| 1:L:172:LEU:HD13 | 1:L:186:THR:HG22 | 0.41 | 1.92 | 5 | 1 |
| 1:I:231:LEU:HD13 | 1:I:231:LEU:O | 0.41 | 2.16 | 3 | 1 |
| 1:G:175:GLU:OE1 | 1:G:185:MET:HE1 | 0.41 | 2.15 | 7 | 1 |
| 1:H:228:ALA:O | 1:H:232:ALA:HB3 | 0.41 | 2.15 | 9 | 1 |
| 1:K:149:SER:C | 1:K:150:ILE:HD12 | 0.41 | 2.39 | 1 | 1 |
| 1:L:191:VAL:HG22 | 1:L:202:LEU:HD22 | 0.41 | 1.92 | 2 | 1 |
| 1:L:150:ILE:O | 1:L:189:LEU:HD12 | 0.41 | 2.15 | 3 | 1 |
| 1:I:201:ILE:HG21 | 1:I:218:CYS:SG | 0.41 | 2.56 | 5 | 1 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:HG3 | 0.41 | 1.93 | 7 | 1 |
| 1:H:215:MET:HE2 | 1:H:216:THR:HA | 0.41 | 1.91 | 4 | 1 |
| 1:G:150:ILE:HD11 | 1:G:168:PHE:CE2 | 0.41 | 2.51 | 5 | 1 |
| 1:I:197:ASP:HB2 | 1:I:221:VAL:HG13 | 0.41 | 1.93 | 9 | 1 |
| 1:J:168:PHE:CZ | 1:J:186:THR:HG22 | 0.40 | 2.52 | 1 | 1 |
| 1:L:161:PHE:CZ | 1:L:202:LEU:HD11 | 0.40 | 2.52 | 1 | 1 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:I:162:ARG:NH2 | 1:I:165:VAL:HG21 | 0.40 | 2.31 | 6 | 1 |
| 1:I:205:LEU:HD21 | 1:I:217:ALA:CB | 0.40 | 2.45 | 7 | 1 |
| 1:J:171:THR:O | 1:J:174:ALA:HB3 | 0.40 | 2.15 | 1 | 1 |
| 1:I:150:ILE:CD1 | 1:I:172:LEU:HD21 | 0.40 | 2.47 | 5 | 1 |
| 1:K:150:ILE:HG23 | 1:K:189:LEU:HG | 0.40 | 1.92 | 10 | 1 |
| 1:H:150:ILE:HG12 | 1:H:172:LEU:HD21 | 0.40 | 1.93 | 4 | 1 |
| 1:K:238:VAL:HG12 | 1:L:236:SER:OG | 0.40 | 2.17 | 5 | 1 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:HG12 | 0.40 | 1.94 | 7 | 1 |
| 1:H:150:ILE:HB | 1:H:185:MET:HE2 | 0.40 | 1.93 | 1 | 1 |
| 1:I:150:ILE:HG23 | 1:I:189:LEU:CG | 0.40 | 2.47 | 1 | 1 |
| 1:H:223:GLY:O | 1:H:227:LYS:HG2 | 0.40 | 2.16 | 4 | 1 |
| 1:G:233:GLU:OE2 | 1:L:238:VAL:HG21 | 0.40 | 2.16 | 6 | 1 |
| 1:H:189:LEU:HD22 | 1:H:189:LEU:N | 0.40 | 2.32 | 9 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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 | G | 92/102 (90%) | 84±2 (91±3%) | 6±2 (7±2%) | 2±1 (2±1%) | 9 | 52 |
| 1 | H | 91/102 (89%) | 78±2 (86±2%) | 10±2 (11±2%) | 2±1 (3±1%) | 6 | 43 |
| 1 | I | 86/102 (84%) | 75±2 (87±2%) | 9±2 (11±2%) | 2±1 (3±1%) | 6 | 42 |
| 1 | J | 93/102 (91%) | 82±3 (88±3%) | 9±3 (10±3%) | 2±1 (3±2%) | 6 | 41 |
| 1 | K | 92/102 (90%) | 82±3 (89±3%) | 8±2 (8±2%) | 2±1 (2±1%) | 7 | 44 |
| 1 | L | 91/102 (89%) | 81±1 (89±2%) | 8±2 (9±2%) | 2±1 (2±1%) | 8 | 51 |
| All | All | 5450/6120 (89%) | 4815 (88%) | 509 (9%) | 126 (2%) | 7 | 45 |

All 40 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 195 | ASN | 10 |
| 1 | K | 195 | ASN | 10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | L | 195 | ASN | 10 |
| 1 | H | 195 | ASN | 9 |
| 1 | I | 195 | ASN | 9 |
| 1 | J | 195 | ASN | 8 |
| 1 | I | 148 | THR | 5 |
| 1 | K | 148 | THR | 5 |
| 1 | H | 190 | LEU | 4 |
| 1 | J | 157 | PRO | 4 |
| 1 | J | 224 | PRO | 4 |
| 1 | G | 157 | PRO | 3 |
| 1 | J | 148 | THR | 3 |
| 1 | J | 239 | THR | 3 |
| 1 | G | 148 | THR | 2 |
| 1 | H | 148 | THR | 2 |
| 1 | L | 156 | GLY | 2 |
| 1 | I | 196 | PRO | 2 |
| 1 | I | 207 | PRO | 2 |
| 1 | G | 239 | THR | 2 |
| 1 | H | 149 | SER | 2 |
| 1 | J | 153 | ILE | 2 |
| 1 | H | 196 | PRO | 2 |
| 1 | K | 196 | PRO | 2 |
| 1 | L | 148 | THR | 2 |
| 1 | I | 227 | LYS | 2 |
| 1 | K | 194 | ALA | 2 |
| 1 | H | 157 | PRO | 1 |
| 1 | I | 176 | GLN | 1 |
| 1 | L | 152 | ASP | 1 |
| 1 | L | 153 | ILE | 1 |
| 1 | H | 221 | VAL | 1 |
| 1 | J | 152 | ASP | 1 |
| 1 | H | 161 | PHE | 1 |
| 1 | I | 210 | THR | 1 |
| 1 | K | 190 | LEU | 1 |
| 1 | H | 152 | ASP | 1 |
| 1 | K | 223 | GLY | 1 |
| 1 | K | 224 | PRO | 1 |
| 1 | L | 149 | SER | 1 |

6.3.2 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 NMR 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 | G | 76/83 (92%) | 72±1 (95±2%) | 4±1 (5±2%) | 25 | 75 |
| 1 | H | 75/83 (90%) | 70±2 (93±3%) | 5±2 (7±3%) | 17 | 65 |
| 1 | I | 73/83 (88%) | 68±1 (94±2%) | 5±1 (6±2%) | 18 | 67 |
| 1 | J | 77/83 (93%) | 72±1 (94±2%) | 5±1 (6±2%) | 19 | 68 |
| 1 | K | 76/83 (92%) | 71±3 (94±3%) | 5±3 (6±3%) | 18 | 67 |
| 1 | L | 75/83 (90%) | 69±2 (92±3%) | 6±2 (8±3%) | 13 | 61 |
| All | All | 4520/4980 (91%) | 4233 (94%) | 287 (6%) | 18 | 67 |

All 109 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 150 | ILE | 10 |
| 1 | K | 150 | ILE | 9 |
| 1 | J | 150 | ILE | 8 |
| 1 | J | 189 | LEU | 8 |
| 1 | G | 168 | PHE | 7 |
| 1 | J | 202 | LEU | 7 |
| 1 | K | 168 | PHE | 7 |
| 1 | L | 150 | ILE | 7 |
| 1 | L | 172 | LEU | 7 |
| 1 | L | 189 | LEU | 7 |
| 1 | H | 150 | ILE | 6 |
| 1 | H | 227 | LYS | 6 |
| 1 | I | 168 | PHE | 6 |
| 1 | H | 168 | PHE | 6 |
| 1 | L | 168 | PHE | 6 |
| 1 | L | 211 | LEU | 6 |
| 1 | I | 211 | LEU | 6 |
| 1 | I | 227 | LYS | 5 |
| 1 | K | 230 | VAL | 5 |
| 1 | L | 230 | VAL | 5 |
| 1 | G | 172 | LEU | 5 |
| 1 | H | 172 | LEU | 4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | J | 168 | PHE | 4 |
| 1 | K | 189 | LEU | 4 |
| 1 | I | 189 | LEU | 4 |
| 1 | K | 172 | LEU | 4 |
| 1 | L | 215 | MET | 3 |
| 1 | H | 166 | ASP | 3 |
| 1 | H | 215 | MET | 3 |
| 1 | I | 173 | ARG | 3 |
| 1 | J | 215 | MET | 3 |
| 1 | L | 227 | LYS | 3 |
| 1 | I | 172 | LEU | 3 |
| 1 | J | 211 | LEU | 3 |
| 1 | I | 202 | LEU | 3 |
| 1 | H | 193 | ASN | 2 |
| 1 | K | 199 | LYS | 2 |
| 1 | L | 193 | ASN | 2 |
| 1 | G | 189 | LEU | 2 |
| 1 | G | 230 | VAL | 2 |
| 1 | H | 173 | ARG | 2 |
| 1 | H | 181 | VAL | 2 |
| 1 | I | 162 | ARG | 2 |
| 1 | J | 203 | LYS | 2 |
| 1 | K | 162 | ARG | 2 |
| 1 | K | 202 | LEU | 2 |
| 1 | K | 203 | LYS | 2 |
| 1 | H | 202 | LEU | 2 |
| 1 | J | 172 | LEU | 2 |
| 1 | J | 227 | LYS | 2 |
| 1 | G | 211 | LEU | 2 |
| 1 | H | 211 | LEU | 2 |
| 1 | I | 150 | ILE | 2 |
| 1 | L | 202 | LEU | 2 |
| 1 | I | 215 | MET | 2 |
| 1 | K | 215 | MET | 2 |
| 1 | L | 175 | GLU | 2 |
| 1 | J | 183 | ASN | 2 |
| 1 | I | 181 | VAL | 2 |
| 1 | G | 215 | MET | 2 |
| 1 | L | 161 | PHE | 2 |
| 1 | K | 181 | VAL | 2 |
| 1 | H | 230 | VAL | 1 |
| 1 | G | 166 | ASP | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 231 | LEU | 1 |
| 1 | G | 239 | THR | 1 |
| 1 | H | 162 | ARG | 1 |
| 1 | H | 231 | LEU | 1 |
| 1 | I | 166 | ASP | 1 |
| 1 | I | 203 | LYS | 1 |
| 1 | J | 162 | ARG | 1 |
| 1 | K | 151 | LEU | 1 |
| 1 | K | 183 | ASN | 1 |
| 1 | L | 212 | GLU | 1 |
| 1 | H | 198 | CYS | 1 |
| 1 | H | 238 | VAL | 1 |
| 1 | I | 231 | LEU | 1 |
| 1 | J | 219 | GLN | 1 |
| 1 | K | 198 | CYS | 1 |
| 1 | K | 231 | LEU | 1 |
| 1 | I | 171 | THR | 1 |
| 1 | G | 175 | GLU | 1 |
| 1 | H | 151 | LEU | 1 |
| 1 | H | 184 | TRP | 1 |
| 1 | I | 175 | GLU | 1 |
| 1 | I | 184 | TRP | 1 |
| 1 | L | 149 | SER | 1 |
| 1 | H | 148 | THR | 1 |
| 1 | H | 163 | ASP | 1 |
| 1 | I | 190 | LEU | 1 |
| 1 | J | 230 | VAL | 1 |
| 1 | L | 200 | THR | 1 |
| 1 | G | 151 | LEU | 1 |
| 1 | H | 169 | TYR | 1 |
| 1 | L | 238 | VAL | 1 |
| 1 | H | 212 | GLU | 1 |
| 1 | H | 216 | THR | 1 |
| 1 | J | 149 | SER | 1 |
| 1 | K | 164 | TYR | 1 |
| 1 | K | 185 | MET | 1 |
| 1 | J | 181 | VAL | 1 |
| 1 | J | 231 | LEU | 1 |
| 1 | K | 166 | ASP | 1 |
| 1 | K | 227 | LYS | 1 |
| 1 | L | 162 | ARG | 1 |
| 1 | L | 173 | ARG | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 202 | LEU | 1 |
| 1 | I | 212 | GLU | 1 |
| 1 | L | 219 | GLN | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|-------|-------|-----|------|--------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | IHP | I | 301 | - | 36,36,36 | 1.67±0.00 | 6±1 (15±1%) |
| 2 | A1CCY | H | 301 | - | 36,36,36 | 2.14±0.00 | 8±0 (22±0%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|-------|-------|-----|------|-------------|-----------|--------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | IHP | I | 301 | - | 60,60,60 | 1.30±0.00 | 7±0 (11±0%) |
| 2 | A1CCY | H | 301 | - | 44,54,54 | 2.32±0.01 | 10±0 (22±0%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|-------|-------|-----|------|---------|--------------|-----------|
| 3 | IHP | I | 301 | - | - | 0±0,30,54,54 | 0±0,1,1,1 |
| 2 | A1CCY | H | 301 | - | - | 0±0,24,32,32 | 0±0,4,4,4 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|-------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | H | 301 | A1CCY | C12-N23 | 6.59 | 1.54 | 1.47 | 4 | 10 |
| 2 | H | 301 | A1CCY | C13-C11 | 5.98 | 1.60 | 1.52 | 9 | 10 |
| 3 | I | 301 | IHP | C6-C5 | 5.42 | 1.63 | 1.52 | 7 | 10 |
| 2 | H | 301 | A1CCY | C18-C13 | 5.05 | 1.47 | 1.39 | 7 | 10 |
| 3 | I | 301 | IHP | P6-O16 | 3.39 | 1.53 | 1.59 | 8 | 10 |
| 2 | H | 301 | A1CCY | C6-C1 | 3.12 | 1.45 | 1.39 | 10 | 10 |
| 3 | I | 301 | IHP | C5-C4 | 2.98 | 1.58 | 1.52 | 2 | 10 |
| 2 | H | 301 | A1CCY | C14-C13 | 2.83 | 1.43 | 1.39 | 7 | 10 |
| 3 | I | 301 | IHP | C2-C1 | 2.82 | 1.58 | 1.52 | 2 | 10 |
| 2 | H | 301 | A1CCY | C8-N10 | 2.59 | 1.52 | 1.48 | 5 | 10 |
| 2 | H | 301 | A1CCY | C27-C26 | 2.53 | 1.34 | 1.41 | 6 | 10 |
| 2 | H | 301 | A1CCY | C2-C1 | 2.25 | 1.36 | 1.39 | 7 | 10 |
| 3 | I | 301 | IHP | P2-O42 | 2.24 | 1.46 | 1.54 | 4 | 10 |
| 3 | I | 301 | IHP | P1-O11 | 2.04 | 1.63 | 1.59 | 7 | 5 |
| 3 | I | 301 | IHP | O13-C3 | 2.00 | 1.37 | 1.44 | 2 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|-------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | H | 301 | A1CCY | C28-N23-C24 | 7.97 | 117.34 | 122.90 | 5 | 10 |
| 2 | H | 301 | A1CCY | C9-C1-C6 | 7.33 | 105.58 | 110.50 | 10 | 10 |
| 2 | H | 301 | A1CCY | C6-C7-C8 | 6.53 | 96.46 | 102.89 | 1 | 10 |
| 3 | I | 301 | IHP | C5-C4-C3 | 3.81 | 102.06 | 110.43 | 2 | 10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|-------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | I | 301 | IHP | O15-C5-C6 | 3.24 | 115.66 | 108.76 | 1 | 10 |
| 2 | H | 301 | A1CCY | C17-C16-C19 | 3.14 | 115.06 | 121.47 | 1 | 10 |
| 2 | H | 301 | A1CCY | C7-C6-C1 | 3.11 | 112.59 | 110.50 | 5 | 10 |
| 3 | I | 301 | IHP | C5-C6-C1 | 3.08 | 103.66 | 110.43 | 4 | 10 |
| 2 | H | 301 | A1CCY | C15-C16-C19 | 2.80 | 127.19 | 121.47 | 1 | 10 |
| 3 | I | 301 | IHP | O34-P4-O14 | 2.68 | 116.27 | 105.85 | 3 | 10 |
| 3 | I | 301 | IHP | C6-C5-C4 | 2.53 | 104.88 | 110.43 | 10 | 10 |
| 2 | H | 301 | A1CCY | O29-C24-N23 | 2.50 | 117.21 | 120.53 | 5 | 10 |
| 3 | I | 301 | IHP | O15-P5-O25 | 2.44 | 100.63 | 109.33 | 9 | 10 |
| 2 | H | 301 | A1CCY | C3-C2-C1 | 2.26 | 117.57 | 120.88 | 9 | 10 |
| 2 | H | 301 | A1CCY | C21-C19-C16 | 2.12 | 115.36 | 110.35 | 5 | 10 |
| 2 | H | 301 | A1CCY | C14-C13-C18 | 2.06 | 115.74 | 118.30 | 7 | 8 |
| 3 | I | 301 | IHP | O46-P6-O36 | 2.06 | 115.53 | 107.80 | 3 | 10 |

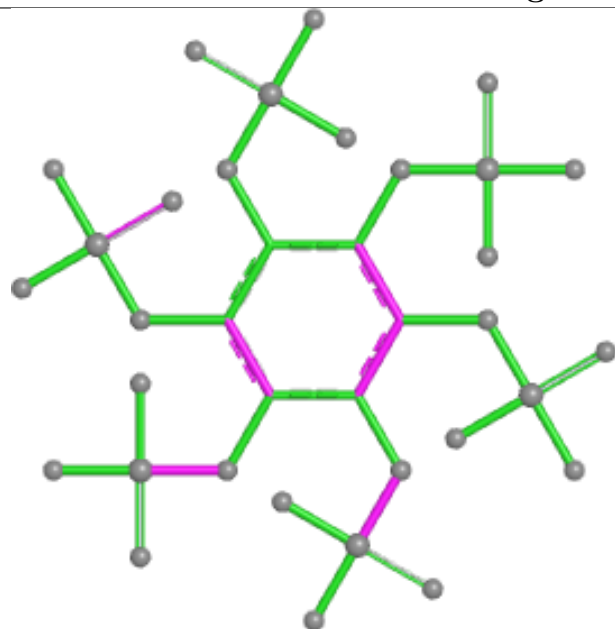
There are no chirality outliers.

There are no torsion outliers.

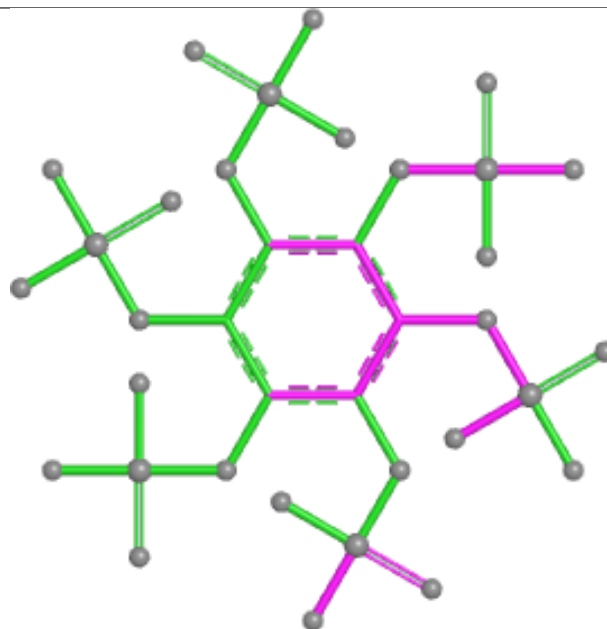
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

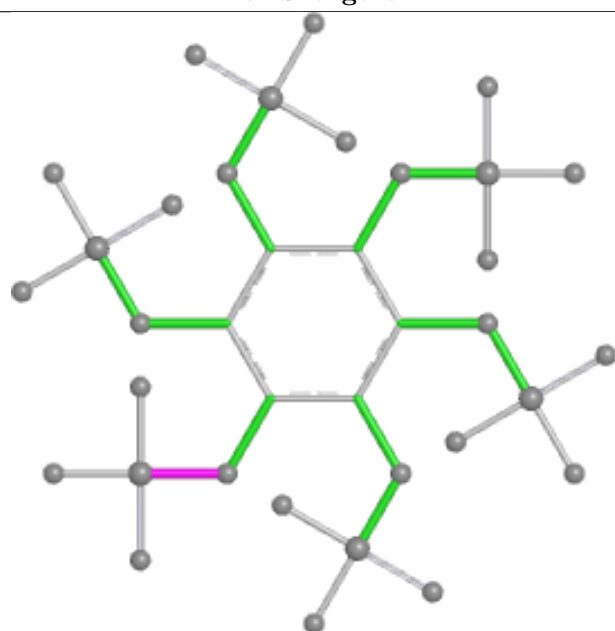
Ligand IHP I 301



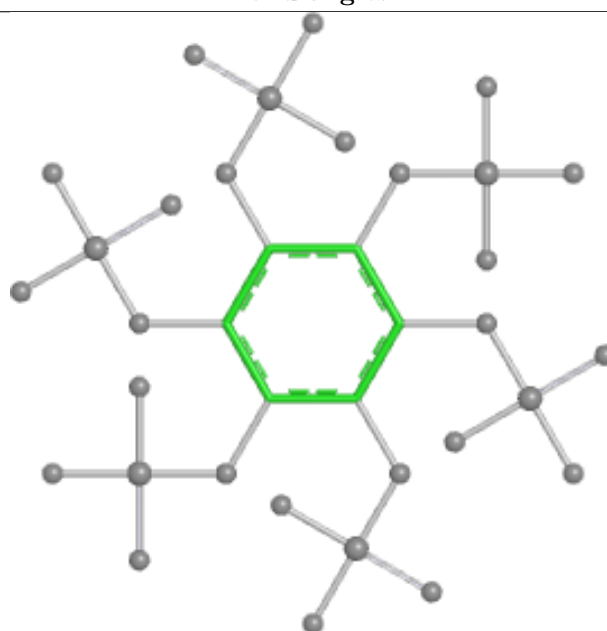
Bond lengths



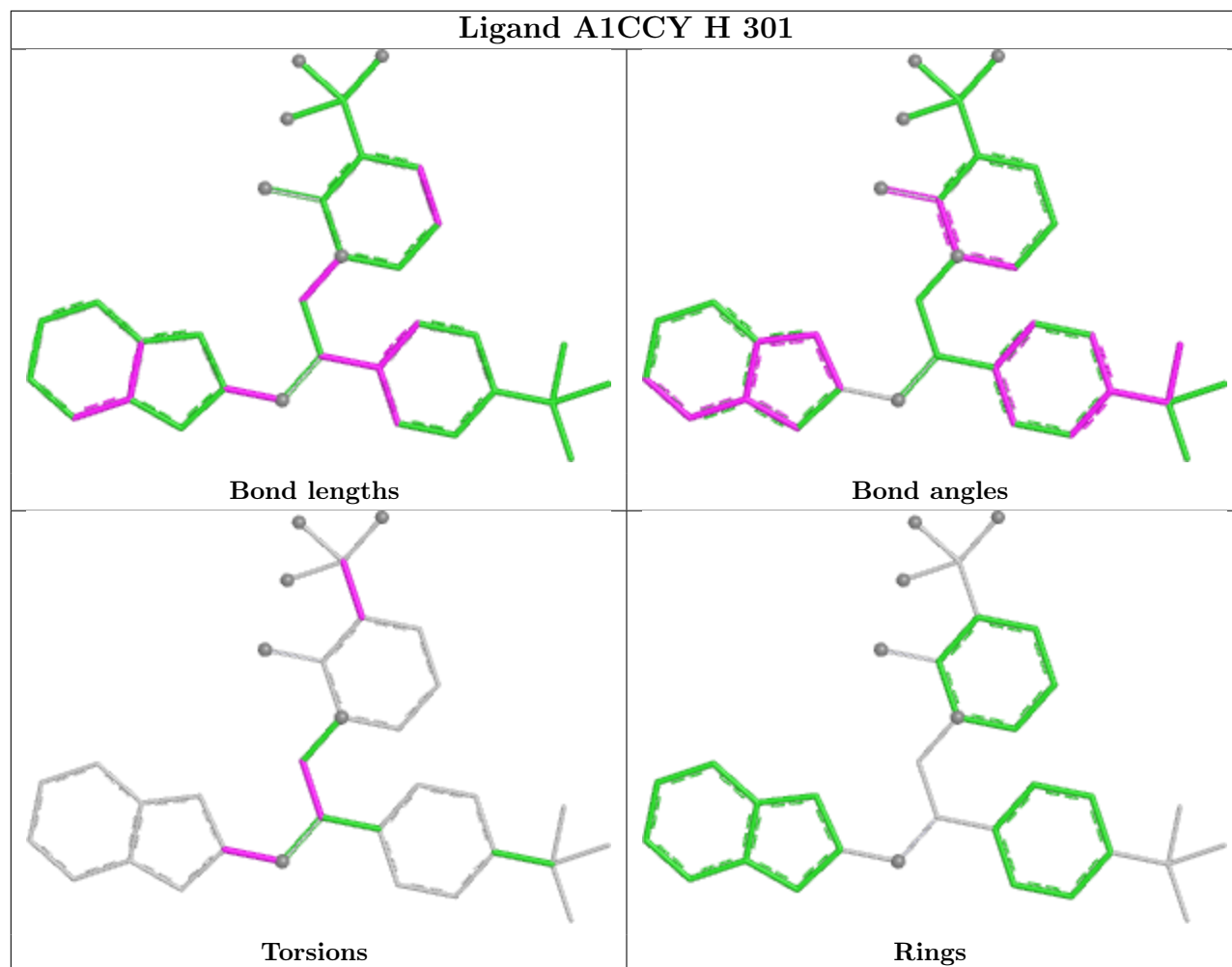
Bond angles



Torsions



Rings



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1000295825_cs_P1.str.V1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|-----|
| Total number of shifts | 516 |
| Number of shifts mapped to atoms | 516 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 96 | -0.80 ± 0.20 | Should be checked |
| $^{13}\text{C}_\beta$ | 87 | 0.10 ± 0.18 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 92 | -0.78 ± 0.21 | Should be applied |
| ^{15}N | 93 | -0.45 ± 0.80 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 474 atoms were assigned a chemical shift out of a possible 7333. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|--------------|-----------------|-----------------|
| Backbone | 257/2702 (10%) | 2/1098 (0%) | 174/1090 (16%) | 81/514 (16%) |
| Sidechain | 198/4296 (5%) | 8/2790 (0%) | 190/1326 (14%) | 0/180 (0%) |

Continued on next page...

Continued from previous page...

| | Total | ¹H | ¹³C | ¹⁵N |
|----------|---------------|----------------------|-----------------------|-----------------------|
| Aromatic | 19/335 (6%) | 1/164 (1%) | 18/160 (11%) | 0/11 (0%) |
| Overall | 474/7333 (6%) | 11/4052 (0%) | 382/2576 (15%) | 81/705 (11%) |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 501 atoms were assigned a chemical shift out of a possible 8046. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|---------------|----------------------|-----------------------|-----------------------|
| Backbone | 278/3042 (9%) | 2/1242 (0%) | 188/1224 (15%) | 88/576 (15%) |
| Sidechain | 204/4662 (4%) | 8/3036 (0%) | 196/1440 (14%) | 0/186 (0%) |
| Aromatic | 19/342 (6%) | 1/168 (1%) | 18/162 (11%) | 0/12 (0%) |
| Overall | 501/8046 (6%) | 11/4446 (0%) | 402/2826 (14%) | 88/774 (11%) |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

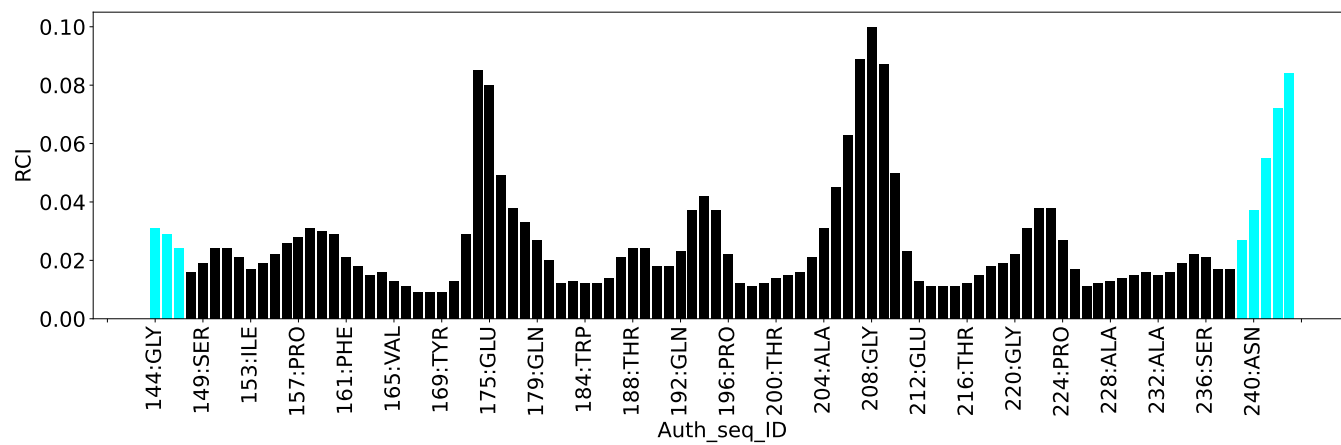
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain G:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description | Value |
|--|-------|
| Total distance restraints | 2529 |
| Intra-residue ($ i-j =0$) | 834 |
| Sequential ($ i-j =1$) | 290 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 522 |
| Long range ($ i-j \geq 5$) | 474 |
| Inter-chain | 409 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 1116 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 5.9 |
| Number of long range restraints per residue ¹ | 0.8 |

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 26.9 | 0.2 |
| 0.2-0.5 (Medium) | 54.3 | 0.5 |
| >0.5 (Large) | 75.5 | 3.06 |

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 159.3 | 9.96 |
| 10.0-20.0 (Medium) | 21.9 | 19.97 |
| >20.0 (Large) | 5.8 | 72.7 |

9 Distance violation analysis ⓘ

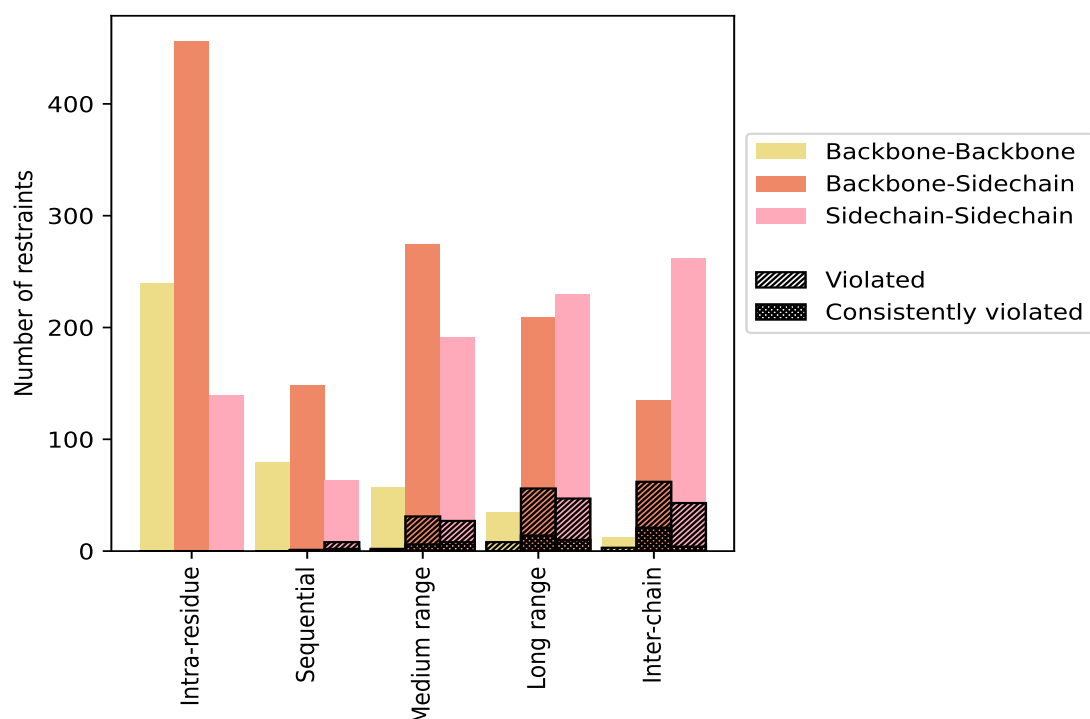
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|--|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|---------------------|---------------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue (i-j =0) | 834 | 33.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 239 | 9.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 456 | 18.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 139 | 5.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential (i-j =1) | 290 | 11.5 | 9 | 3.1 | 0.4 | 3 | 1.0 | 0.1 |
| Backbone-Backbone | 79 | 3.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 148 | 5.9 | 1 | 0.7 | 0.0 | 1 | 0.7 | 0.0 |
| Sidechain-Sidechain | 63 | 2.5 | 8 | 12.7 | 0.3 | 2 | 3.2 | 0.1 |
| Medium range (i-j >1 & i-j <5) | 522 | 20.6 | 60 | 11.5 | 2.4 | 15 | 2.9 | 0.6 |
| Backbone-Backbone | 57 | 2.3 | 2 | 3.5 | 0.1 | 1 | 1.8 | 0.0 |
| Backbone-Sidechain | 274 | 10.8 | 31 | 11.3 | 1.2 | 6 | 2.2 | 0.2 |
| Sidechain-Sidechain | 191 | 7.6 | 27 | 14.1 | 1.1 | 8 | 4.2 | 0.3 |
| Long range (i-j ≥5) | 474 | 18.7 | 111 | 23.4 | 4.4 | 24 | 5.1 | 0.9 |
| Backbone-Backbone | 35 | 1.4 | 8 | 22.9 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 209 | 8.3 | 56 | 26.8 | 2.2 | 14 | 6.7 | 0.6 |
| Sidechain-Sidechain | 230 | 9.1 | 47 | 20.4 | 1.9 | 10 | 4.3 | 0.4 |
| Inter-chain | 409 | 16.2 | 108 | 26.4 | 4.3 | 25 | 6.1 | 1.0 |
| Backbone-Backbone | 12 | 0.5 | 3 | 25.0 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 135 | 5.3 | 62 | 45.9 | 2.5 | 21 | 15.6 | 0.8 |
| Sidechain-Sidechain | 262 | 10.4 | 43 | 16.4 | 1.7 | 4 | 1.5 | 0.2 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 2529 | 100.0 | 288 | 11.4 | 11.4 | 67 | 2.6 | 2.6 |
| Backbone-Backbone | 422 | 16.7 | 13 | 3.1 | 0.5 | 1 | 0.2 | 0.0 |
| Backbone-Sidechain | 1222 | 48.3 | 150 | 12.3 | 5.9 | 42 | 3.4 | 1.7 |
| Sidechain-Sidechain | 885 | 35.0 | 125 | 14.1 | 4.9 | 24 | 2.7 | 0.9 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

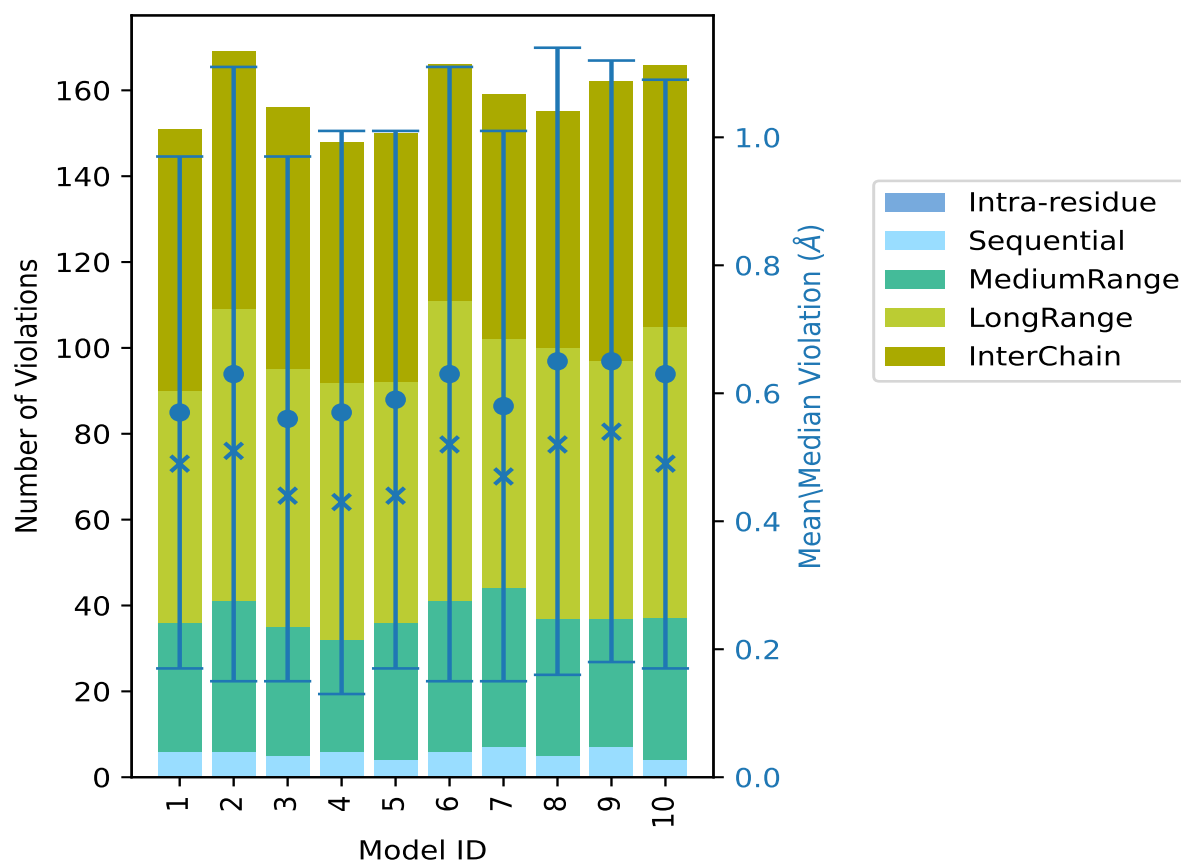
9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 0 | 6 | 30 | 54 | 61 | 151 | 0.57 | 1.89 | 0.4 | 0.49 |
| 2 | 0 | 6 | 35 | 68 | 60 | 169 | 0.63 | 2.24 | 0.48 | 0.51 |
| 3 | 0 | 5 | 30 | 60 | 61 | 156 | 0.56 | 1.95 | 0.41 | 0.44 |
| 4 | 0 | 6 | 26 | 60 | 56 | 148 | 0.57 | 2.21 | 0.44 | 0.43 |
| 5 | 0 | 4 | 32 | 56 | 58 | 150 | 0.59 | 2.29 | 0.42 | 0.44 |
| 6 | 0 | 6 | 35 | 70 | 55 | 166 | 0.63 | 2.26 | 0.48 | 0.52 |
| 7 | 0 | 7 | 37 | 58 | 57 | 159 | 0.58 | 2.13 | 0.43 | 0.47 |
| 8 | 0 | 5 | 32 | 63 | 55 | 155 | 0.65 | 3.06 | 0.49 | 0.52 |
| 9 | 0 | 7 | 30 | 60 | 65 | 162 | 0.65 | 2.37 | 0.47 | 0.54 |
| 10 | 0 | 4 | 33 | 68 | 61 | 166 | 0.63 | 2.6 | 0.46 | 0.49 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2241(IR:834, SQ:281, MR:462, LR:363, IC:301) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 12 | 22 | 22 | 56 | 1 | 10.0 |
| 0 | 2 | 10 | 12 | 10 | 34 | 2 | 20.0 |
| 0 | 0 | 5 | 10 | 16 | 31 | 3 | 30.0 |

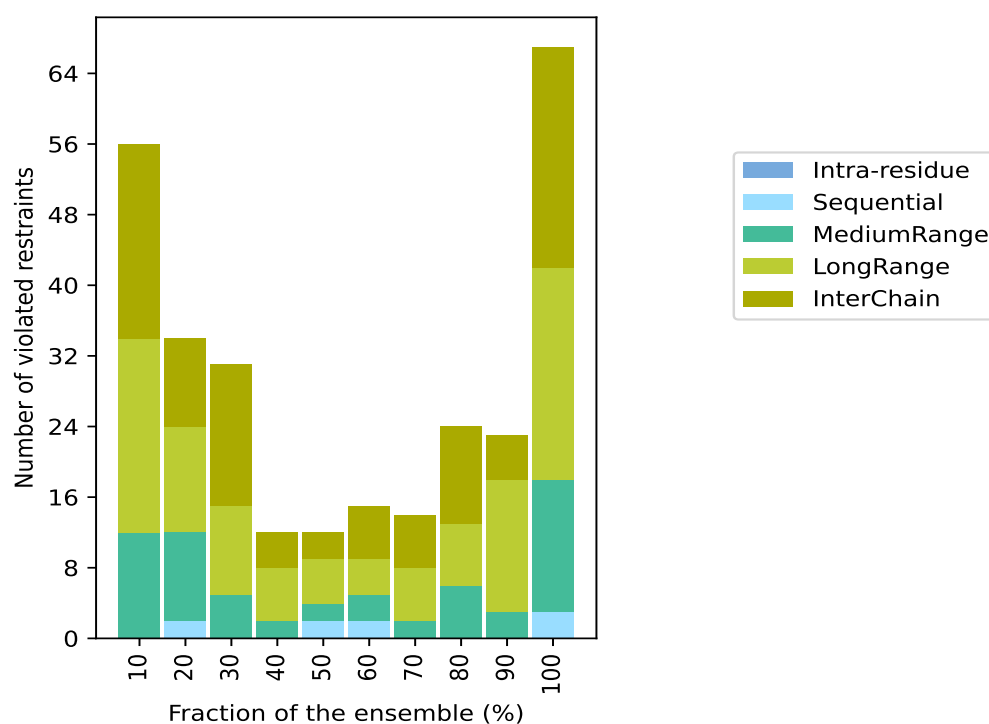
Continued on next page...

Continued from previous page...

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 2 | 6 | 4 | 12 | 4 | 40.0 |
| 0 | 2 | 2 | 5 | 3 | 12 | 5 | 50.0 |
| 0 | 2 | 3 | 4 | 6 | 15 | 6 | 60.0 |
| 0 | 0 | 2 | 6 | 6 | 14 | 7 | 70.0 |
| 0 | 0 | 6 | 7 | 11 | 24 | 8 | 80.0 |
| 0 | 0 | 3 | 15 | 5 | 23 | 9 | 90.0 |
| 0 | 3 | 15 | 24 | 25 | 67 | 10 | 100.0 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

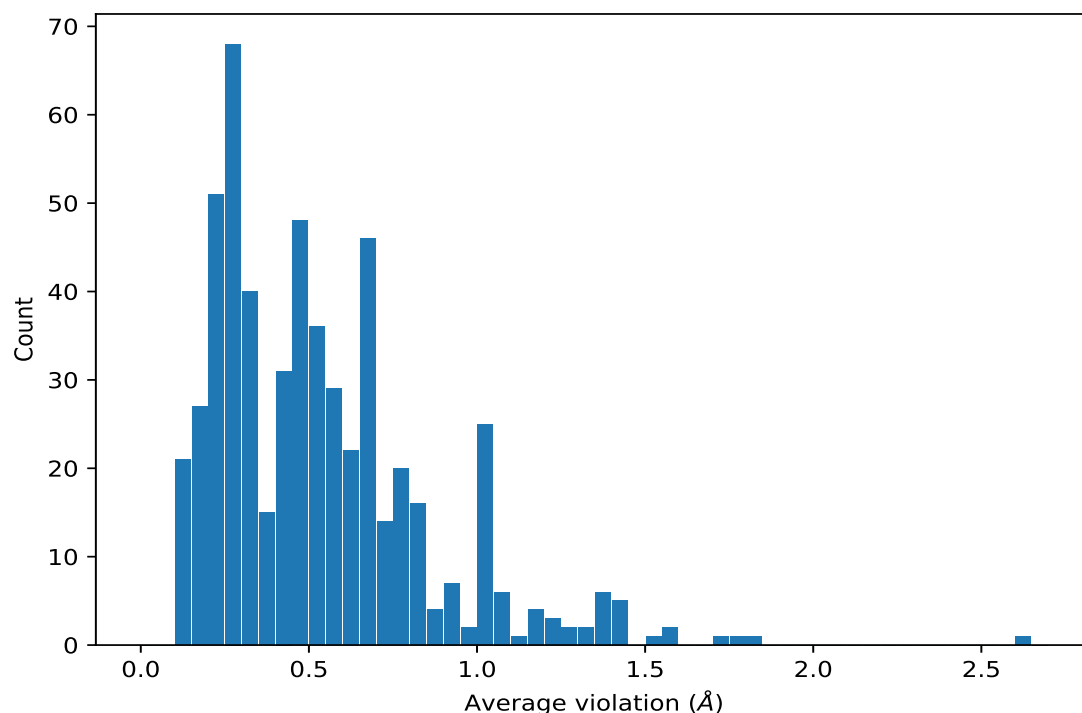


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|----------------|---------------------|----------|---------------------|------------|
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 10 | 1.83 | 0.39 | 1.98 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 10 | 1.71 | 0.27 | 1.77 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 10 | 1.59 | 0.08 | 1.6 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 10 | 1.55 | 0.27 | 1.48 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 10 | 1.5 | 0.17 | 1.46 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 10 | 1.43 | 0.35 | 1.59 |
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 10 | 1.38 | 0.62 | 1.41 |
| (1,1024) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 10 | 1.38 | 0.62 | 1.41 |
| (1,1024) | 1:171:L:THR:CG2 | 1:152:L:ASP:CB | 10 | 1.38 | 0.62 | 1.41 |
| (1,1024) | 1:171:G:THR:CG2 | 1:152:G:ASP:CB | 10 | 1.38 | 0.62 | 1.41 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 10 | 1.38 | 0.2 | 1.31 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 10 | 1.35 | 0.21 | 1.39 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 10 | 1.33 | 0.29 | 1.25 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 10 | 1.32 | 0.25 | 1.29 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 10 | 1.16 | 0.31 | 1.03 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|-----------------|---------------------|----------|---------------------|--------|
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 10 | 1.11 | 0.56 | 0.95 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 10 | 1.09 | 0.18 | 1.1 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 10 | 1.07 | 0.07 | 1.1 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 10 | 1.05 | 0.25 | 1.06 |
| (1,1201) | 1:153:K:ILE:CG2 | 1:165:K:VAL:CB | 10 | 1.05 | 0.25 | 1.06 |
| (1,1201) | 1:153:H:ILE:CG2 | 1:165:H:VAL:CB | 10 | 1.05 | 0.25 | 1.06 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 10 | 1.03 | 0.1 | 1.06 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 10 | 1.01 | 0.22 | 0.98 |
| (1,1400) | 1:194:I:ALA:CA | 1:197:I:ASP:CA | 10 | 1.0 | 0.05 | 1.02 |
| (1,1400) | 1:194:L:ALA:CA | 1:197:L:ASP:CA | 10 | 1.0 | 0.05 | 1.02 |
| (1,1400) | 1:194:K:ALA:CA | 1:197:K:ASP:CA | 10 | 1.0 | 0.05 | 1.02 |
| (1,471) | 1:163:K:ASP:CB | 1:161:K:PHE:CG | 10 | 1.0 | 0.22 | 1.04 |
| (1,471) | 1:163:G:ASP:CB | 1:161:G:PHE:CG | 10 | 1.0 | 0.22 | 1.04 |
| (1,471) | 1:163:L:ASP:CB | 1:161:L:PHE:CG | 10 | 1.0 | 0.22 | 1.04 |
| (1,471) | 1:163:H:ASP:CB | 1:161:H:PHE:CG | 10 | 1.0 | 0.22 | 1.04 |
| (1,471) | 1:163:I:ASP:CB | 1:161:I:PHE:CG | 10 | 1.0 | 0.22 | 1.04 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG1 | 10 | 1.0 | 0.27 | 1.02 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 10 | 1.0 | 0.27 | 1.02 |
| (1,1462) | 1:153:H:ILE:CG2 | 1:165:H:VAL:CG2 | 10 | 1.0 | 0.27 | 1.02 |
| (1,1462) | 1:153:K:ILE:CG2 | 1:165:K:VAL:CG2 | 10 | 1.0 | 0.27 | 1.02 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 10 | 0.99 | 0.11 | 0.96 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 10 | 0.95 | 0.24 | 0.89 |
| (1,57) | 1:154:L:ARG:CG | 1:192:L:GLN:CA | 10 | 0.95 | 0.24 | 0.89 |
| (1,57) | 1:154:J:ARG:CG | 1:192:J:GLN:CA | 10 | 0.95 | 0.24 | 0.89 |
| (1,57) | 1:154:H:ARG:CG | 1:192:H:GLN:CA | 10 | 0.95 | 0.24 | 0.89 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 10 | 0.92 | 0.1 | 0.92 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 10 | 0.89 | 0.82 | 0.61 |
| (1,1561) | 1:175:J:GLU:CB | 1:185:J:MET:CB | 10 | 0.89 | 0.82 | 0.61 |
| (1,1561) | 1:175:K:GLU:CB | 1:185:K:MET:CB | 10 | 0.89 | 0.82 | 0.61 |
| (1,1561) | 1:175:H:GLU:CB | 1:185:H:MET:CB | 10 | 0.89 | 0.82 | 0.61 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 10 | 0.82 | 0.18 | 0.75 |
| (1,1609) | 1:155:G:GLN:CB | 1:197:G:ASP:CB | 10 | 0.82 | 0.18 | 0.75 |
| (1,1609) | 1:155:K:GLN:CB | 1:197:K:ASP:CB | 10 | 0.82 | 0.18 | 0.75 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 10 | 0.82 | 0.42 | 0.7 |
| (1,662) | 1:150:K:ILE:CG2 | 1:168:K:PHE:C | 10 | 0.82 | 0.42 | 0.7 |
| (1,662) | 1:150:H:ILE:CG2 | 1:168:H:PHE:C | 10 | 0.82 | 0.42 | 0.7 |
| (1,662) | 1:150:L:ILE:CG2 | 1:168:L:PHE:C | 10 | 0.82 | 0.42 | 0.7 |
| (1,1029) | 1:167:L:ARG:CB | 1:169:L:TYR:CD1 | 10 | 0.79 | 0.24 | 0.86 |
| (1,1029) | 1:167:J:ARG:CB | 1:169:J:TYR:CD1 | 10 | 0.79 | 0.24 | 0.86 |
| (1,1029) | 1:167:I:ARG:CB | 1:169:I:TYR:CD1 | 10 | 0.79 | 0.24 | 0.86 |
| (1,1029) | 1:167:H:ARG:CB | 1:169:H:TYR:CD1 | 10 | 0.79 | 0.24 | 0.86 |
| (1,1029) | 1:167:K:ARG:CB | 1:169:K:TYR:CD1 | 10 | 0.79 | 0.24 | 0.86 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-----------------|----------------|---------------------|----------|---------------------|--------|
| (1,299) | 1:201:L:ILE:CG2 | 1:197:L:ASP:CB | 10 | 0.78 | 0.13 | 0.76 |
| (1,299) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 10 | 0.78 | 0.13 | 0.76 |
| (1,299) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CB | 10 | 0.78 | 0.13 | 0.76 |
| (1,299) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 10 | 0.78 | 0.13 | 0.76 |
| (1,263) | 1:151:L:LEU:CD1 | 1:153:L:ILE:CB | 10 | 0.73 | 0.32 | 0.75 |
| (1,263) | 1:151:K:LEU:CD1 | 1:153:K:ILE:CB | 10 | 0.73 | 0.32 | 0.75 |
| (1,263) | 1:151:H:LEU:CD1 | 1:153:H:ILE:CB | 10 | 0.73 | 0.32 | 0.75 |
| (1,263) | 1:151:G:LEU:CD1 | 1:153:G:ILE:CB | 10 | 0.73 | 0.32 | 0.75 |
| (1,1552) | 1:153:J:ILE:CG1 | 1:172:J:LEU:CA | 10 | 0.7 | 0.17 | 0.64 |
| (1,1552) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 10 | 0.7 | 0.17 | 0.64 |
| (1,1552) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 10 | 0.7 | 0.17 | 0.64 |
| (1,1552) | 1:153:I:ILE:CG1 | 1:172:I:LEU:CA | 10 | 0.7 | 0.17 | 0.64 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 10 | 0.7 | 0.36 | 0.56 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 10 | 0.69 | 0.13 | 0.69 |
| (1,1234) | 1:191:L:VAL:CG1 | 1:198:L:CYS:CA | 10 | 0.69 | 0.13 | 0.69 |
| (1,1234) | 1:191:G:VAL:CG1 | 1:198:G:CYS:CA | 10 | 0.69 | 0.13 | 0.69 |
| (1,1234) | 1:191:I:VAL:CG1 | 1:198:I:CYS:CA | 10 | 0.69 | 0.13 | 0.69 |
| (1,1234) | 1:191:J:VAL:CG1 | 1:198:J:CYS:CA | 10 | 0.69 | 0.13 | 0.69 |
| (1,1106) | 1:174:J:ALA:CB | 1:182:J:LYS:CE | 10 | 0.68 | 0.18 | 0.63 |
| (1,1106) | 1:174:L:ALA:CB | 1:182:L:LYS:CE | 10 | 0.68 | 0.18 | 0.63 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 10 | 0.68 | 0.18 | 0.63 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 10 | 0.68 | 0.21 | 0.74 |
| (1,384) | 1:189:I:LEU:CG | 1:164:I:TYR:CZ | 10 | 0.68 | 0.21 | 0.74 |
| (1,384) | 1:189:G:LEU:CG | 1:164:G:TYR:CZ | 10 | 0.68 | 0.21 | 0.74 |
| (1,107) | 1:150:H:ILE:CA | 1:164:H:TYR:CZ | 10 | 0.68 | 0.37 | 0.64 |
| (1,107) | 1:150:G:ILE:CA | 1:164:G:TYR:CZ | 10 | 0.68 | 0.37 | 0.64 |
| (1,107) | 1:150:K:ILE:CA | 1:164:K:TYR:CZ | 10 | 0.68 | 0.37 | 0.64 |
| (1,107) | 1:150:I:ILE:CA | 1:164:I:TYR:CZ | 10 | 0.68 | 0.37 | 0.64 |
| (1,107) | 1:150:L:ILE:CA | 1:164:L:TYR:CZ | 10 | 0.68 | 0.37 | 0.64 |
| (1,607) | 1:205:K:LEU:CB | 1:208:K:GLY:CA | 10 | 0.67 | 0.18 | 0.62 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 10 | 0.67 | 0.18 | 0.62 |
| (1,607) | 1:205:J:LEU:CB | 1:208:J:GLY:CA | 10 | 0.67 | 0.18 | 0.62 |
| (1,607) | 1:205:H:LEU:CB | 1:208:H:GLY:CA | 10 | 0.67 | 0.18 | 0.62 |
| (1,183) | 1:151:K:LEU:CG | 1:153:K:ILE:CB | 10 | 0.66 | 0.14 | 0.64 |
| (1,183) | 1:151:J:LEU:CG | 1:153:J:ILE:CB | 10 | 0.66 | 0.14 | 0.64 |
| (1,183) | 1:151:L:LEU:CG | 1:153:L:ILE:CB | 10 | 0.66 | 0.14 | 0.64 |
| (1,183) | 1:151:H:LEU:CG | 1:153:H:ILE:CB | 10 | 0.66 | 0.14 | 0.64 |
| (1,183) | 1:151:I:LEU:CG | 1:153:I:ILE:CB | 10 | 0.66 | 0.14 | 0.64 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 10 | 0.66 | 0.13 | 0.6 |
| (1,861) | 1:153:I:ILE:CG2 | 1:169:I:TYR:C | 10 | 0.66 | 0.13 | 0.6 |
| (1,861) | 1:153:L:ILE:CG2 | 1:169:L:TYR:C | 10 | 0.66 | 0.13 | 0.6 |
| (1,350) | 1:190:I:LEU:CG | 1:187:I:GLU:CG | 10 | 0.65 | 0.11 | 0.65 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|-----------------|---------------------|----------|---------------------|--------|
| (1,350) | 1:190:J:LEU:CG | 1:187:J:GLU:CG | 10 | 0.65 | 0.11 | 0.65 |
| (1,350) | 1:190:K:LEU:CG | 1:187:K:GLU:CG | 10 | 0.65 | 0.11 | 0.65 |
| (1,350) | 1:190:H:LEU:CG | 1:187:H:GLU:CG | 10 | 0.65 | 0.11 | 0.65 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 10 | 0.64 | 0.14 | 0.6 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 10 | 0.63 | 0.29 | 0.61 |
| (1,155) | 1:155:L:GLN:CB | 1:196:L:PRO:CA | 10 | 0.61 | 0.05 | 0.6 |
| (1,155) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 10 | 0.61 | 0.05 | 0.6 |
| (1,155) | 1:155:K:GLN:CB | 1:196:K:PRO:CA | 10 | 0.61 | 0.05 | 0.6 |
| (1,155) | 1:155:I:GLN:CB | 1:196:I:PRO:CA | 10 | 0.61 | 0.05 | 0.6 |
| (1,155) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 10 | 0.61 | 0.05 | 0.6 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 10 | 0.58 | 0.18 | 0.56 |
| (1,1623) | 1:214:J:MET:CB | 1:198:J:CYS:CA | 10 | 0.58 | 0.18 | 0.56 |
| (1,912) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 10 | 0.58 | 0.21 | 0.53 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 10 | 0.58 | 0.21 | 0.53 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 10 | 0.56 | 0.25 | 0.55 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 10 | 0.55 | 0.14 | 0.6 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 10 | 0.55 | 0.32 | 0.64 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 10 | 0.55 | 0.33 | 0.42 |
| (1,500) | 1:172:H:LEU:CD1 | 1:153:H:ILE:CG1 | 10 | 0.55 | 0.33 | 0.42 |
| (1,500) | 1:172:L:LEU:CD1 | 1:153:L:ILE:CG1 | 10 | 0.55 | 0.33 | 0.42 |
| (1,500) | 1:172:J:LEU:CD1 | 1:153:J:ILE:CG1 | 10 | 0.55 | 0.33 | 0.42 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 10 | 0.55 | 0.04 | 0.55 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 10 | 0.53 | 0.34 | 0.35 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 10 | 0.52 | 0.2 | 0.54 |
| (1,1084) | 1:192:I:GLN:CA | 1:164:I:TYR:CZ | 10 | 0.51 | 0.18 | 0.45 |
| (1,1084) | 1:192:G:GLN:CA | 1:164:G:TYR:CZ | 10 | 0.51 | 0.18 | 0.45 |
| (1,1084) | 1:192:K:GLN:CA | 1:164:K:TYR:CZ | 10 | 0.51 | 0.18 | 0.45 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 10 | 0.51 | 0.18 | 0.45 |
| (1,31) | 1:215:H:MET:CG | 1:219:H:GLN:C | 10 | 0.5 | 0.43 | 0.37 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 10 | 0.5 | 0.43 | 0.37 |
| (1,31) | 1:215:K:MET:CG | 1:219:K:GLN:C | 10 | 0.5 | 0.43 | 0.37 |
| (1,31) | 1:215:I:MET:CG | 1:219:I:GLN:C | 10 | 0.5 | 0.43 | 0.37 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 10 | 0.49 | 0.11 | 0.5 |
| (1,1203) | 1:190:I:LEU:CD1 | 1:155:I:GLN:CG | 10 | 0.49 | 0.11 | 0.5 |
| (1,1203) | 1:190:K:LEU:CD1 | 1:155:K:GLN:CG | 10 | 0.49 | 0.11 | 0.5 |
| (1,104) | 1:198:L:CYS:CB | 1:199:L:LYS:CE | 10 | 0.49 | 0.11 | 0.5 |
| (1,104) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 10 | 0.49 | 0.11 | 0.5 |
| (1,104) | 1:198:I:CYS:CB | 1:199:I:LYS:CE | 10 | 0.49 | 0.11 | 0.5 |
| (1,104) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 10 | 0.49 | 0.11 | 0.5 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 10 | 0.48 | 0.16 | 0.47 |
| (1,563) | 1:235:G:MET:CB | 1:233:H:GLU:CG | 10 | 0.48 | 0.16 | 0.47 |
| (1,1288) | 1:201:J:ILE:CG1 | 1:214:J:MET:CA | 10 | 0.46 | 0.11 | 0.44 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-----------------|-----------------|---------------------|----------|---------------------|--------|
| (1,1288) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 10 | 0.46 | 0.11 | 0.44 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 10 | 0.46 | 0.11 | 0.44 |
| (1,1288) | 1:201:L:ILE:CG1 | 1:214:L:MET:CA | 10 | 0.46 | 0.11 | 0.44 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 10 | 0.45 | 0.12 | 0.46 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 10 | 0.42 | 0.07 | 0.46 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 10 | 0.42 | 0.07 | 0.46 |
| (1,95) | 1:179:J:GLN:CB | 1:177:J:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,95) | 1:179:L:GLN:CB | 1:177:L:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,95) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,95) | 1:179:H:GLN:CB | 1:177:H:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,95) | 1:179:K:GLN:CB | 1:177:K:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,95) | 1:179:I:GLN:CB | 1:177:I:ALA:CA | 10 | 0.42 | 0.06 | 0.42 |
| (1,454) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 10 | 0.34 | 0.11 | 0.34 |
| (1,454) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 10 | 0.34 | 0.11 | 0.34 |
| (1,454) | 1:201:K:ILE:CG1 | 1:205:K:LEU:CA | 10 | 0.34 | 0.11 | 0.34 |
| (1,454) | 1:201:I:ILE:CG1 | 1:205:I:LEU:CA | 10 | 0.34 | 0.11 | 0.34 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 10 | 0.34 | 0.13 | 0.32 |
| (1,986) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CA | 10 | 0.34 | 0.13 | 0.32 |
| (1,986) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CA | 10 | 0.34 | 0.13 | 0.32 |
| (1,1428) | 1:214:L:MET:CB | 1:205:L:LEU:CA | 10 | 0.32 | 0.09 | 0.34 |
| (1,1428) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 10 | 0.32 | 0.09 | 0.34 |
| (1,1428) | 1:214:G:MET:CB | 1:205:G:LEU:CA | 10 | 0.32 | 0.09 | 0.34 |
| (1,1428) | 1:214:H:MET:CB | 1:205:H:LEU:CA | 10 | 0.32 | 0.09 | 0.34 |
| (1,249) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 10 | 0.31 | 0.06 | 0.3 |
| (1,249) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 10 | 0.31 | 0.06 | 0.3 |
| (1,249) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 10 | 0.31 | 0.06 | 0.3 |
| (1,249) | 1:196:J:PRO:CD | 1:200:J:THR:CB | 10 | 0.31 | 0.06 | 0.3 |
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 10 | 0.28 | 0.05 | 0.29 |
| (1,1621) | 1:204:G:ALA:CB | 1:206:G:GLY:C | 10 | 0.28 | 0.05 | 0.29 |
| (1,1621) | 1:204:L:ALA:CB | 1:206:L:GLY:C | 10 | 0.28 | 0.05 | 0.29 |
| (1,1621) | 1:204:H:ALA:CB | 1:206:H:GLY:C | 10 | 0.28 | 0.05 | 0.29 |
| (1,1619) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 10 | 0.28 | 0.04 | 0.28 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 10 | 0.28 | 0.04 | 0.28 |
| (1,1619) | 1:160:H:PRO:CG | 1:161:H:PHE:CG | 10 | 0.28 | 0.04 | 0.28 |
| (1,1619) | 1:160:J:PRO:CG | 1:161:J:PHE:CG | 10 | 0.28 | 0.04 | 0.28 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE2 | 9 | 1.21 | 0.4 | 1.2 |
| (1,156) | 1:187:K:GLU:CA | 1:169:K:TYR:CE2 | 9 | 1.21 | 0.4 | 1.2 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE1 | 9 | 1.21 | 0.4 | 1.2 |
| (1,1339) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 9 | 1.04 | 0.57 | 1.04 |
| (1,1339) | 1:151:G:LEU:CG | 1:189:G:LEU:CB | 9 | 1.04 | 0.57 | 1.04 |
| (1,1339) | 1:151:H:LEU:CG | 1:189:H:LEU:CB | 9 | 1.04 | 0.57 | 1.04 |
| (1,1339) | 1:151:I:LEU:CG | 1:189:I:LEU:CB | 9 | 1.04 | 0.57 | 1.04 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|-----------------|---------------------|----------|---------------------|--------|
| (1,859) | 1:157:K:PRO:CG | 1:197:K:ASP:CB | 9 | 1.0 | 0.34 | 1.11 |
| (1,859) | 1:157:H:PRO:CG | 1:197:H:ASP:CB | 9 | 1.0 | 0.34 | 1.11 |
| (1,859) | 1:157:J:PRO:CG | 1:197:J:ASP:CB | 9 | 1.0 | 0.34 | 1.11 |
| (1,746) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 9 | 0.79 | 0.27 | 0.87 |
| (1,746) | 1:221:J:VAL:CG1 | 1:230:J:VAL:CG2 | 9 | 0.79 | 0.27 | 0.87 |
| (1,746) | 1:221:H:VAL:CG2 | 1:230:H:VAL:CG2 | 9 | 0.79 | 0.27 | 0.87 |
| (1,746) | 1:221:I:VAL:CG1 | 1:230:I:VAL:CG2 | 9 | 0.79 | 0.27 | 0.87 |
| (1,746) | 1:221:H:VAL:CG1 | 1:230:H:VAL:CG2 | 9 | 0.79 | 0.27 | 0.87 |
| (1,396) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 9 | 0.75 | 0.34 | 0.82 |
| (1,396) | 1:174:H:ALA:CA | 1:148:H:THR:CA | 9 | 0.75 | 0.34 | 0.82 |
| (1,396) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 9 | 0.75 | 0.34 | 0.82 |
| (1,396) | 1:174:I:ALA:CA | 1:148:I:THR:CA | 9 | 0.75 | 0.34 | 0.82 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 9 | 0.74 | 0.74 | 0.3 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 9 | 0.64 | 0.22 | 0.66 |
| (1,61) | 1:150:G:ILE:CG2 | 1:182:G:LYS:C | 9 | 0.64 | 0.4 | 0.6 |
| (1,61) | 1:150:I:ILE:CG2 | 1:182:I:LYS:C | 9 | 0.64 | 0.4 | 0.6 |
| (1,61) | 1:150:H:ILE:CG2 | 1:182:H:LYS:C | 9 | 0.64 | 0.4 | 0.6 |
| (1,61) | 1:150:L:ILE:CG2 | 1:182:L:LYS:C | 9 | 0.64 | 0.4 | 0.6 |
| (1,61) | 1:150:J:ILE:CG2 | 1:182:J:LYS:C | 9 | 0.64 | 0.4 | 0.6 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 9 | 0.56 | 0.18 | 0.54 |
| (1,434) | 1:230:H:VAL:CG2 | 1:221:H:VAL:CA | 9 | 0.56 | 0.18 | 0.54 |
| (1,434) | 1:230:G:VAL:CG2 | 1:221:G:VAL:CA | 9 | 0.56 | 0.18 | 0.54 |
| (1,434) | 1:230:L:VAL:CG2 | 1:221:L:VAL:CA | 9 | 0.56 | 0.18 | 0.54 |
| (1,761) | 1:172:L:LEU:CD1 | 1:189:L:LEU:CG | 9 | 0.55 | 0.27 | 0.5 |
| (1,761) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CG | 9 | 0.55 | 0.27 | 0.5 |
| (1,761) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CG | 9 | 0.55 | 0.27 | 0.5 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 9 | 0.54 | 0.3 | 0.51 |
| (1,430) | 1:162:K:ARG:CA | 1:218:K:CYS:CA | 9 | 0.54 | 0.3 | 0.51 |
| (1,43) | 1:165:L:VAL:CG2 | 1:202:L:LEU:CG | 9 | 0.5 | 0.18 | 0.44 |
| (1,43) | 1:165:G:VAL:CG2 | 1:202:G:LEU:CG | 9 | 0.5 | 0.18 | 0.44 |
| (1,43) | 1:165:H:VAL:CG2 | 1:202:H:LEU:CG | 9 | 0.5 | 0.18 | 0.44 |
| (1,43) | 1:165:I:VAL:CG2 | 1:202:I:LEU:CG | 9 | 0.5 | 0.18 | 0.44 |
| (1,1533) | 1:214:I:MET:CG | 1:190:I:LEU:CB | 9 | 0.46 | 0.14 | 0.45 |
| (1,1533) | 1:214:G:MET:CG | 1:190:G:LEU:CB | 9 | 0.46 | 0.14 | 0.45 |
| (1,1533) | 1:214:L:MET:CG | 1:190:L:LEU:CB | 9 | 0.46 | 0.14 | 0.45 |
| (1,1533) | 1:214:H:MET:CG | 1:190:H:LEU:CB | 9 | 0.46 | 0.14 | 0.45 |
| (1,378) | 1:177:L:ALA:CB | 1:185:L:MET:CA | 9 | 0.44 | 0.23 | 0.43 |
| (1,378) | 1:177:I:ALA:CB | 1:185:I:MET:CA | 9 | 0.44 | 0.23 | 0.43 |
| (1,378) | 1:177:K:ALA:CB | 1:185:K:MET:CA | 9 | 0.44 | 0.23 | 0.43 |
| (1,378) | 1:177:H:ALA:CB | 1:185:H:MET:CA | 9 | 0.44 | 0.23 | 0.43 |
| (1,891) | 1:221:L:VAL:CG2 | 1:219:L:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |
| (1,891) | 1:221:J:VAL:CG2 | 1:219:J:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|--------------------|---------------------|----------|---------------------|--------|
| (1,891) | 1:221:H:VAL:CG2 | 1:219:H:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |
| (1,891) | 1:221:G:VAL:CG2 | 1:219:G:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |
| (1,891) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |
| (1,891) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 9 | 0.41 | 0.08 | 0.41 |
| (1,1176) | 1:190:K:LEU:CD1 | 1:166:K:ASP:CA | 9 | 0.39 | 0.1 | 0.38 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 9 | 0.39 | 0.1 | 0.38 |
| (1,1176) | 1:190:J:LEU:CD1 | 1:166:J:ASP:CA | 9 | 0.39 | 0.1 | 0.38 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 9 | 0.37 | 0.14 | 0.4 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 9 | 0.37 | 0.14 | 0.4 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 9 | 0.37 | 0.14 | 0.4 |
| (1,1818) | 1:191:I:VAL:N | 1:199:I:LYS:CE | 9 | 0.37 | 0.09 | 0.4 |
| (1,1818) | 1:191:H:VAL:N | 1:199:H:LYS:CE | 9 | 0.37 | 0.09 | 0.4 |
| (1,1818) | 1:191:J:VAL:N | 1:199:J:LYS:CE | 9 | 0.37 | 0.09 | 0.4 |
| (1,1818) | 1:191:K:VAL:N | 1:199:K:LYS:CE | 9 | 0.37 | 0.09 | 0.4 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 9 | 0.3 | 0.17 | 0.24 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 9 | 0.3 | 0.17 | 0.24 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 9 | 0.29 | 0.1 | 0.27 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 9 | 0.29 | 0.1 | 0.27 |
| (1,1396) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 9 | 0.28 | 0.09 | 0.28 |
| (1,1396) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 9 | 0.28 | 0.09 | 0.28 |
| (1,1396) | 1:172:G:LEU:CG | 1:183:G:ASN:CA | 9 | 0.28 | 0.09 | 0.28 |
| (1,897) | 1:153:J:ILE:CD1 | 1:151:J:LEU:C | 9 | 0.26 | 0.05 | 0.25 |
| (1,897) | 1:153:K:ILE:CD1 | 1:151:K:LEU:C | 9 | 0.26 | 0.05 | 0.25 |
| (1,897) | 1:153:L:ILE:CD1 | 1:151:L:LEU:C | 9 | 0.26 | 0.05 | 0.25 |
| (1,897) | 1:153:I:ILE:CD1 | 1:151:I:LEU:C | 9 | 0.26 | 0.05 | 0.25 |
| (1,667) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 9 | 0.2 | 0.08 | 0.21 |
| (1,667) | 1:191:H:VAL:CG1 | 1:194:H:ALA:C | 9 | 0.2 | 0.08 | 0.21 |
| (1,667) | 1:191:J:VAL:CG1 | 1:194:J:ALA:C | 9 | 0.2 | 0.08 | 0.21 |
| (1,667) | 1:191:L:VAL:CG1 | 1:194:L:ALA:C | 9 | 0.2 | 0.08 | 0.21 |
| (1,667) | 1:191:G:VAL:CG1 | 1:194:G:ALA:C | 9 | 0.2 | 0.08 | 0.21 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 8 | 1.76 | 0.33 | 1.81 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 8 | 1.02 | 0.62 | 1.25 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 8 | 0.97 | 0.15 | 0.94 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 8 | 0.76 | 0.39 | 0.7 |
| (1,1447) | 1:152:I:ASP:CB | 1:149:I:SER:CB | 8 | 0.72 | 0.43 | 0.64 |
| (1,1447) | 1:152:H:ASP:CB | 1:149:H:SER:CB | 8 | 0.72 | 0.43 | 0.64 |
| (1,1447) | 1:152:G:ASP:CB | 1:149:G:SER:CB | 8 | 0.72 | 0.43 | 0.64 |
| (1,1447) | 1:152:L:ASP:CB | 1:149:L:SER:CB | 8 | 0.72 | 0.43 | 0.64 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 8 | 0.64 | 0.37 | 0.63 |
| (1,1070) | 1:150:J:ILE:CD1 | 1:167:J:ARG:CA | 8 | 0.62 | 0.42 | 0.44 |
| (1,1070) | 1:150:K:ILE:CD1 | 1:167:K:ARG:CA | 8 | 0.62 | 0.42 | 0.44 |
| (1,1070) | 1:150:H:ILE:CD1 | 1:167:H:ARG:CA | 8 | 0.62 | 0.42 | 0.44 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-----------------|--------------------|---------------------|----------|---------------------|--------|
| (1,1070) | 1:150:L:ILE:CD1 | 1:167:L:ARG:CA | 8 | 0.62 | 0.42 | 0.44 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 8 | 0.6 | 0.27 | 0.71 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 8 | 0.6 | 0.23 | 0.66 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 8 | 0.48 | 0.22 | 0.42 |
| (1,1297) | 1:180:J:GLU:CG | 1:184:J:TRP:CA | 8 | 0.48 | 0.22 | 0.42 |
| (1,1297) | 1:180:L:GLU:CG | 1:184:L:TRP:CA | 8 | 0.48 | 0.22 | 0.42 |
| (1,1073) | 1:154:J:ARG:CG | 1:151:J:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,1073) | 1:154:I:ARG:CG | 1:151:I:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,1073) | 1:154:H:ARG:CG | 1:151:H:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,1073) | 1:154:K:ARG:CG | 1:151:K:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,1073) | 1:154:L:ARG:CG | 1:151:L:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,1073) | 1:154:G:ARG:CG | 1:151:G:LEU:CA | 8 | 0.47 | 0.29 | 0.46 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 8 | 0.46 | 0.13 | 0.52 |
| (1,981) | 1:150:J:ILE:CG2 | 1:190:J:LEU:CA | 8 | 0.46 | 0.2 | 0.37 |
| (1,981) | 1:150:K:ILE:CG2 | 1:190:K:LEU:CA | 8 | 0.46 | 0.2 | 0.37 |
| (1,981) | 1:150:H:ILE:CG2 | 1:190:H:LEU:CA | 8 | 0.46 | 0.2 | 0.37 |
| (1,981) | 1:150:I:ILE:CG2 | 1:190:I:LEU:CA | 8 | 0.46 | 0.2 | 0.37 |
| (1,981) | 1:150:L:ILE:CG2 | 1:190:L:LEU:CA | 8 | 0.46 | 0.2 | 0.37 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 8 | 0.42 | 0.23 | 0.46 |
| (1,1331) | 1:205:J:LEU:CD1 | 1:210:J:THR:CA | 8 | 0.4 | 0.23 | 0.34 |
| (1,1331) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 8 | 0.4 | 0.23 | 0.34 |
| (1,1331) | 1:205:L:LEU:CD1 | 1:210:L:THR:CA | 8 | 0.4 | 0.23 | 0.34 |
| (1,1331) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 8 | 0.4 | 0.23 | 0.34 |
| (1,939) | 1:189:G:LEU:CA | 1:153:G:ILE:C | 8 | 0.35 | 0.18 | 0.33 |
| (1,939) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 8 | 0.35 | 0.18 | 0.33 |
| (1,939) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 8 | 0.35 | 0.18 | 0.33 |
| (1,939) | 1:189:L:LEU:CA | 1:153:L:ILE:C | 8 | 0.35 | 0.18 | 0.33 |
| (1,1267) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 8 | 0.33 | 0.12 | 0.35 |
| (1,1267) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 8 | 0.33 | 0.12 | 0.35 |
| (1,1267) | 1:172:H:LEU:CD1 | 1:183:H:ASN:CB | 8 | 0.33 | 0.12 | 0.35 |
| (1,1267) | 1:172:G:LEU:CD1 | 1:183:G:ASN:CB | 8 | 0.33 | 0.12 | 0.35 |
| (1,1267) | 1:172:L:LEU:CD1 | 1:183:L:ASN:CB | 8 | 0.33 | 0.12 | 0.35 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 8 | 0.33 | 0.14 | 0.32 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 8 | 0.33 | 0.14 | 0.32 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 8 | 0.28 | 0.1 | 0.28 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 8 | 0.28 | 0.1 | 0.28 |
| (1,1498) | 1:190:L:LEU:CG | 1:187:L:GLU:CB | 8 | 0.26 | 0.11 | 0.24 |
| (1,1498) | 1:190:J:LEU:CG | 1:187:J:GLU:CB | 8 | 0.26 | 0.11 | 0.24 |
| (1,1498) | 1:190:I:LEU:CG | 1:187:I:GLU:CB | 8 | 0.26 | 0.11 | 0.24 |
| (1,1498) | 1:190:K:LEU:CG | 1:187:K:GLU:CB | 8 | 0.26 | 0.11 | 0.24 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 8 | 0.25 | 0.07 | 0.26 |
| (1,1337) | 1:185:L:MET:CG | 1:182:L:LYS:CE | 8 | 0.25 | 0.07 | 0.26 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|-------------------|---------------------|----------|---------------------|--------|
| (1,1337) | 1:185:I:MET:CG | 1:182:I:LYS:CE | 8 | 0.25 | 0.07 | 0.26 |
| (1,1590) | 1:198:I:CYS:CB | 1:214:I:MET:CA | 8 | 0.24 | 0.07 | 0.22 |
| (1,1590) | 1:198:J:CYS:CB | 1:214:J:MET:CA | 8 | 0.24 | 0.07 | 0.22 |
| (1,1590) | 1:198:K:CYS:CB | 1:214:K:MET:CA | 8 | 0.24 | 0.07 | 0.22 |
| (1,297) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 8 | 0.2 | 0.03 | 0.2 |
| (1,297) | 1:202:J:LEU:CG | 1:194:J:ALA:CA | 8 | 0.2 | 0.03 | 0.2 |
| (1,297) | 1:202:H:LEU:CG | 1:194:H:ALA:CA | 8 | 0.2 | 0.03 | 0.2 |
| (1,1591) | 1:190:J:LEU:CD1 | 1:194:J:ALA:C | 8 | 0.19 | 0.05 | 0.18 |
| (1,1591) | 1:190:K:LEU:CD1 | 1:194:K:ALA:C | 8 | 0.19 | 0.05 | 0.18 |
| (1,1591) | 1:190:I:LEU:CD1 | 1:194:I:ALA:C | 8 | 0.19 | 0.05 | 0.18 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 7 | 1.03 | 0.21 | 0.95 |
| (1,1531) | 1:148:J:THR:CA | 1:174:J:ALA:C | 7 | 0.65 | 0.34 | 0.57 |
| (1,1531) | 1:148:K:THR:CA | 1:174:K:ALA:C | 7 | 0.65 | 0.34 | 0.57 |
| (1,1531) | 1:148:I:THR:CA | 1:174:I:ALA:C | 7 | 0.65 | 0.34 | 0.57 |
| (1,1531) | 1:148:H:THR:CA | 1:174:H:ALA:C | 7 | 0.65 | 0.34 | 0.57 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 7 | 0.52 | 0.3 | 0.61 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 7 | 0.51 | 0.35 | 0.4 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 7 | 0.5 | 0.16 | 0.51 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 7 | 0.48 | 0.33 | 0.37 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 7 | 0.48 | 0.33 | 0.37 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 7 | 0.3 | 0.14 | 0.23 |
| (1,1457) | 1:165:J:VAL:CG2 | 1:214:J:MET:CA | 7 | 0.3 | 0.14 | 0.23 |
| (1,721) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 7 | 0.28 | 0.06 | 0.25 |
| (1,721) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 7 | 0.28 | 0.06 | 0.25 |
| (1,721) | 1:191:J:VAL:CG1 | 1:193:J:ASN:CA | 7 | 0.28 | 0.06 | 0.25 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 7 | 0.28 | 0.15 | 0.21 |
| (1,914) | 1:221:K:VAL:CG1 | 1:223:K:GLY:CA | 7 | 0.26 | 0.12 | 0.2 |
| (1,914) | 1:221:H:VAL:CG1 | 1:223:H:GLY:CA | 7 | 0.26 | 0.12 | 0.2 |
| (1,914) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 7 | 0.26 | 0.12 | 0.2 |
| (1,914) | 1:221:L:VAL:CG1 | 1:223:L:GLY:CA | 7 | 0.26 | 0.12 | 0.2 |
| (1,475) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 7 | 0.25 | 0.09 | 0.23 |
| (1,475) | 1:153:H:ILE:CD1 | 1:193:H:ASN:CG | 7 | 0.25 | 0.09 | 0.23 |
| (1,475) | 1:153:J:ILE:CD1 | 1:193:J:ASN:CG | 7 | 0.25 | 0.09 | 0.23 |
| (1,1028) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 7 | 0.23 | 0.08 | 0.21 |
| (1,1028) | 1:190:L:LEU:CD1 | 1:169:L:TYR:CB | 7 | 0.23 | 0.08 | 0.21 |
| (1,1028) | 1:190:G:LEU:CD1 | 1:169:G:TYR:CB | 7 | 0.23 | 0.08 | 0.21 |
| (1,903) | 1:197:I:ASP:CB | 1:218:I:CYS:CA | 7 | 0.21 | 0.05 | 0.2 |
| (1,903) | 1:197:K:ASP:CB | 1:218:K:CYS:CA | 7 | 0.21 | 0.05 | 0.2 |
| (1,903) | 1:197:J:ASP:CB | 1:218:J:CYS:CA | 7 | 0.21 | 0.05 | 0.2 |
| (1,62) | 1:156:I:GLY:CA | 1:164:I:TYR:CA | 7 | 0.18 | 0.04 | 0.17 |
| (1,62) | 1:156:H:GLY:CA | 1:164:H:TYR:CA | 7 | 0.18 | 0.04 | 0.17 |
| (1,62) | 1:156:G:GLY:CA | 1:164:G:TYR:CA | 7 | 0.18 | 0.04 | 0.17 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|-----------------|---------------------|----------|---------------------|--------|
| (1,62) | 1:156:K:GLY:CA | 1:164:K:TYR:CA | 7 | 0.18 | 0.04 | 0.17 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 6 | 0.82 | 0.51 | 0.9 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 6 | 0.82 | 0.51 | 0.9 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 6 | 0.82 | 0.51 | 0.9 |
| (1,1525) | 1:211:K:LEU:CD1 | 1:213:K:GLU:C | 6 | 0.74 | 0.44 | 0.76 |
| (1,1525) | 1:211:L:LEU:CD1 | 1:213:L:GLU:C | 6 | 0.74 | 0.44 | 0.76 |
| (1,1525) | 1:211:I:LEU:CD1 | 1:213:I:GLU:C | 6 | 0.74 | 0.44 | 0.76 |
| (1,1525) | 1:211:J:LEU:CD1 | 1:213:J:GLU:C | 6 | 0.74 | 0.44 | 0.76 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 6 | 0.63 | 0.51 | 0.38 |
| (1,1191) | 1:171:L:THR:CG2 | 1:175:L:GLU:CA | 6 | 0.63 | 0.56 | 0.29 |
| (1,1191) | 1:171:K:THR:CG2 | 1:175:K:GLU:CA | 6 | 0.63 | 0.56 | 0.29 |
| (1,1191) | 1:171:H:THR:CG2 | 1:175:H:GLU:CA | 6 | 0.63 | 0.56 | 0.29 |
| (1,353) | 1:150:G:ILE:CD1 | 1:151:G:LEU:CD1 | 6 | 0.55 | 0.18 | 0.53 |
| (1,353) | 1:150:K:ILE:CD1 | 1:151:K:LEU:CD1 | 6 | 0.55 | 0.18 | 0.53 |
| (1,353) | 1:150:H:ILE:CD1 | 1:151:H:LEU:CD1 | 6 | 0.55 | 0.18 | 0.53 |
| (1,353) | 1:150:I:ILE:CD1 | 1:151:I:LEU:CD1 | 6 | 0.55 | 0.18 | 0.53 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 6 | 0.55 | 0.17 | 0.51 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 6 | 0.51 | 0.27 | 0.43 |
| (1,405) | 1:150:J:ILE:CG1 | 1:171:J:THR:CA | 6 | 0.43 | 0.23 | 0.42 |
| (1,405) | 1:150:I:ILE:CG1 | 1:171:I:THR:CA | 6 | 0.43 | 0.23 | 0.42 |
| (1,405) | 1:150:K:ILE:CG1 | 1:171:K:THR:CA | 6 | 0.43 | 0.23 | 0.42 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 6 | 0.42 | 0.22 | 0.34 |
| (1,1291) | 1:219:K:GLN:CB | 1:160:K:PRO:CA | 6 | 0.42 | 0.22 | 0.34 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 6 | 0.32 | 0.13 | 0.29 |
| (1,882) | 1:153:H:ILE:CG1 | 1:148:H:THR:CB | 6 | 0.29 | 0.07 | 0.31 |
| (1,882) | 1:153:J:ILE:CG1 | 1:148:J:THR:CB | 6 | 0.29 | 0.07 | 0.31 |
| (1,882) | 1:153:L:ILE:CG1 | 1:148:L:THR:CB | 6 | 0.29 | 0.07 | 0.31 |
| (1,882) | 1:153:K:ILE:CG1 | 1:148:K:THR:CB | 6 | 0.29 | 0.07 | 0.31 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 6 | 0.27 | 0.1 | 0.26 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 6 | 0.25 | 0.07 | 0.24 |
| (1,608) | 1:211:J:LEU:CD2 | 1:190:J:LEU:C | 6 | 0.24 | 0.13 | 0.18 |
| (1,608) | 1:211:L:LEU:CD2 | 1:190:L:LEU:C | 6 | 0.24 | 0.13 | 0.18 |
| (1,608) | 1:211:I:LEU:CD2 | 1:190:I:LEU:C | 6 | 0.24 | 0.13 | 0.18 |
| (1,1307) | 1:211:L:LEU:CB | 1:212:L:GLU:CD | 6 | 0.2 | 0.04 | 0.22 |
| (1,1307) | 1:211:H:LEU:CB | 1:212:H:GLU:CD | 6 | 0.2 | 0.04 | 0.22 |
| (1,1307) | 1:211:G:LEU:CB | 1:212:G:GLU:CD | 6 | 0.2 | 0.04 | 0.22 |
| (1,1307) | 1:211:I:LEU:CB | 1:212:I:GLU:CD | 6 | 0.2 | 0.04 | 0.22 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 5 | 0.72 | 0.23 | 0.64 |
| (1,444) | 1:185:H:MET:CE | 1:189:H:LEU:CD1 | 5 | 0.48 | 0.08 | 0.49 |
| (1,444) | 1:185:G:MET:CE | 1:189:G:LEU:CD1 | 5 | 0.48 | 0.08 | 0.49 |
| (1,444) | 1:185:K:MET:CE | 1:189:K:LEU:CD1 | 5 | 0.48 | 0.08 | 0.49 |
| (1,455) | 1:230:G:VAL:CG1 | 1:233:G:GLU:CD | 5 | 0.48 | 0.23 | 0.46 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|--------------------|---------------------|----------|---------------------|--------|
| (1,455) | 1:230:K:VAL:CG1 | 1:233:K:GLU:CD | 5 | 0.48 | 0.23 | 0.46 |
| (1,455) | 1:230:L:VAL:CG2 | 1:233:L:GLU:CD | 5 | 0.48 | 0.23 | 0.46 |
| (1,455) | 1:230:L:VAL:CG1 | 1:233:L:GLU:CD | 5 | 0.48 | 0.23 | 0.46 |
| (1,455) | 1:230:J:VAL:CG2 | 1:233:J:GLU:CD | 5 | 0.48 | 0.23 | 0.46 |
| (1,666) | 1:207:H:PRO:CG | 1:202:H:LEU:CA | 5 | 0.34 | 0.16 | 0.29 |
| (1,666) | 1:207:K:PRO:CG | 1:202:K:LEU:CA | 5 | 0.34 | 0.16 | 0.29 |
| (1,666) | 1:207:L:PRO:CG | 1:202:L:LEU:CA | 5 | 0.34 | 0.16 | 0.29 |
| (1,284) | 1:150:L:ILE:CD1 | 1:190:L:LEU:CD1 | 5 | 0.28 | 0.13 | 0.24 |
| (1,284) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 5 | 0.28 | 0.13 | 0.24 |
| (1,284) | 1:150:I:ILE:CD1 | 1:190:I:LEU:CD1 | 5 | 0.28 | 0.13 | 0.24 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 5 | 0.27 | 0.1 | 0.26 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 5 | 0.26 | 0.11 | 0.24 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 5 | 0.26 | 0.11 | 0.24 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 5 | 0.26 | 0.11 | 0.24 |
| (1,251) | 1:151:G:LEU:CD1 | 1:150:G:ILE:CG1 | 5 | 0.25 | 0.12 | 0.19 |
| (1,251) | 1:151:K:LEU:CD1 | 1:150:K:ILE:CG1 | 5 | 0.25 | 0.12 | 0.19 |
| (1,251) | 1:151:L:LEU:CD1 | 1:150:L:ILE:CG1 | 5 | 0.25 | 0.12 | 0.19 |
| (1,1432) | 1:153:K:ILE:CG2 | 1:165:K:VAL:C | 5 | 0.23 | 0.13 | 0.16 |
| (1,1432) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 5 | 0.23 | 0.13 | 0.16 |
| (1,1432) | 1:153:L:ILE:CG2 | 1:165:L:VAL:C | 5 | 0.23 | 0.13 | 0.16 |
| (1,1432) | 1:153:H:ILE:CG2 | 1:165:H:VAL:C | 5 | 0.23 | 0.13 | 0.16 |
| (1,103) | 1:190:I:LEU:CG | 1:164:I:TYR:CB | 5 | 0.19 | 0.07 | 0.23 |
| (1,103) | 1:190:H:LEU:CG | 1:164:H:TYR:CB | 5 | 0.19 | 0.07 | 0.23 |
| (1,959) | 1:158:H:LYS:CD | 1:159:H:GLU:CD | 5 | 0.17 | 0.04 | 0.17 |
| (1,959) | 1:158:I:LYS:CD | 1:159:I:GLU:CD | 5 | 0.17 | 0.04 | 0.17 |
| (1,23) | 1:153:J:ILE:CG2 | 1:167:J:ARG:CG | 5 | 0.14 | 0.01 | 0.13 |
| (1,23) | 1:153:K:ILE:CG2 | 1:167:K:ARG:CG | 5 | 0.14 | 0.01 | 0.13 |
| (1,1452) | 1:238:L:VAL:CG1 | 1:241:L:THR:CA | 4 | 1.42 | 0.68 | 1.4 |
| (1,1452) | 1:238:H:VAL:CG2 | 1:241:H:THR:CA | 4 | 1.42 | 0.68 | 1.4 |
| (1,797) | 1:238:I:VAL:CG1 | 1:243:I:THR:CA | 4 | 0.66 | 0.33 | 0.75 |
| (1,797) | 1:238:I:VAL:CG2 | 1:243:I:THR:CA | 4 | 0.66 | 0.33 | 0.75 |
| (1,797) | 1:238:K:VAL:CG2 | 1:243:K:THR:CA | 4 | 0.66 | 0.33 | 0.75 |
| (1,797) | 1:238:K:VAL:CG2 | 1:243:L:THR:CA | 4 | 0.66 | 0.33 | 0.75 |
| (1,962) | 1:244:K:ILE:CA | 1:238:K:VAL:CA | 4 | 0.56 | 0.32 | 0.46 |
| (1,962) | 1:244:I:ILE:CA | 1:238:I:VAL:CA | 4 | 0.56 | 0.32 | 0.46 |
| (1,962) | 1:244:L:ILE:CA | 1:238:L:VAL:CA | 4 | 0.56 | 0.32 | 0.46 |
| (1,696) | 1:151:G:LEU:CG | 1:189:G:LEU:CG | 4 | 0.53 | 0.16 | 0.55 |
| (1,696) | 1:151:H:LEU:CG | 1:189:H:LEU:CG | 4 | 0.53 | 0.16 | 0.55 |
| (1,696) | 1:151:J:LEU:CG | 1:189:J:LEU:CG | 4 | 0.53 | 0.16 | 0.55 |
| (1,1046) | 1:238:L:VAL:CG1 | 1:244:L:ILE:CB | 4 | 0.45 | 0.15 | 0.4 |
| (1,1046) | 1:238:H:VAL:CG2 | 1:244:H:ILE:CB | 4 | 0.45 | 0.15 | 0.4 |
| (1,1046) | 1:238:K:VAL:CG2 | 1:244:L:ILE:CB | 4 | 0.45 | 0.15 | 0.4 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|--------------------|-------------------|---------------------|----------|---------------------|--------|
| (1,1046) | 1:238:H:VAL:CG1 | 1:244:H:ILE:CB | 4 | 0.45 | 0.15 | 0.4 |
| (1,2144) | 1:156:L:GLY:CA | 1:160:G:PRO:CD | 4 | 0.37 | 0.13 | 0.33 |
| (1,2360) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:F32 | 4 | 0.36 | 0.21 | 0.33 |
| (1,2293) | 2:301:H:A1CCY:F32 | 1:222:H:GLY:CA | 4 | 0.3 | 0.19 | 0.3 |
| (1,1661) | 1:150:H:ILE:CG1 | 1:175:H:GLU:CB | 4 | 0.24 | 0.16 | 0.18 |
| (1,1661) | 1:150:K:ILE:CG1 | 1:182:K:LYS:CB | 4 | 0.24 | 0.16 | 0.18 |
| (1,1661) | 1:150:J:ILE:CG1 | 1:182:J:LYS:CB | 4 | 0.24 | 0.16 | 0.18 |
| (1,433) | 1:187:L:GLU:CB | 1:184:L:TRP:CZ3 | 4 | 0.23 | 0.05 | 0.25 |
| (1,433) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 4 | 0.23 | 0.05 | 0.25 |
| (1,2173) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 4 | 0.18 | 0.03 | 0.18 |
| (1,2173) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 4 | 0.18 | 0.03 | 0.18 |
| (1,1063) | 1:190:H:LEU:CD1 | 1:161:H:PHE:CA | 4 | 0.12 | 0.01 | 0.12 |
| (1,1110) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 3 | 1.19 | 0.66 | 0.79 |
| (1,1110) | 1:244:L:ILE:CG1 | 1:237:G:GLN:CB | 3 | 1.19 | 0.66 | 0.79 |
| (1,1110) | 1:244:J:ILE:CG1 | 1:237:K:GLN:CB | 3 | 1.19 | 0.66 | 0.79 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ1 | 3 | 0.81 | 0.85 | 0.33 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ2 | 3 | 0.81 | 0.85 | 0.33 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ3 | 3 | 0.81 | 0.85 | 0.33 |
| (1,2235) | 2:301:H:A1CCY:F32 | 1:226:I:HIS:CA | 3 | 0.8 | 0.22 | 0.79 |
| (1,1030) | 1:148:H:THR:CB | 1:174:H:ALA:C | 3 | 0.52 | 0.24 | 0.66 |
| (1,1030) | 1:148:K:THR:CB | 1:174:K:ALA:C | 3 | 0.52 | 0.24 | 0.66 |
| (1,1030) | 1:148:G:THR:CB | 1:174:G:ALA:C | 3 | 0.52 | 0.24 | 0.66 |
| (1,2161) | 1:162:L:ARG:CG | 1:152:K:ASP:CB | 3 | 0.52 | 0.25 | 0.64 |
| (1,1465) | 1:150:J:ILE:CG2 | 1:153:J:ILE:CG1 | 3 | 0.52 | 0.14 | 0.55 |
| (1,1465) | 1:150:K:ILE:CG2 | 1:153:K:ILE:CG1 | 3 | 0.52 | 0.14 | 0.55 |
| (1,1465) | 1:150:I:ILE:CG2 | 1:153:I:ILE:CG1 | 3 | 0.52 | 0.14 | 0.55 |
| (1,631) | 1:244:I:ILE:CG1 | 1:238:I:VAL:CA | 3 | 0.51 | 0.15 | 0.43 |
| (1,631) | 1:244:H:ILE:CG1 | 1:238:H:VAL:CA | 3 | 0.51 | 0.15 | 0.43 |
| (1,631) | 1:244:L:ILE:CG1 | 1:238:L:VAL:CA | 3 | 0.51 | 0.15 | 0.43 |
| (1,2341) | 3:301:I:IHP:P1 | 1:158:L:LYS:HA | 3 | 0.5 | 0.23 | 0.66 |
| (1,2377) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:F32 | 3 | 0.48 | 0.07 | 0.5 |
| (1,2279) | 2:301:H:A1CCY:H8 | 1:232:H:ALA:CA | 3 | 0.44 | 0.27 | 0.36 |
| (1,40) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 3 | 0.42 | 0.22 | 0.51 |
| (1,40) | 1:219:J:GLN:CG | 1:160:J:PRO:CA | 3 | 0.42 | 0.22 | 0.51 |
| (1,2230) | 2:301:H:A1CCY:F33 | 1:223:I:GLY:CA | 3 | 0.38 | 0.34 | 0.15 |
| (1,2242) | 2:301:H:A1CCY:H12A | 1:232:I:ALA:CA | 3 | 0.35 | 0.18 | 0.47 |
| (1,2242) | 2:301:H:A1CCY:H12B | 1:232:I:ALA:CA | 3 | 0.35 | 0.18 | 0.47 |
| (1,1335) | 1:217:J:ALA:CB | 1:221:J:VAL:CG2 | 3 | 0.34 | 0.02 | 0.34 |
| (1,1335) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 3 | 0.34 | 0.02 | 0.34 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ1 | 3 | 0.31 | 0.06 | 0.32 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ2 | 3 | 0.31 | 0.06 | 0.32 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ3 | 3 | 0.31 | 0.06 | 0.32 |

Continued on next page

Continued from previous page...

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|--------------------|--------------------|---------------------|----------|---------------------|--------|
| (1,833) | 1:235:L:MET:CB | 1:239:L:THR:CA | 3 | 0.31 | 0.1 | 0.36 |
| (1,833) | 1:235:H:MET:CB | 1:239:H:THR:CA | 3 | 0.31 | 0.1 | 0.36 |
| (1,294) | 1:152:G:ASP:CB | 1:148:G:THR:CB | 3 | 0.3 | 0.12 | 0.38 |
| (1,294) | 1:152:L:ASP:CB | 1:148:L:THR:CB | 3 | 0.3 | 0.12 | 0.38 |
| (1,1218) | 1:202:H:LEU:CD1 | 1:205:H:LEU:CA | 3 | 0.28 | 0.13 | 0.26 |
| (1,1218) | 1:202:I:LEU:CD1 | 1:205:I:LEU:CA | 3 | 0.28 | 0.13 | 0.26 |
| (1,1218) | 1:202:J:LEU:CD1 | 1:205:J:LEU:CA | 3 | 0.28 | 0.13 | 0.26 |
| (1,811) | 1:185:G:MET:CE | 1:151:G:LEU:CG | 3 | 0.24 | 0.11 | 0.21 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD2 | 3 | 0.22 | 0.07 | 0.17 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD3 | 3 | 0.22 | 0.07 | 0.17 |
| (1,561) | 1:172:K:LEU:CG | 1:153:K:ILE:CB | 3 | 0.21 | 0.09 | 0.17 |
| (1,561) | 1:172:H:LEU:CG | 1:153:H:ILE:CB | 3 | 0.21 | 0.09 | 0.17 |
| (1,2391) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F33 | 3 | 0.2 | 0.08 | 0.17 |
| (1,876) | 1:153:K:ILE:CG2 | 1:164:K:TYR:CA | 3 | 0.2 | 0.02 | 0.19 |
| (1,876) | 1:153:J:ILE:CG2 | 1:164:J:TYR:CA | 3 | 0.2 | 0.02 | 0.19 |
| (1,876) | 1:153:G:ILE:CG2 | 1:164:G:TYR:CA | 3 | 0.2 | 0.02 | 0.19 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12A | 3 | 0.2 | 0.03 | 0.18 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12B | 3 | 0.2 | 0.03 | 0.18 |
| (1,2258) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CA | 3 | 0.19 | 0.04 | 0.16 |
| (1,2282) | 2:301:H:A1CCY:H12A | 1:232:H:ALA:CB | 3 | 0.18 | 0.05 | 0.2 |
| (1,2282) | 2:301:H:A1CCY:H12B | 1:232:H:ALA:CB | 3 | 0.18 | 0.05 | 0.2 |
| (1,854) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 3 | 0.17 | 0.02 | 0.16 |
| (1,2128) | 1:195:H:ASN:CA | 1:219:I:GLN:CA | 3 | 0.17 | 0.01 | 0.16 |
| (1,2396) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F33 | 3 | 0.17 | 0.04 | 0.16 |
| (1,804) | 1:190:I:LEU:CA | 1:165:I:VAL:CA | 3 | 0.16 | 0.05 | 0.13 |
| (1,804) | 1:190:H:LEU:CA | 1:165:H:VAL:CA | 3 | 0.16 | 0.05 | 0.13 |
| (1,1246) | 1:218:I:CYS:CB | 1:226:I:HIS:CD2 | 3 | 0.13 | 0.02 | 0.13 |
| (1,1246) | 1:218:H:CYS:CB | 1:226:H:HIS:CD2 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2159) | 1:223:I:GLY:CA | 1:157:H:PRO:CD | 2 | 2.65 | 0.41 | 2.65 |
| (1,952) | 1:175:H:GLU:CB | 1:148:H:THR:CB | 2 | 1.41 | 0.18 | 1.41 |
| (1,952) | 1:175:L:GLU:CB | 1:148:L:THR:CB | 2 | 1.41 | 0.18 | 1.41 |
| (1,684) | 1:175:L:GLU:CB | 1:171:L:THR:CB | 2 | 1.27 | 0.04 | 1.27 |
| (1,684) | 1:175:K:GLU:CB | 1:171:K:THR:CB | 2 | 1.27 | 0.04 | 1.27 |
| (1,2236) | 2:301:H:A1CCY:F31 | 1:224:I:PRO:CA | 2 | 1.06 | 0.05 | 1.06 |
| (1,1624) | 1:150:H:ILE:CD1 | 1:175:H:GLU:CB | 2 | 1.0 | 0.72 | 1.0 |
| (1,1624) | 1:150:J:ILE:CD1 | 1:175:J:GLU:CB | 2 | 1.0 | 0.72 | 1.0 |
| (1,1519) | 1:175:H:GLU:CB | 1:148:H:THR:CA | 2 | 0.92 | 0.57 | 0.92 |
| (1,1519) | 1:175:L:GLU:CB | 1:148:L:THR:CA | 2 | 0.92 | 0.57 | 0.92 |
| (1,244) | 1:175:L:GLU:CB | 1:171:L:THR:CA | 2 | 0.82 | 0.0 | 0.82 |
| (1,244) | 1:175:K:GLU:CB | 1:171:K:THR:CA | 2 | 0.82 | 0.0 | 0.82 |
| (1,2238) | 2:301:H:A1CCY:F33 | 1:224:I:PRO:CA | 2 | 0.76 | 0.04 | 0.76 |
| (1,2288) | 2:301:H:A1CCY:F33 | 1:157:H:PRO:CG | 2 | 0.68 | 0.28 | 0.68 |

Continued on next page

Continued from previous page...

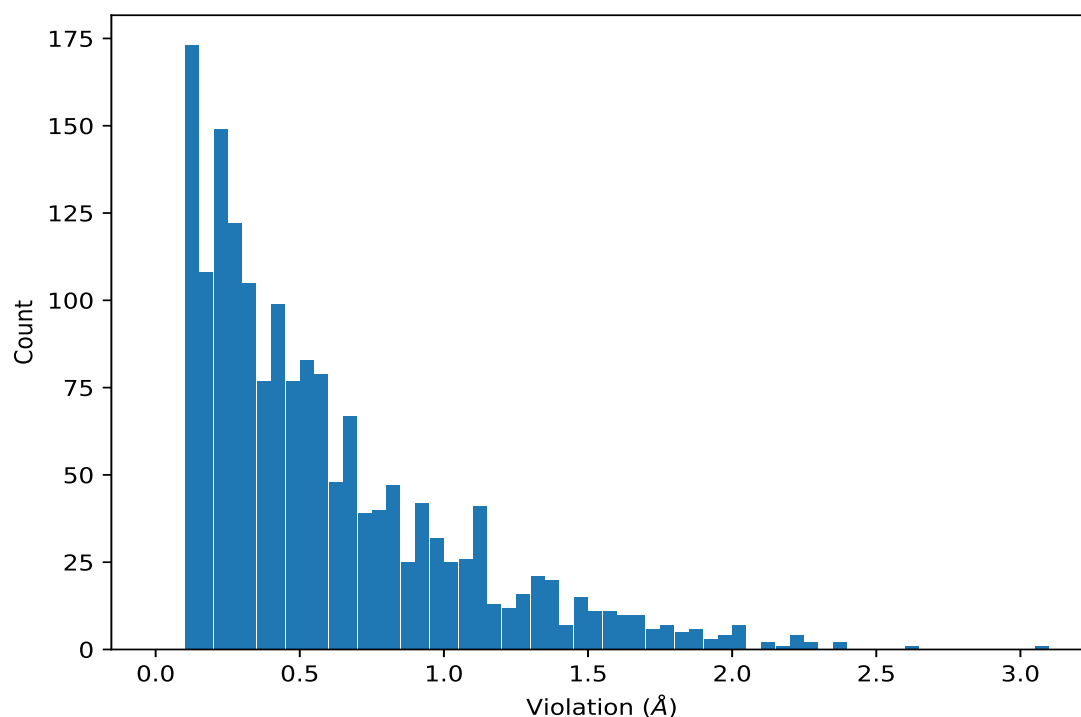
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median |
|----------|-------------------|--------------------|---------------------|----------|---------------------|--------|
| (1,176) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 2 | 0.52 | 0.24 | 0.52 |
| (1,176) | 1:244:J:ILE:CG1 | 1:237:K:GLN:CA | 2 | 0.52 | 0.24 | 0.52 |
| (1,169) | 1:161:J:PHE:CD1 | 1:165:J:VAL:C | 2 | 0.39 | 0.03 | 0.39 |
| (1,169) | 1:161:K:PHE:CD1 | 1:165:K:VAL:C | 2 | 0.39 | 0.03 | 0.39 |
| (1,590) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 2 | 0.31 | 0.03 | 0.31 |
| (1,2139) | 1:156:G:GLY:CA | 1:160:H:PRO:CD | 2 | 0.28 | 0.13 | 0.28 |
| (1,1351) | 1:162:I:ARG:CG | 1:161:I:PHE:CD1 | 2 | 0.26 | 0.11 | 0.26 |
| (1,2153) | 1:219:J:GLN:CG | 1:155:I:GLN:CA | 2 | 0.26 | 0.15 | 0.26 |
| (1,403) | 1:189:G:LEU:CG | 1:151:G:LEU:CB | 2 | 0.26 | 0.14 | 0.26 |
| (1,403) | 1:189:H:LEU:CG | 1:151:H:LEU:CB | 2 | 0.26 | 0.14 | 0.26 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22A | 2 | 0.24 | 0.1 | 0.24 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22B | 2 | 0.24 | 0.1 | 0.24 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22C | 2 | 0.24 | 0.1 | 0.24 |
| (1,2152) | 1:219:K:GLN:CG | 1:155:J:GLN:CA | 2 | 0.24 | 0.05 | 0.24 |
| (1,1262) | 1:190:I:LEU:CD1 | 1:202:I:LEU:CG | 2 | 0.2 | 0.04 | 0.2 |
| (1,787) | 1:218:I:CYS:CB | 1:197:I:ASP:CB | 2 | 0.2 | 0.09 | 0.2 |
| (1,1280) | 1:214:H:MET:CG | 1:207:H:PRO:CA | 2 | 0.2 | 0.0 | 0.2 |
| (1,1147) | 1:153:K:ILE:CB | 1:193:K:ASN:CA | 2 | 0.19 | 0.03 | 0.19 |
| (1,1147) | 1:153:L:ILE:CB | 1:193:L:ASN:CA | 2 | 0.19 | 0.03 | 0.19 |
| (1,2215) | 1:225:J:GLY:CA | 1:196:I:PRO:CD | 2 | 0.19 | 0.06 | 0.19 |
| (1,1544) | 1:214:L:MET:CA | 1:210:L:THR:CB | 2 | 0.18 | 0.06 | 0.18 |
| (1,1544) | 1:214:I:MET:CA | 1:210:I:THR:CB | 2 | 0.18 | 0.06 | 0.18 |
| (1,878) | 1:184:G:TRP:CD1 | 1:188:G:THR:C | 2 | 0.16 | 0.06 | 0.16 |
| (1,827) | 1:160:I:PRO:CB | 1:161:I:PHE:CD2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,827) | 1:160:H:PRO:CB | 1:161:H:PHE:CD2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,2254) | 2:301:H:A1CCY:F32 | 1:195:H:ASN:CA | 2 | 0.15 | 0.03 | 0.15 |
| (1,271) | 1:194:L:ALA:CB | 1:154:L:ARG:CG | 2 | 0.14 | 0.03 | 0.14 |
| (1,271) | 1:194:G:ALA:CB | 1:154:G:ARG:CG | 2 | 0.14 | 0.03 | 0.14 |
| (1,275) | 1:187:I:GLU:CB | 1:183:I:ASN:CB | 2 | 0.14 | 0.0 | 0.14 |
| (1,275) | 1:187:K:GLU:CB | 1:183:K:ASN:CB | 2 | 0.14 | 0.0 | 0.14 |
| (1,1565) | 1:234:G:ALA:CB | 1:238:G:VAL:CA | 2 | 0.14 | 0.04 | 0.14 |
| (1,1565) | 1:234:J:ALA:CB | 1:238:J:VAL:CA | 2 | 0.14 | 0.04 | 0.14 |
| (1,656) | 1:167:I:ARG:CB | 1:159:I:GLU:CG | 2 | 0.13 | 0.03 | 0.13 |
| (1,656) | 1:167:K:ARG:CB | 1:159:K:GLU:CG | 2 | 0.13 | 0.03 | 0.13 |
| (1,1395) | 1:211:K:LEU:CD2 | 1:209:K:ALA:CA | 2 | 0.12 | 0.01 | 0.12 |
| (1,1395) | 1:211:I:LEU:CD2 | 1:209:I:ALA:CA | 2 | 0.12 | 0.01 | 0.12 |
| (1,703) | 1:205:K:LEU:CG | 1:218:K:CYS:CA | 2 | 0.12 | 0.02 | 0.12 |
| (1,703) | 1:205:I:LEU:CG | 1:218:I:CYS:CA | 2 | 0.12 | 0.02 | 0.12 |
| (1,414) | 1:171:G:THR:CA | 1:168:G:PHE:CG | 2 | 0.12 | 0.0 | 0.12 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|----------------|----------|---------------|
| (1,2159) | 1:223:I:GLY:CA | 1:157:H:PRO:CD | 8 | 3.06 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 10 | 2.6 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 9 | 2.37 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 9 | 2.35 |
| (1,1561) | 1:175:K:GLU:CB | 1:185:K:MET:CB | 5 | 2.29 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 6 | 2.26 |
| (1,2159) | 1:223:I:GLY:CA | 1:157:H:PRO:CD | 2 | 2.24 |
| (1,1024) | 1:171:G:THR:CG2 | 1:152:G:ASP:CB | 6 | 2.22 |
| (1,1452) | 1:238:L:VAL:CG1 | 1:241:L:THR:CA | 4 | 2.21 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 2 | 2.2 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,1024) | 1:171:G:THR:CG2 | 1:152:G:ASP:CB | 9 | 2.17 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 7 | 2.13 |
| (1,1110) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 2 | 2.12 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 4 | 2.05 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 10 | 2.03 |
| (1,1024) | 1:171:G:THR:CG2 | 1:152:G:ASP:CB | 7 | 2.02 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ1 | 9 | 2.0 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ2 | 9 | 2.0 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ3 | 9 | 2.0 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 5 | 2.0 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 8 | 1.99 |
| (1,1452) | 1:238:L:VAL:CG1 | 1:241:L:THR:CA | 8 | 1.99 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 6 | 1.97 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 4 | 1.96 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 3 | 1.95 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 5 | 1.92 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 8 | 1.91 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 2 | 1.89 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 1 | 1.89 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 7 | 1.89 |
| (1,662) | 1:150:K:ILE:CG2 | 1:168:K:PHE:C | 3 | 1.88 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 10 | 1.87 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 4 | 1.86 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 6 | 1.83 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE2 | 1 | 1.83 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 8 | 1.82 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 3 | 1.82 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 6 | 1.81 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 7 | 1.79 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 6 | 1.78 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 9 | 1.76 |
| (1,1339) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 6 | 1.76 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 8 | 1.75 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 1 | 1.75 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 3 | 1.75 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 5 | 1.74 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 8 | 1.73 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 2 | 1.72 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 2 | 1.72 |
| (1,1624) | 1:150:H:ILE:CD1 | 1:175:H:GLU:CB | 10 | 1.72 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 8 | 1.71 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 2 | 1.69 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,1339) | 1:151:G:LEU:CG | 1:189:G:LEU:CB | 2 | 1.69 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 5 | 1.68 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 4 | 1.68 |
| (1,1447) | 1:152:G:ASP:CB | 1:149:G:SER:CB | 6 | 1.68 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 9 | 1.67 |
| (1,31) | 1:215:H:MET:CG | 1:219:H:GLN:C | 9 | 1.67 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 1 | 1.66 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 8 | 1.66 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 9 | 1.66 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 3 | 1.64 |
| (1,1339) | 1:151:G:LEU:CG | 1:189:G:LEU:CB | 9 | 1.63 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 9 | 1.62 |
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 10 | 1.62 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 3 | 1.61 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 7 | 1.61 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 7 | 1.6 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 1 | 1.6 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 10 | 1.6 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 6 | 1.6 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 8 | 1.59 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 2 | 1.59 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 7 | 1.59 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 1 | 1.59 |
| (1,952) | 1:175:H:GLU:CB | 1:148:H:THR:CB | 10 | 1.59 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 6 | 1.58 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 7 | 1.57 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 8 | 1.57 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 4 | 1.56 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 2 | 1.56 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 8 | 1.55 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 8 | 1.54 |
| (1,1024) | 1:171:L:THR:CG2 | 1:152:L:ASP:CB | 5 | 1.54 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 10 | 1.54 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 5 | 1.53 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE2 | 9 | 1.53 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 6 | 1.52 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 5 | 1.52 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 3 | 1.52 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 2 | 1.52 |
| (1,1191) | 1:171:K:THR:CG2 | 1:175:K:GLU:CA | 10 | 1.5 |
| (1,156) | 1:187:K:GLU:CA | 1:169:K:TYR:CE2 | 8 | 1.5 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 4 | 1.49 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 1 | 1.49 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 1 | 1.49 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 1 | 1.49 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 2 | 1.49 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 9 | 1.49 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 4 | 1.49 |
| (1,1519) | 1:175:H:GLU:CB | 1:148:H:THR:CA | 10 | 1.49 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 2 | 1.48 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 2 | 1.48 |
| (1,1201) | 1:153:K:ILE:CG2 | 1:165:K:VAL:CB | 2 | 1.48 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 1 | 1.47 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 6 | 1.46 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 2 | 1.46 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 4 | 1.46 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 9 | 1.45 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 10 | 1.45 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 6 | 1.44 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 8 | 1.44 |
| (1,859) | 1:157:K:PRO:CG | 1:197:K:ASP:CB | 9 | 1.44 |
| (1,2246) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CB | 6 | 1.43 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 8 | 1.42 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 6 | 1.4 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 7 | 1.4 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 6 | 1.4 |
| (1,1462) | 1:153:H:ILE:CG2 | 1:165:H:VAL:CG2 | 6 | 1.4 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 3 | 1.39 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 4 | 1.39 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 6 | 1.39 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 9 | 1.39 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 7 | 1.39 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 3 | 1.38 |
| (1,263) | 1:151:L:LEU:CD1 | 1:153:L:ILE:CB | 3 | 1.38 |
| (1,61) | 1:150:G:ILE:CG2 | 1:182:G:LYS:C | 2 | 1.38 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 2 | 1.37 |
| (1,1462) | 1:153:K:ILE:CG2 | 1:165:K:VAL:CG2 | 10 | 1.37 |
| (1,1070) | 1:150:K:ILE:CD1 | 1:167:K:ARG:CA | 3 | 1.37 |
| (1,156) | 1:187:K:GLU:CA | 1:169:K:TYR:CE2 | 2 | 1.37 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 3 | 1.36 |
| (1,500) | 1:172:J:LEU:CD1 | 1:153:J:ILE:CG1 | 9 | 1.36 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 1 | 1.35 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 1 | 1.35 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 4 | 1.34 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,1201) | 1:153:H:ILE:CG2 | 1:165:H:VAL:CB | 6 | 1.34 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 2 | 1.33 |
| (1,859) | 1:157:J:PRO:CG | 1:197:J:ASP:CB | 4 | 1.33 |
| (1,396) | 1:174:H:ALA:CA | 1:148:H:THR:CA | 8 | 1.33 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 7 | 1.33 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 7 | 1.32 |
| (1,107) | 1:150:G:ILE:CA | 1:164:G:TYR:CZ | 7 | 1.32 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 3 | 1.31 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 7 | 1.31 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 10 | 1.31 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 3 | 1.31 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 10 | 1.31 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 2 | 1.31 |
| (1,1191) | 1:171:K:THR:CG2 | 1:175:K:GLU:CA | 5 | 1.31 |
| (1,684) | 1:175:L:GLU:CB | 1:171:L:THR:CB | 10 | 1.31 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 6 | 1.3 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 10 | 1.3 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 10 | 1.3 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 2 | 1.3 |
| (1,57) | 1:154:J:ARG:CG | 1:192:J:GLN:CA | 3 | 1.3 |
| (1,2227) | 2:301:H:A1CCY:F33 | 1:220:I:GLY:CA | 9 | 1.29 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 9 | 1.29 |
| (1,471) | 1:163:L:ASP:CB | 1:161:L:PHE:CG | 4 | 1.29 |
| (1,1024) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 3 | 1.28 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 7 | 1.27 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 2 | 1.27 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 9 | 1.27 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 8 | 1.27 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 5 | 1.25 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 7 | 1.25 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 7 | 1.25 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 7 | 1.25 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 4 | 1.25 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 1 | 1.25 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 5 | 1.25 |
| (1,1525) | 1:211:K:LEU:CD1 | 1:213:K:GLU:C | 1 | 1.25 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 6 | 1.24 |
| (1,1339) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 7 | 1.24 |
| (1,684) | 1:175:K:GLU:CB | 1:171:K:THR:CB | 5 | 1.24 |
| (1,2289) | 2:301:H:A1CCY:F31 | 1:196:H:PRO:CA | 5 | 1.23 |
| (1,2276) | 2:301:H:A1CCY:H11 | 1:232:H:ALA:CA | 9 | 1.23 |
| (1,952) | 1:175:L:GLU:CB | 1:148:L:THR:CB | 5 | 1.23 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,859) | 1:157:J:PRO:CG | 1:197:J:ASP:CB | 10 | 1.22 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 2 | 1.22 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 1 | 1.21 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 10 | 1.21 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 8 | 1.21 |
| (1,1531) | 1:148:H:THR:CA | 1:174:H:ALA:C | 10 | 1.21 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 8 | 1.2 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 5 | 1.2 |
| (1,471) | 1:163:K:ASP:CB | 1:161:K:PHE:CG | 10 | 1.2 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE2 | 10 | 1.2 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 4 | 1.18 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 8 | 1.18 |
| (1,1029) | 1:167:L:ARG:CB | 1:169:L:TYR:CD1 | 8 | 1.18 |
| (1,746) | 1:221:H:VAL:CG2 | 1:230:H:VAL:CG2 | 6 | 1.18 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 9 | 1.17 |
| (1,2224) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CD | 6 | 1.17 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 9 | 1.17 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 10 | 1.16 |
| (1,471) | 1:163:I:ASP:CB | 1:161:I:PHE:CG | 9 | 1.16 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 10 | 1.15 |
| (1,1525) | 1:211:L:LEU:CD1 | 1:213:L:GLU:C | 9 | 1.15 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 5 | 1.15 |
| (1,1070) | 1:150:L:ILE:CD1 | 1:167:L:ARG:CA | 9 | 1.15 |
| (1,61) | 1:150:H:ILE:CG2 | 1:182:H:LYS:C | 9 | 1.15 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 5 | 1.14 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 4 | 1.14 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 1 | 1.14 |
| (1,746) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 10 | 1.14 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 1 | 1.14 |
| (1,57) | 1:154:J:ARG:CG | 1:192:J:GLN:CA | 8 | 1.14 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 2 | 1.13 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 2 | 1.13 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 1 | 1.13 |
| (1,1201) | 1:153:K:ILE:CG2 | 1:165:K:VAL:CB | 10 | 1.13 |
| (1,859) | 1:157:K:PRO:CG | 1:197:K:ASP:CB | 1 | 1.13 |
| (2,3) | 2:301:H:A1CCY:H28 | 1:197:H:ASP:N | 6 | 1.12 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 10 | 1.12 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 4 | 1.12 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 3 | 1.12 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 9 | 1.12 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 10 | 1.12 |
| (1,471) | 1:163:G:ASP:CB | 1:161:G:PHE:CG | 2 | 1.12 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 8 | 1.11 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 4 | 1.11 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 10 | 1.11 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 5 | 1.11 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 6 | 1.11 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 4 | 1.11 |
| (1,2236) | 2:301:H:A1CCY:F31 | 1:224:I:PRO:CA | 8 | 1.11 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 3 | 1.11 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 4 | 1.11 |
| (1,859) | 1:157:K:PRO:CG | 1:197:K:ASP:CB | 6 | 1.11 |
| (1,859) | 1:157:J:PRO:CG | 1:197:J:ASP:CB | 8 | 1.11 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 10 | 1.1 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 10 | 1.1 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 10 | 1.1 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 6 | 1.1 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 1 | 1.1 |
| (1,1400) | 1:194:K:ALA:CA | 1:197:K:ASP:CA | 8 | 1.1 |
| (1,962) | 1:244:K:ILE:CA | 1:238:K:VAL:CA | 10 | 1.1 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 5 | 1.09 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 9 | 1.09 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 10 | 1.09 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 1 | 1.09 |
| (1,761) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CG | 8 | 1.09 |
| (1,156) | 1:187:K:GLU:CA | 1:169:K:TYR:CE2 | 6 | 1.09 |
| (1,107) | 1:150:L:ILE:CA | 1:164:L:TYR:CZ | 6 | 1.09 |
| (1,2235) | 2:301:H:A1CCY:F32 | 1:226:I:HIS:CA | 6 | 1.08 |
| (1,1525) | 1:211:L:LEU:CD1 | 1:213:L:GLU:C | 2 | 1.08 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG1 | 5 | 1.08 |
| (1,1106) | 1:174:J:ALA:CB | 1:182:J:LYS:CE | 10 | 1.08 |
| (1,430) | 1:162:K:ARG:CA | 1:218:K:CYS:CA | 9 | 1.08 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE1 | 3 | 1.08 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 10 | 1.07 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 9 | 1.07 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 1 | 1.07 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 7 | 1.07 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 2 | 1.07 |
| (1,471) | 1:163:K:ASP:CB | 1:161:K:PHE:CG | 1 | 1.07 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 5 | 1.06 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 5 | 1.06 |
| (1,1400) | 1:194:L:ALA:CA | 1:197:L:ASP:CA | 3 | 1.06 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 5 | 1.05 |
| (1,1609) | 1:155:G:GLN:CB | 1:197:G:ASP:CB | 2 | 1.05 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,1552) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 9 | 1.05 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 6 | 1.05 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 2 | 1.04 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 9 | 1.04 |
| (1,1339) | 1:151:H:LEU:CG | 1:189:H:LEU:CB | 3 | 1.04 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 5 | 1.03 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 10 | 1.03 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 2 | 1.03 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 5 | 1.03 |
| (1,1400) | 1:194:K:ALA:CA | 1:197:K:ASP:CA | 6 | 1.03 |
| (1,1400) | 1:194:L:ALA:CA | 1:197:L:ASP:CA | 10 | 1.03 |
| (1,1339) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 1 | 1.03 |
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 1 | 1.03 |
| (1,396) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 6 | 1.03 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 10 | 1.02 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 2 | 1.02 |
| (1,1531) | 1:148:K:THR:CA | 1:174:K:ALA:C | 5 | 1.02 |
| (1,1400) | 1:194:I:ALA:CA | 1:197:I:ASP:CA | 5 | 1.02 |
| (1,1400) | 1:194:K:ALA:CA | 1:197:K:ASP:CA | 7 | 1.02 |
| (1,263) | 1:151:H:LEU:CD1 | 1:153:H:ILE:CB | 4 | 1.02 |
| (1,2236) | 2:301:H:A1CCY:F31 | 1:224:I:PRO:CA | 2 | 1.01 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 6 | 1.01 |
| (1,1029) | 1:167:I:ARG:CB | 1:169:I:TYR:CD1 | 6 | 1.01 |
| (1,797) | 1:238:I:VAL:CG2 | 1:243:I:THR:CA | 1 | 1.01 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 4 | 1.01 |
| (1,471) | 1:163:L:ASP:CB | 1:161:L:PHE:CG | 7 | 1.01 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 10 | 1.0 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 7 | 0.99 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 3 | 0.99 |
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 8 | 0.99 |
| (1,183) | 1:151:H:LEU:CG | 1:153:H:ILE:CB | 8 | 0.99 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 4 | 0.98 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 10 | 0.98 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 5 | 0.98 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 1 | 0.98 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 7 | 0.98 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 3 | 0.98 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 8 | 0.98 |
| (1,396) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 1 | 0.98 |
| (1,384) | 1:189:I:LEU:CG | 1:164:I:TYR:CZ | 7 | 0.98 |
| (1,299) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 8 | 0.98 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 1 | 0.97 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 2 | 0.97 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 8 | 0.97 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 7 | 0.97 |
| (1,1400) | 1:194:I:ALA:CA | 1:197:I:ASP:CA | 2 | 0.97 |
| (1,786) | 1:165:L:VAL:CG2 | 1:159:L:GLU:CD | 1 | 0.97 |
| (1,299) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 9 | 0.97 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 1 | 0.96 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 1 | 0.96 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 4 | 0.96 |
| (1,2288) | 2:301:H:A1CCY:F33 | 1:157:H:PRO:CG | 6 | 0.96 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 7 | 0.96 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 7 | 0.96 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 6 | 0.96 |
| (1,1400) | 1:194:L:ALA:CA | 1:197:L:ASP:CA | 4 | 0.96 |
| (1,761) | 1:172:L:LEU:CD1 | 1:189:L:LEU:CG | 2 | 0.96 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 2 | 0.96 |
| (1,430) | 1:162:K:ARG:CA | 1:218:K:CYS:CA | 2 | 0.96 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 7 | 0.95 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 10 | 0.95 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 7 | 0.95 |
| (1,2233) | 2:301:H:A1CCY:F33 | 1:227:I:LYS:CA | 8 | 0.95 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 3 | 0.95 |
| (1,1400) | 1:194:I:ALA:CA | 1:197:I:ASP:CA | 1 | 0.95 |
| (1,1073) | 1:154:K:ARG:CG | 1:151:K:LEU:CA | 7 | 0.95 |
| (1,471) | 1:163:L:ASP:CB | 1:161:L:PHE:CG | 3 | 0.95 |
| (1,378) | 1:177:H:ALA:CB | 1:185:H:MET:CA | 10 | 0.95 |
| (1,107) | 1:150:G:ILE:CA | 1:164:G:TYR:CZ | 2 | 0.95 |
| (1,2247) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CB | 9 | 0.94 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 10 | 0.94 |
| (1,1029) | 1:167:J:ARG:CB | 1:169:J:TYR:CD1 | 2 | 0.94 |
| (1,1029) | 1:167:I:ARG:CB | 1:169:I:TYR:CD1 | 7 | 0.94 |
| (1,57) | 1:154:H:ARG:CG | 1:192:H:GLN:CA | 5 | 0.94 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 7 | 0.93 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 8 | 0.93 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 3 | 0.93 |
| (1,1552) | 1:153:I:ILE:CG1 | 1:172:I:LEU:CA | 10 | 0.93 |
| (1,746) | 1:221:J:VAL:CG1 | 1:230:J:VAL:CG2 | 3 | 0.93 |
| (1,107) | 1:150:L:ILE:CA | 1:164:L:TYR:CZ | 9 | 0.93 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 6 | 0.92 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 2 | 0.92 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 2 | 0.92 |
| (1,662) | 1:150:L:ILE:CG2 | 1:168:L:PHE:C | 7 | 0.92 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,471) | 1:163:I:ASP:CB | 1:161:I:PHE:CG | 8 | 0.92 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 9 | 0.91 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 2 | 0.91 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 9 | 0.91 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 7 | 0.91 |
| (1,1400) | 1:194:I:ALA:CA | 1:197:I:ASP:CA | 9 | 0.91 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 8 | 0.91 |
| (1,156) | 1:187:K:GLU:CA | 1:169:K:TYR:CE2 | 7 | 0.91 |
| (1,2265) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CA | 5 | 0.9 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 4 | 0.9 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 5 | 0.9 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 9 | 0.9 |
| (1,912) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 3 | 0.9 |
| (1,746) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 5 | 0.9 |
| (1,607) | 1:205:H:LEU:CB | 1:208:H:GLY:CA | 9 | 0.9 |
| (1,500) | 1:172:H:LEU:CD1 | 1:153:H:ILE:CG1 | 3 | 0.9 |
| (1,299) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 2 | 0.9 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 8 | 0.89 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 9 | 0.89 |
| (1,1447) | 1:152:I:ASP:CB | 1:149:I:SER:CB | 2 | 0.89 |
| (1,353) | 1:150:K:ILE:CD1 | 1:151:K:LEU:CD1 | 6 | 0.89 |
| (1,263) | 1:151:G:LEU:CD1 | 1:153:G:ILE:CB | 7 | 0.89 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 7 | 0.88 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 10 | 0.88 |
| (1,2266) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CA | 5 | 0.88 |
| (1,1561) | 1:175:J:GLU:CB | 1:185:J:MET:CB | 2 | 0.88 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 4 | 0.88 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 4 | 0.88 |
| (1,1029) | 1:167:L:ARG:CB | 1:169:L:TYR:CD1 | 1 | 0.88 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 2 | 0.88 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 3 | 0.87 |
| (1,2230) | 2:301:H:A1CCY:F33 | 1:223:I:GLY:CA | 9 | 0.87 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 6 | 0.87 |
| (1,1552) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 6 | 0.87 |
| (1,746) | 1:221:H:VAL:CG2 | 1:230:H:VAL:CG2 | 4 | 0.87 |
| (1,471) | 1:163:H:ASP:CB | 1:161:H:PHE:CG | 6 | 0.87 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 10 | 0.86 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 6 | 0.86 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 3 | 0.86 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 7 | 0.86 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 5 | 0.86 |
| (1,1073) | 1:154:L:ARG:CG | 1:151:L:LEU:CA | 9 | 0.86 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 8 | 0.85 |
| (1,1084) | 1:192:G:GLN:CA | 1:164:G:TYR:CZ | 2 | 0.85 |
| (1,43) | 1:165:H:VAL:CG2 | 1:202:H:LEU:CG | 9 | 0.85 |
| (1,1447) | 1:152:H:ASP:CB | 1:149:H:SER:CB | 3 | 0.84 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 7 | 0.84 |
| (1,1070) | 1:150:J:ILE:CD1 | 1:167:J:ARG:CA | 1 | 0.84 |
| (1,1029) | 1:167:K:ARG:CB | 1:169:K:TYR:CD1 | 9 | 0.84 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 1 | 0.84 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 4 | 0.83 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 7 | 0.83 |
| (1,2268) | 2:301:H:A1CCY:F32 | 1:198:H:CYS:CA | 6 | 0.83 |
| (1,2256) | 2:301:H:A1CCY:F31 | 1:159:H:GLU:CA | 6 | 0.83 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 10 | 0.83 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 4 | 0.83 |
| (1,434) | 1:230:G:VAL:CG2 | 1:221:G:VAL:CA | 6 | 0.83 |
| (1,434) | 1:230:L:VAL:CG2 | 1:221:L:VAL:CA | 10 | 0.83 |
| (1,384) | 1:189:G:LEU:CG | 1:164:G:TYR:CZ | 6 | 0.83 |
| (1,350) | 1:190:I:LEU:CG | 1:187:I:GLU:CG | 1 | 0.83 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 4 | 0.82 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 7 | 0.82 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 6 | 0.82 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 7 | 0.82 |
| (1,455) | 1:230:L:VAL:CG2 | 1:233:L:GLU:CD | 5 | 0.82 |
| (1,396) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 3 | 0.82 |
| (1,396) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 5 | 0.82 |
| (1,263) | 1:151:H:LEU:CD1 | 1:153:H:ILE:CB | 9 | 0.82 |
| (1,244) | 1:175:K:GLU:CB | 1:171:K:THR:CA | 5 | 0.82 |
| (1,244) | 1:175:L:GLU:CB | 1:171:L:THR:CA | 10 | 0.82 |
| (1,183) | 1:151:L:LEU:CG | 1:153:L:ILE:CB | 10 | 0.82 |
| (1,57) | 1:154:H:ARG:CG | 1:192:H:GLN:CA | 10 | 0.82 |
| (1,2269) | 2:301:H:A1CCY:F33 | 1:198:H:CYS:CA | 3 | 0.81 |
| (1,2225) | 2:301:H:A1CCY:F31 | 1:220:I:GLY:CA | 4 | 0.81 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 1 | 0.81 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 7 | 0.81 |
| (1,1234) | 1:191:J:VAL:CG1 | 1:198:J:CYS:CA | 9 | 0.81 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 6 | 0.81 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 10 | 0.8 |
| (1,2279) | 2:301:H:A1CCY:H8 | 1:232:H:ALA:CA | 2 | 0.8 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 8 | 0.8 |
| (1,2238) | 2:301:H:A1CCY:F33 | 1:224:I:PRO:CA | 8 | 0.8 |
| (1,1452) | 1:238:H:VAL:CG2 | 1:241:H:THR:CA | 7 | 0.8 |
| (1,1106) | 1:174:L:ALA:CB | 1:182:L:LYS:CE | 8 | 0.8 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,861) | 1:153:L:ILE:CG2 | 1:169:L:TYR:C | 6 | 0.8 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 5 | 0.8 |
| (1,396) | 1:174:H:ALA:CA | 1:148:H:THR:CA | 10 | 0.8 |
| (1,299) | 1:201:L:ILE:CG2 | 1:197:L:ASP:CB | 1 | 0.8 |
| (1,263) | 1:151:H:LEU:CD1 | 1:153:H:ILE:CB | 8 | 0.8 |
| (1,2235) | 2:301:H:A1CCY:F32 | 1:226:I:HIS:CA | 2 | 0.79 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 10 | 0.79 |
| (1,1561) | 1:175:J:GLU:CB | 1:185:J:MET:CB | 8 | 0.79 |
| (1,1110) | 1:244:J:ILE:CG1 | 1:237:K:GLN:CB | 7 | 0.79 |
| (1,1106) | 1:174:L:ALA:CB | 1:182:L:LYS:CE | 2 | 0.79 |
| (1,607) | 1:205:J:LEU:CB | 1:208:J:GLY:CA | 8 | 0.79 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 1 | 0.78 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 6 | 0.78 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 9 | 0.78 |
| (1,1447) | 1:152:I:ASP:CB | 1:149:I:SER:CB | 1 | 0.78 |
| (1,405) | 1:150:I:ILE:CG1 | 1:171:I:THR:CA | 3 | 0.78 |
| (1,61) | 1:150:I:ILE:CG2 | 1:182:I:LYS:C | 3 | 0.78 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 2 | 0.78 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 5 | 0.77 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 9 | 0.77 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 4 | 0.77 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG2 | 7 | 0.77 |
| (1,981) | 1:150:K:ILE:CG2 | 1:190:K:LEU:CA | 3 | 0.77 |
| (1,350) | 1:190:J:LEU:CG | 1:187:J:GLU:CG | 4 | 0.77 |
| (1,299) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CB | 10 | 0.77 |
| (1,2297) | 2:301:H:A1CCY:F33 | 1:222:I:GLY:CA | 3 | 0.76 |
| (1,2239) | 2:301:H:A1CCY:H11 | 1:231:I:LEU:CA | 3 | 0.76 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 4 | 0.76 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 10 | 0.76 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 9 | 0.76 |
| (1,797) | 1:238:I:VAL:CG1 | 1:243:I:THR:CA | 10 | 0.76 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 5 | 0.76 |
| (1,299) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 7 | 0.76 |
| (1,176) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 2 | 0.76 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 9 | 0.76 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 4 | 0.75 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 8 | 0.75 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 8 | 0.75 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 8 | 0.75 |
| (1,2161) | 1:162:L:ARG:CG | 1:152:K:ASP:CB | 6 | 0.75 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 5 | 0.75 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 4 | 0.75 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 9 | 0.75 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 10 | 0.75 |
| (1,384) | 1:189:I:LEU:CG | 1:164:I:TYR:CZ | 9 | 0.75 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 7 | 0.74 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 6 | 0.74 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 8 | 0.74 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 8 | 0.74 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 2 | 0.74 |
| (1,1234) | 1:191:G:VAL:CG1 | 1:198:G:CYS:CA | 7 | 0.74 |
| (1,797) | 1:238:K:VAL:CG2 | 1:243:L:THR:CA | 3 | 0.74 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 2 | 0.74 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 6 | 0.74 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 4 | 0.73 |
| (1,2165) | 1:162:H:ARG:CG | 1:152:G:ASP:CB | 4 | 0.73 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 8 | 0.73 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 6 | 0.73 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 4 | 0.73 |
| (1,981) | 1:150:L:ILE:CG2 | 1:190:L:LEU:CA | 7 | 0.73 |
| (1,859) | 1:157:K:PRO:CG | 1:197:K:ASP:CB | 7 | 0.73 |
| (1,696) | 1:151:H:LEU:CG | 1:189:H:LEU:CG | 6 | 0.73 |
| (1,61) | 1:150:H:ILE:CG2 | 1:182:H:LYS:C | 4 | 0.73 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 3 | 0.72 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 10 | 0.72 |
| (1,2238) | 2:301:H:A1CCY:F33 | 1:224:I:PRO:CA | 2 | 0.72 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 10 | 0.72 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 3 | 0.72 |
| (1,1331) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 6 | 0.72 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 9 | 0.72 |
| (1,1234) | 1:191:L:VAL:CG1 | 1:198:L:CYS:CA | 3 | 0.72 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 4 | 0.72 |
| (1,1030) | 1:148:H:THR:CB | 1:174:H:ALA:C | 10 | 0.72 |
| (1,746) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 1 | 0.72 |
| (1,631) | 1:244:H:ILE:CG1 | 1:238:H:VAL:CA | 3 | 0.72 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 10 | 0.72 |
| (1,299) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 6 | 0.72 |
| (1,107) | 1:150:G:ILE:CA | 1:164:G:TYR:CZ | 8 | 0.72 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 10 | 0.71 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 8 | 0.71 |
| (1,1084) | 1:192:K:GLN:CA | 1:164:K:TYR:CZ | 9 | 0.71 |
| (1,1046) | 1:238:K:VAL:CG2 | 1:244:L:ILE:CB | 3 | 0.71 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 6 | 0.71 |
| (1,350) | 1:190:J:LEU:CG | 1:187:J:GLU:CG | 2 | 0.71 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 5 | 0.7 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 5 | 0.7 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 5 | 0.7 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 9 | 0.7 |
| (1,1609) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 1 | 0.7 |
| (1,1201) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CB | 1 | 0.7 |
| (1,350) | 1:190:J:LEU:CG | 1:187:J:GLU:CG | 9 | 0.7 |
| (1,263) | 1:151:K:LEU:CD1 | 1:153:K:ILE:CB | 6 | 0.7 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 10 | 0.69 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 7 | 0.69 |
| (1,1452) | 1:238:H:VAL:CG2 | 1:241:H:THR:CA | 6 | 0.69 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 10 | 0.69 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 10 | 0.69 |
| (1,263) | 1:151:L:LEU:CD1 | 1:153:L:ILE:CB | 10 | 0.69 |
| (1,155) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 6 | 0.69 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 5 | 0.68 |
| (1,2257) | 2:301:H:A1CCY:F32 | 1:159:H:GLU:CA | 6 | 0.68 |
| (1,2244) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CD | 4 | 0.68 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 1 | 0.68 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 2 | 0.68 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 7 | 0.68 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 2 | 0.68 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 5 | 0.68 |
| (1,662) | 1:150:H:ILE:CG2 | 1:168:H:PHE:C | 4 | 0.68 |
| (1,662) | 1:150:L:ILE:CG2 | 1:168:L:PHE:C | 9 | 0.68 |
| (1,420) | 1:240:K:ASN:CB | 1:237:K:GLN:CA | 8 | 0.68 |
| (1,350) | 1:190:I:LEU:CG | 1:187:I:GLU:CG | 6 | 0.68 |
| (1,2360) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:F32 | 9 | 0.67 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 8 | 0.67 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 7 | 0.67 |
| (1,1533) | 1:214:G:MET:CG | 1:190:G:LEU:CB | 2 | 0.67 |
| (1,1531) | 1:148:K:THR:CA | 1:174:K:ALA:C | 8 | 0.67 |
| (1,1465) | 1:150:I:ILE:CG2 | 1:153:I:ILE:CG1 | 7 | 0.67 |
| (1,1331) | 1:205:J:LEU:CD1 | 1:210:J:THR:CA | 2 | 0.67 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 4 | 0.67 |
| (1,299) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 4 | 0.67 |
| (1,183) | 1:151:K:LEU:CG | 1:153:K:ILE:CB | 2 | 0.67 |
| (1,183) | 1:151:J:LEU:CG | 1:153:J:ILE:CB | 4 | 0.67 |
| (1,155) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 8 | 0.67 |
| (1,43) | 1:165:I:VAL:CG2 | 1:202:I:LEU:CG | 8 | 0.67 |
| (1,2341) | 3:301:I:IHP:P1 | 1:158:L:LYS:HA | 5 | 0.66 |
| (1,2341) | 3:301:I:IHP:P1 | 1:158:L:LYS:HA | 10 | 0.66 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 3 | 0.66 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 5 | 0.66 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 5 | 0.66 |
| (1,1609) | 1:155:K:GLN:CB | 1:197:K:ASP:CB | 7 | 0.66 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG1 | 8 | 0.66 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 5 | 0.66 |
| (1,1234) | 1:191:L:VAL:CG1 | 1:198:L:CYS:CA | 6 | 0.66 |
| (1,1110) | 1:244:L:ILE:CG1 | 1:237:G:GLN:CB | 6 | 0.66 |
| (1,1030) | 1:148:K:THR:CB | 1:174:K:ALA:C | 5 | 0.66 |
| (1,1029) | 1:167:J:ARG:CB | 1:169:J:TYR:CD1 | 3 | 0.66 |
| (1,500) | 1:172:L:LEU:CD1 | 1:153:L:ILE:CG1 | 5 | 0.66 |
| (1,155) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 4 | 0.66 |
| (1,57) | 1:154:K:ARG:CG | 1:192:K:GLN:CA | 4 | 0.66 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 7 | 0.65 |
| (1,2357) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:F32 | 9 | 0.65 |
| (1,2252) | 2:301:H:A1CCY:F32 | 1:223:H:GLY:CA | 4 | 0.65 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 1 | 0.65 |
| (1,1552) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 5 | 0.65 |
| (1,1552) | 1:153:J:ILE:CG1 | 1:172:J:LEU:CA | 7 | 0.65 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 5 | 0.65 |
| (1,1331) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 8 | 0.65 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 6 | 0.65 |
| (1,939) | 1:189:G:LEU:CA | 1:153:G:ILE:C | 5 | 0.65 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 6 | 0.65 |
| (1,405) | 1:150:J:ILE:CG1 | 1:171:J:THR:CA | 1 | 0.65 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 9 | 0.64 |
| (1,2161) | 1:162:L:ARG:CG | 1:152:K:ASP:CB | 8 | 0.64 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 3 | 0.64 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 9 | 0.64 |
| (1,1552) | 1:153:J:ILE:CG1 | 1:172:J:LEU:CA | 2 | 0.64 |
| (1,1552) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 8 | 0.64 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 6 | 0.64 |
| (1,1288) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 2 | 0.64 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 8 | 0.64 |
| (1,183) | 1:151:K:LEU:CG | 1:153:K:ILE:CB | 5 | 0.64 |
| (1,104) | 1:198:L:CYS:CB | 1:199:L:LYS:CE | 1 | 0.64 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 6 | 0.63 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 6 | 0.63 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 9 | 0.63 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 10 | 0.63 |
| (1,1609) | 1:155:K:GLN:CB | 1:197:K:ASP:CB | 5 | 0.63 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 1 | 0.63 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1084) | 1:192:I:GLN:CA | 1:164:I:TYR:CZ | 1 | 0.63 |
| (1,1084) | 1:192:G:GLN:CA | 1:164:G:TYR:CZ | 5 | 0.63 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 7 | 0.63 |
| (1,353) | 1:150:G:ILE:CD1 | 1:151:G:LEU:CD1 | 7 | 0.63 |
| (1,183) | 1:151:K:LEU:CG | 1:153:K:ILE:CB | 3 | 0.63 |
| (1,57) | 1:154:L:ARG:CG | 1:192:L:GLN:CA | 2 | 0.63 |
| (1,40) | 1:219:J:GLN:CG | 1:160:J:PRO:CA | 10 | 0.63 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 8 | 0.62 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 9 | 0.62 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 4 | 0.62 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 7 | 0.62 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 1 | 0.62 |
| (1,1029) | 1:167:I:ARG:CB | 1:169:I:TYR:CD1 | 10 | 0.62 |
| (1,981) | 1:150:I:ILE:CG2 | 1:190:I:LEU:CA | 6 | 0.62 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 4 | 0.62 |
| (1,378) | 1:177:I:ALA:CB | 1:185:I:MET:CA | 2 | 0.62 |
| (1,350) | 1:190:I:LEU:CG | 1:187:I:GLU:CG | 3 | 0.62 |
| (1,299) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CB | 5 | 0.62 |
| (1,155) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 9 | 0.62 |
| (1,155) | 1:155:I:GLN:CB | 1:196:I:PRO:CA | 10 | 0.62 |
| (1,104) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 8 | 0.62 |
| (1,43) | 1:165:L:VAL:CG2 | 1:202:L:LEU:CG | 2 | 0.62 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 3 | 0.61 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 1 | 0.61 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 2 | 0.61 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 4 | 0.61 |
| (1,666) | 1:207:L:PRO:CG | 1:202:L:LEU:CA | 9 | 0.61 |
| (1,444) | 1:185:K:MET:CE | 1:189:K:LEU:CD1 | 10 | 0.61 |
| (1,434) | 1:230:H:VAL:CG2 | 1:221:H:VAL:CA | 4 | 0.61 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 5 | 0.61 |
| (1,350) | 1:190:H:LEU:CG | 1:187:H:GLU:CG | 8 | 0.61 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 1 | 0.6 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 2 | 0.6 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 3 | 0.6 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 5 | 0.6 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 4 | 0.6 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 1 | 0.6 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 3 | 0.6 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 9 | 0.6 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 2 | 0.6 |
| (1,696) | 1:151:G:LEU:CG | 1:189:G:LEU:CG | 2 | 0.6 |
| (1,183) | 1:151:L:LEU:CG | 1:153:L:ILE:CB | 7 | 0.6 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,61) | 1:150:G:ILE:CG2 | 1:182:G:LYS:C | 1 | 0.6 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 3 | 0.59 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 6 | 0.59 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 2 | 0.59 |
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 2 | 0.59 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 1 | 0.59 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 9 | 0.59 |
| (1,607) | 1:205:K:LEU:CB | 1:208:K:GLY:CA | 3 | 0.59 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 8 | 0.59 |
| (1,155) | 1:155:L:GLN:CB | 1:196:L:PRO:CA | 1 | 0.59 |
| (1,155) | 1:155:I:GLN:CB | 1:196:I:PRO:CA | 7 | 0.59 |
| (1,104) | 1:198:I:CYS:CB | 1:199:I:LYS:CE | 4 | 0.59 |
| (1,104) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 6 | 0.59 |
| (1,43) | 1:165:H:VAL:CG2 | 1:202:H:LEU:CG | 6 | 0.59 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 9 | 0.58 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 2 | 0.58 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 9 | 0.58 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 2 | 0.58 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 4 | 0.58 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 1 | 0.58 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 7 | 0.58 |
| (1,2144) | 1:156:L:GLY:CA | 1:160:G:PRO:CD | 9 | 0.58 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 9 | 0.58 |
| (1,861) | 1:153:L:ILE:CG2 | 1:169:L:TYR:C | 5 | 0.58 |
| (1,455) | 1:230:G:VAL:CG1 | 1:233:G:GLU:CD | 1 | 0.58 |
| (1,384) | 1:189:I:LEU:CG | 1:164:I:TYR:CZ | 4 | 0.58 |
| (1,183) | 1:151:I:LEU:CG | 1:153:I:ILE:CB | 9 | 0.58 |
| (1,155) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 2 | 0.58 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 8 | 0.57 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 3 | 0.57 |
| (1,1552) | 1:153:J:ILE:CG1 | 1:172:J:LEU:CA | 4 | 0.57 |
| (1,1533) | 1:214:H:MET:CG | 1:190:H:LEU:CB | 8 | 0.57 |
| (1,1533) | 1:214:G:MET:CG | 1:190:G:LEU:CB | 9 | 0.57 |
| (1,1531) | 1:148:J:THR:CA | 1:174:J:ALA:C | 1 | 0.57 |
| (1,1462) | 1:153:L:ILE:CG2 | 1:165:L:VAL:CG1 | 1 | 0.57 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 2 | 0.57 |
| (1,1234) | 1:191:K:VAL:CG1 | 1:198:K:CYS:CA | 10 | 0.57 |
| (1,1203) | 1:190:K:LEU:CD1 | 1:155:K:GLN:CG | 8 | 0.57 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 3 | 0.57 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 9 | 0.57 |
| (1,353) | 1:150:G:ILE:CD1 | 1:151:G:LEU:CD1 | 1 | 0.57 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 9 | 0.56 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 9 | 0.56 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 6 | 0.56 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 6 | 0.56 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 6 | 0.56 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 9 | 0.56 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 10 | 0.56 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 10 | 0.56 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 8 | 0.56 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 2 | 0.56 |
| (1,1106) | 1:174:L:ALA:CB | 1:182:L:LYS:CE | 4 | 0.56 |
| (1,861) | 1:153:J:ILE:CG2 | 1:169:J:TYR:C | 2 | 0.56 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 1 | 0.56 |
| (1,299) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 3 | 0.56 |
| (1,107) | 1:150:K:ILE:CA | 1:164:K:TYR:CZ | 3 | 0.56 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 3 | 0.55 |
| (1,2377) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:F32 | 2 | 0.55 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 5 | 0.55 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 3 | 0.55 |
| (1,1531) | 1:148:K:THR:CA | 1:174:K:ALA:C | 6 | 0.55 |
| (1,1465) | 1:150:J:ILE:CG2 | 1:153:J:ILE:CG1 | 1 | 0.55 |
| (1,1106) | 1:174:K:ALA:CB | 1:182:K:LYS:CE | 7 | 0.55 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 9 | 0.55 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 9 | 0.55 |
| (1,350) | 1:190:H:LEU:CG | 1:187:H:GLU:CG | 10 | 0.55 |
| (1,155) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 3 | 0.55 |
| (1,104) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 9 | 0.55 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 1 | 0.54 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 1 | 0.54 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 1 | 0.54 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 9 | 0.54 |
| (1,2235) | 2:301:H:A1CCY:F32 | 1:226:I:HIS:CA | 8 | 0.54 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 5 | 0.54 |
| (1,1533) | 1:214:L:MET:CG | 1:190:L:LEU:CB | 6 | 0.54 |
| (1,1288) | 1:201:J:ILE:CG1 | 1:214:J:MET:CA | 1 | 0.54 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 6 | 0.54 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 8 | 0.54 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 6 | 0.54 |
| (1,861) | 1:153:I:ILE:CG2 | 1:169:I:TYR:C | 3 | 0.54 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 10 | 0.54 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 1 | 0.54 |
| (1,183) | 1:151:J:LEU:CG | 1:153:J:ILE:CB | 6 | 0.54 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 9 | 0.53 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 9 | 0.53 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 5 | 0.53 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 10 | 0.53 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 2 | 0.53 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 1 | 0.53 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 8 | 0.53 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 9 | 0.53 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 7 | 0.53 |
| (1,1818) | 1:191:I:VAL:N | 1:199:I:LYS:CE | 8 | 0.53 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 6 | 0.53 |
| (1,1552) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 3 | 0.53 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 3 | 0.53 |
| (1,378) | 1:177:K:ALA:CB | 1:185:K:MET:CA | 7 | 0.53 |
| (1,350) | 1:190:K:LEU:CG | 1:187:K:GLU:CG | 7 | 0.53 |
| (1,155) | 1:155:K:GLN:CB | 1:196:K:PRO:CA | 5 | 0.53 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 2 | 0.52 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 7 | 0.52 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 6 | 0.52 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 6 | 0.52 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 6 | 0.52 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 8 | 0.52 |
| (1,1661) | 1:150:H:ILE:CG1 | 1:175:H:GLU:CB | 8 | 0.52 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 8 | 0.52 |
| (1,1267) | 1:172:G:LEU:CD1 | 1:183:G:ASN:CB | 6 | 0.52 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 8 | 0.52 |
| (1,939) | 1:189:L:LEU:CA | 1:153:L:ILE:C | 8 | 0.52 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 7 | 0.52 |
| (1,891) | 1:221:H:VAL:CG2 | 1:219:H:GLN:CG | 6 | 0.52 |
| (1,746) | 1:221:J:VAL:CG1 | 1:230:J:VAL:CG2 | 7 | 0.52 |
| (1,454) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 2 | 0.52 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 7 | 0.52 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 1 | 0.51 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 1 | 0.51 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 4 | 0.51 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 4 | 0.51 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 5 | 0.51 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 10 | 0.51 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 7 | 0.51 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 10 | 0.51 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 1 | 0.51 |
| (1,1447) | 1:152:H:ASP:CB | 1:149:H:SER:CB | 10 | 0.51 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 2 | 0.51 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------------|-------------------|----------|---------------|
| (1,1073) | 1:154:H:ARG:CG | 1:151:H:LEU:CA | 5 | 0.51 |
| (1,859) | 1:157:H:PRO:CG | 1:197:H:ASP:CB | 2 | 0.51 |
| (1,761) | 1:172:L:LEU:CD1 | 1:189:L:LEU:CG | 1 | 0.51 |
| (1,761) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CG | 10 | 0.51 |
| (1,746) | 1:221:H:VAL:CG1 | 1:230:H:VAL:CG2 | 9 | 0.51 |
| (1,444) | 1:185:G:MET:CE | 1:189:G:LEU:CD1 | 6 | 0.51 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 3 | 0.51 |
| (1,430) | 1:162:K:ARG:CA | 1:218:K:CYS:CA | 7 | 0.51 |
| (1,95) | 1:179:I:GLN:CB | 1:177:I:ALA:CA | 9 | 0.51 |
| (1,40) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 4 | 0.51 |
| (1,2377) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:F32 | 9 | 0.5 |
| (1,2293) | 2:301:H:A1CCY:F32 | 1:222:H:GLY:CA | 3 | 0.5 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 3 | 0.5 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 1 | 0.5 |
| (1,1552) | 1:153:J:ILE:CG1 | 1:172:J:LEU:CA | 1 | 0.5 |
| (1,1203) | 1:190:I:LEU:CD1 | 1:155:I:GLN:CG | 3 | 0.5 |
| (1,1203) | 1:190:K:LEU:CD1 | 1:155:K:GLN:CG | 5 | 0.5 |
| (1,939) | 1:189:G:LEU:CA | 1:153:G:ILE:C | 1 | 0.5 |
| (1,761) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CG | 3 | 0.5 |
| (1,696) | 1:151:G:LEU:CG | 1:189:G:LEU:CG | 9 | 0.5 |
| (1,608) | 1:211:L:LEU:CD2 | 1:190:L:LEU:C | 4 | 0.5 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 3 | 0.5 |
| (1,563) | 1:235:G:MET:CB | 1:233:H:GLU:CG | 10 | 0.5 |
| (1,353) | 1:150:H:ILE:CD1 | 1:151:H:LEU:CD1 | 3 | 0.5 |
| (1,183) | 1:151:K:LEU:CG | 1:153:K:ILE:CB | 1 | 0.5 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 1 | 0.49 |
| (1,2263) | 2:301:H:A1CCY:F32 | 1:227:H:LYS:CA | 5 | 0.49 |
| (1,2242) | 2:301:H:A1CCY:H12A | 1:232:I:ALA:CA | 2 | 0.49 |
| (1,2242) | 2:301:H:A1CCY:H12B | 1:232:I:ALA:CA | 2 | 0.49 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 7 | 0.49 |
| (1,1561) | 1:175:H:GLU:CB | 1:185:H:MET:CB | 7 | 0.49 |
| (1,1339) | 1:151:H:LEU:CG | 1:189:H:LEU:CB | 4 | 0.49 |
| (1,1203) | 1:190:H:LEU:CD1 | 1:155:H:GLN:CG | 9 | 0.49 |
| (1,607) | 1:205:K:LEU:CB | 1:208:K:GLY:CA | 1 | 0.49 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 9 | 0.49 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 1 | 0.49 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 8 | 0.49 |
| (1,444) | 1:185:K:MET:CE | 1:189:K:LEU:CD1 | 9 | 0.49 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 4 | 0.48 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 4 | 0.48 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 4 | 0.48 |
| (1,2293) | 2:301:H:A1CCY:F32 | 1:222:H:GLY:CA | 9 | 0.48 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------------|-----------------|----------|---------------|
| (1,2241) | 2:301:H:A1CCY:H9A | 1:232:I:ALA:CA | 2 | 0.48 |
| (1,2241) | 2:301:H:A1CCY:H9B | 1:232:I:ALA:CA | 2 | 0.48 |
| (1,1447) | 1:152:L:ASP:CB | 1:149:L:SER:CB | 7 | 0.48 |
| (1,1432) | 1:153:H:ILE:CG2 | 1:165:H:VAL:C | 9 | 0.48 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 10 | 0.48 |
| (1,891) | 1:221:J:VAL:CG2 | 1:219:J:GLN:CG | 10 | 0.48 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 2 | 0.48 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 3 | 0.48 |
| (1,396) | 1:174:I:ALA:CA | 1:148:I:THR:CA | 7 | 0.48 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 10 | 0.48 |
| (1,2242) | 2:301:H:A1CCY:H12A | 1:232:I:ALA:CA | 9 | 0.47 |
| (1,2242) | 2:301:H:A1CCY:H12B | 1:232:I:ALA:CA | 9 | 0.47 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 5 | 0.47 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 1 | 0.47 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 4 | 0.47 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 2 | 0.47 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 3 | 0.47 |
| (1,1396) | 1:172:G:LEU:CG | 1:183:G:ASN:CA | 9 | 0.47 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 9 | 0.47 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 8 | 0.47 |
| (1,1073) | 1:154:K:ARG:CG | 1:151:K:LEU:CA | 6 | 0.47 |
| (1,1070) | 1:150:J:ILE:CD1 | 1:167:J:ARG:CA | 7 | 0.47 |
| (1,1029) | 1:167:H:ARG:CB | 1:169:H:TYR:CD1 | 5 | 0.47 |
| (1,962) | 1:244:I:ILE:CA | 1:238:I:VAL:CA | 2 | 0.47 |
| (1,891) | 1:221:G:VAL:CG2 | 1:219:G:GLN:CG | 7 | 0.47 |
| (1,607) | 1:205:I:LEU:CB | 1:208:I:GLY:CA | 5 | 0.47 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 7 | 0.47 |
| (1,378) | 1:177:L:ALA:CB | 1:185:L:MET:CA | 6 | 0.47 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 1 | 0.46 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 8 | 0.46 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 10 | 0.46 |
| (1,1313) | 1:185:L:MET:CE | 1:175:L:GLU:C | 10 | 0.46 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 8 | 0.46 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 10 | 0.46 |
| (1,1073) | 1:154:G:ARG:CG | 1:151:G:LEU:CA | 10 | 0.46 |
| (1,891) | 1:221:L:VAL:CG2 | 1:219:L:GLN:CG | 4 | 0.46 |
| (1,607) | 1:205:J:LEU:CB | 1:208:J:GLY:CA | 4 | 0.46 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 1 | 0.46 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 8 | 0.46 |
| (1,455) | 1:230:J:VAL:CG2 | 1:233:J:GLU:CD | 10 | 0.46 |
| (1,107) | 1:150:G:ILE:CA | 1:164:G:TYR:CZ | 5 | 0.46 |
| (1,95) | 1:179:J:GLN:CB | 1:177:J:ALA:CA | 1 | 0.46 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 9 | 0.45 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 9 | 0.45 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 9 | 0.45 |
| (1,1533) | 1:214:G:MET:CG | 1:190:G:LEU:CB | 3 | 0.45 |
| (1,1267) | 1:172:L:LEU:CD1 | 1:183:L:ASN:CB | 9 | 0.45 |
| (1,1218) | 1:202:H:LEU:CD1 | 1:205:H:LEU:CA | 8 | 0.45 |
| (1,962) | 1:244:K:ILE:CA | 1:238:K:VAL:CA | 3 | 0.45 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 4 | 0.45 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 7 | 0.45 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 4 | 0.45 |
| (1,471) | 1:163:L:ASP:CB | 1:161:L:PHE:CG | 5 | 0.45 |
| (1,454) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 7 | 0.45 |
| (1,454) | 1:201:K:ILE:CG1 | 1:205:K:LEU:CA | 8 | 0.45 |
| (1,350) | 1:190:K:LEU:CG | 1:187:K:GLU:CG | 5 | 0.45 |
| (1,284) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 4 | 0.45 |
| (1,95) | 1:179:L:GLN:CB | 1:177:L:ALA:CA | 2 | 0.45 |
| (1,95) | 1:179:I:GLN:CB | 1:177:I:ALA:CA | 8 | 0.45 |
| (1,61) | 1:150:G:ILE:CG2 | 1:182:G:LYS:C | 8 | 0.45 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 3 | 0.44 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 3 | 0.44 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 3 | 0.44 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 7 | 0.44 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 3 | 0.44 |
| (1,2155) | 1:223:G:GLY:CA | 1:157:L:PRO:CD | 10 | 0.44 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 5 | 0.44 |
| (1,1533) | 1:214:G:MET:CG | 1:190:G:LEU:CB | 10 | 0.44 |
| (1,1498) | 1:190:L:LEU:CG | 1:187:L:GLU:CB | 8 | 0.44 |
| (1,1428) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 5 | 0.44 |
| (1,1428) | 1:214:H:MET:CB | 1:205:H:LEU:CA | 10 | 0.44 |
| (1,1084) | 1:192:K:GLN:CA | 1:164:K:TYR:CZ | 3 | 0.44 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 10 | 0.44 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 2 | 0.44 |
| (1,249) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 3 | 0.44 |
| (1,104) | 1:198:I:CYS:CB | 1:199:I:LYS:CE | 10 | 0.44 |
| (1,43) | 1:165:G:VAL:CG2 | 1:202:G:LEU:CG | 10 | 0.44 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 9 | 0.43 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 9 | 0.43 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 4 | 0.43 |
| (1,2156) | 1:223:L:GLY:CA | 1:157:K:PRO:CD | 4 | 0.43 |
| (1,1533) | 1:214:L:MET:CG | 1:190:L:LEU:CB | 5 | 0.43 |
| (1,1525) | 1:211:I:LEU:CD1 | 1:213:I:GLU:C | 6 | 0.43 |
| (1,1288) | 1:201:J:ILE:CG1 | 1:214:J:MET:CA | 5 | 0.43 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1106) | 1:174:J:ALA:CB | 1:182:J:LYS:CE | 1 | 0.43 |
| (1,631) | 1:244:L:ILE:CG1 | 1:238:L:VAL:CA | 4 | 0.43 |
| (1,475) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 2 | 0.43 |
| (1,405) | 1:150:J:ILE:CG1 | 1:171:J:THR:CA | 7 | 0.43 |
| (1,378) | 1:177:L:ALA:CB | 1:185:L:MET:CA | 1 | 0.43 |
| (1,251) | 1:151:K:LEU:CD1 | 1:150:K:ILE:CG1 | 6 | 0.43 |
| (1,95) | 1:179:K:GLN:CB | 1:177:K:ALA:CA | 7 | 0.43 |
| (1,43) | 1:165:G:VAL:CG2 | 1:202:G:LEU:CG | 5 | 0.43 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 7 | 0.42 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 7 | 0.42 |
| (1,2360) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:F32 | 1 | 0.42 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 8 | 0.42 |
| (1,1818) | 1:191:I:VAL:N | 1:199:I:LYS:CE | 6 | 0.42 |
| (1,1818) | 1:191:H:VAL:N | 1:199:H:LYS:CE | 9 | 0.42 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 1 | 0.42 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 7 | 0.42 |
| (1,1331) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 9 | 0.42 |
| (1,1234) | 1:191:I:VAL:CG1 | 1:198:I:CYS:CA | 8 | 0.42 |
| (1,1070) | 1:150:K:ILE:CD1 | 1:167:K:ARG:CA | 5 | 0.42 |
| (1,1046) | 1:238:H:VAL:CG2 | 1:244:H:ILE:CB | 10 | 0.42 |
| (1,914) | 1:221:L:VAL:CG1 | 1:223:L:GLY:CA | 8 | 0.42 |
| (1,761) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CG | 7 | 0.42 |
| (1,455) | 1:230:K:VAL:CG1 | 1:233:K:GLU:CD | 4 | 0.42 |
| (1,454) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 3 | 0.42 |
| (1,405) | 1:150:J:ILE:CG1 | 1:171:J:THR:CA | 6 | 0.42 |
| (1,169) | 1:161:J:PHE:CD1 | 1:165:J:VAL:C | 9 | 0.42 |
| (1,104) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 2 | 0.42 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 1 | 0.41 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 1 | 0.41 |
| (1,2288) | 2:301:H:A1CCY:F33 | 1:157:H:PRO:CG | 4 | 0.41 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 1 | 0.41 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 2 | 0.41 |
| (1,2153) | 1:219:J:GLN:CG | 1:155:I:GLN:CA | 4 | 0.41 |
| (1,2139) | 1:156:G:GLY:CA | 1:160:H:PRO:CD | 5 | 0.41 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 5 | 0.41 |
| (1,1428) | 1:214:G:MET:CB | 1:205:G:LEU:CA | 3 | 0.41 |
| (1,912) | 1:235:L:MET:CB | 1:230:L:VAL:CA | 8 | 0.41 |
| (1,891) | 1:221:J:VAL:CG2 | 1:219:J:GLN:CG | 3 | 0.41 |
| (1,859) | 1:157:H:PRO:CG | 1:197:H:ASP:CB | 3 | 0.41 |
| (1,666) | 1:207:K:PRO:CG | 1:202:K:LEU:CA | 7 | 0.41 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 5 | 0.41 |
| (1,263) | 1:151:L:LEU:CD1 | 1:153:L:ILE:CB | 1 | 0.41 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,203) | 1:189:H:LEU:CD1 | 1:145:H:GLY:CA | 10 | 0.41 |
| (1,95) | 1:179:J:GLN:CB | 1:177:J:ALA:CA | 3 | 0.41 |
| (1,95) | 1:179:J:GLN:CB | 1:177:J:ALA:CA | 4 | 0.41 |
| (1,95) | 1:179:H:GLN:CB | 1:177:H:ALA:CA | 6 | 0.41 |
| (1,61) | 1:150:H:ILE:CG2 | 1:182:H:LYS:C | 5 | 0.41 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 5 | 0.4 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 5 | 0.4 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 10 | 0.4 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 10 | 0.4 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 5 | 0.4 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 5 | 0.4 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 1 | 0.4 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 8 | 0.4 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 8 | 0.4 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 8 | 0.4 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 6 | 0.4 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 3 | 0.4 |
| (1,1818) | 1:191:J:VAL:N | 1:199:J:LYS:CE | 4 | 0.4 |
| (1,1818) | 1:191:I:VAL:N | 1:199:I:LYS:CE | 7 | 0.4 |
| (1,1428) | 1:214:L:MET:CB | 1:205:L:LEU:CA | 6 | 0.4 |
| (1,1176) | 1:190:K:LEU:CD1 | 1:166:K:ASP:CA | 1 | 0.4 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 7 | 0.4 |
| (1,1029) | 1:167:I:ARG:CB | 1:169:I:TYR:CD1 | 4 | 0.4 |
| (1,986) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CA | 2 | 0.4 |
| (1,891) | 1:221:J:VAL:CG2 | 1:219:J:GLN:CG | 5 | 0.4 |
| (1,833) | 1:235:L:MET:CB | 1:239:L:THR:CA | 3 | 0.4 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 7 | 0.4 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 10 | 0.4 |
| (1,444) | 1:185:H:MET:CE | 1:189:H:LEU:CD1 | 5 | 0.4 |
| (1,444) | 1:185:H:MET:CE | 1:189:H:LEU:CD1 | 7 | 0.4 |
| (1,263) | 1:151:K:LEU:CD1 | 1:153:K:ILE:CB | 5 | 0.4 |
| (1,104) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 3 | 0.4 |
| (1,104) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 5 | 0.4 |
| (1,2291) | 2:301:H:A1CCY:F33 | 1:196:H:PRO:CA | 5 | 0.39 |
| (1,1818) | 1:191:J:VAL:N | 1:199:J:LYS:CE | 10 | 0.39 |
| (1,1498) | 1:190:L:LEU:CG | 1:187:L:GLU:CB | 1 | 0.39 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 1 | 0.39 |
| (1,1138) | 1:189:J:LEU:CB | 1:184:J:TRP:CD2 | 10 | 0.39 |
| (1,986) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CA | 7 | 0.39 |
| (1,981) | 1:150:J:ILE:CG2 | 1:190:J:LEU:CA | 10 | 0.39 |
| (1,811) | 1:185:G:MET:CE | 1:151:G:LEU:CG | 9 | 0.39 |
| (1,631) | 1:244:I:ILE:CG1 | 1:238:I:VAL:CA | 8 | 0.39 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,403) | 1:189:H:LEU:CG | 1:151:H:LEU:CB | 2 | 0.39 |
| (1,284) | 1:150:L:ILE:CD1 | 1:190:L:LEU:CD1 | 2 | 0.39 |
| (1,249) | 1:196:J:PRO:CD | 1:200:J:THR:CB | 4 | 0.39 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 5 | 0.39 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 2 | 0.38 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 2 | 0.38 |
| (1,2377) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:F32 | 6 | 0.38 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ1 | 5 | 0.38 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ2 | 5 | 0.38 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ3 | 5 | 0.38 |
| (1,2222) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CD | 9 | 0.38 |
| (1,2219) | 2:301:H:A1CCY:F31 | 1:224:I:PRO:CG | 8 | 0.38 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 4 | 0.38 |
| (1,1531) | 1:148:J:THR:CA | 1:174:J:ALA:C | 3 | 0.38 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 1 | 0.38 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 9 | 0.38 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 1 | 0.38 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 3 | 0.38 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 6 | 0.38 |
| (1,1046) | 1:238:L:VAL:CG1 | 1:244:L:ILE:CB | 8 | 0.38 |
| (1,914) | 1:221:K:VAL:CG1 | 1:223:K:GLY:CA | 2 | 0.38 |
| (1,882) | 1:153:H:ILE:CG1 | 1:148:H:THR:CB | 7 | 0.38 |
| (1,294) | 1:152:G:ASP:CB | 1:148:G:THR:CB | 7 | 0.38 |
| (1,294) | 1:152:G:ASP:CB | 1:148:G:THR:CB | 9 | 0.38 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 3 | 0.37 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 3 | 0.37 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 3 | 0.37 |
| (1,2201) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 9 | 0.37 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 7 | 0.37 |
| (1,1590) | 1:198:K:CYS:CB | 1:214:K:MET:CA | 6 | 0.37 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 4 | 0.37 |
| (1,1525) | 1:211:I:LEU:CD1 | 1:213:I:GLU:C | 7 | 0.37 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 1 | 0.37 |
| (1,1351) | 1:162:I:ARG:CG | 1:161:I:PHE:CD1 | 9 | 0.37 |
| (1,1288) | 1:201:L:ILE:CG1 | 1:214:L:MET:CA | 7 | 0.37 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 9 | 0.37 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 4 | 0.37 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 10 | 0.37 |
| (1,1028) | 1:190:G:LEU:CD1 | 1:169:G:TYR:CB | 8 | 0.37 |
| (1,939) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 7 | 0.37 |
| (1,721) | 1:191:J:VAL:CG1 | 1:193:J:ASN:CA | 5 | 0.37 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 4 | 0.37 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,454) | 1:201:K:ILE:CG1 | 1:205:K:LEU:CA | 6 | 0.37 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 10 | 0.37 |
| (1,353) | 1:150:K:ILE:CD1 | 1:151:K:LEU:CD1 | 2 | 0.37 |
| (1,251) | 1:151:L:LEU:CD1 | 1:150:L:ILE:CG1 | 9 | 0.37 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 6 | 0.36 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 6 | 0.36 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 2 | 0.36 |
| (1,2279) | 2:301:H:A1CCY:H8 | 1:232:H:ALA:CA | 8 | 0.36 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 3 | 0.36 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 3 | 0.36 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 5 | 0.36 |
| (1,1623) | 1:214:J:MET:CB | 1:198:J:CYS:CA | 4 | 0.36 |
| (1,1428) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 4 | 0.36 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 8 | 0.36 |
| (1,1335) | 1:217:J:ALA:CB | 1:221:J:VAL:CG2 | 2 | 0.36 |
| (1,1297) | 1:180:J:GLU:CG | 1:184:J:TRP:CA | 3 | 0.36 |
| (1,1288) | 1:201:L:ILE:CG1 | 1:214:L:MET:CA | 8 | 0.36 |
| (1,1070) | 1:150:J:ILE:CD1 | 1:167:J:ARG:CA | 6 | 0.36 |
| (1,914) | 1:221:L:VAL:CG1 | 1:223:L:GLY:CA | 6 | 0.36 |
| (1,833) | 1:235:L:MET:CB | 1:239:L:THR:CA | 2 | 0.36 |
| (1,761) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CG | 9 | 0.36 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 1 | 0.36 |
| (1,434) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 8 | 0.36 |
| (1,249) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 10 | 0.36 |
| (1,169) | 1:161:K:PHE:CD1 | 1:165:K:VAL:C | 2 | 0.36 |
| (1,126) | 1:156:J:GLY:CA | 1:196:J:PRO:CD | 6 | 0.36 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 8 | 0.35 |
| (1,1621) | 1:204:G:ALA:CB | 1:206:G:GLY:C | 6 | 0.35 |
| (1,1619) | 1:160:H:PRO:CG | 1:161:H:PHE:CG | 4 | 0.35 |
| (1,1519) | 1:175:L:GLU:CB | 1:148:L:THR:CA | 5 | 0.35 |
| (1,1457) | 1:165:J:VAL:CG2 | 1:214:J:MET:CA | 3 | 0.35 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 6 | 0.35 |
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 3 | 0.35 |
| (1,1267) | 1:172:H:LEU:CD1 | 1:183:H:ASN:CB | 4 | 0.35 |
| (1,1267) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 7 | 0.35 |
| (1,1267) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 8 | 0.35 |
| (1,981) | 1:150:L:ILE:CG2 | 1:190:L:LEU:CA | 9 | 0.35 |
| (1,788) | 1:165:J:VAL:CG1 | 1:211:J:LEU:CA | 2 | 0.35 |
| (1,746) | 1:221:I:VAL:CG1 | 1:230:I:VAL:CG2 | 8 | 0.35 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 9 | 0.35 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 5 | 0.35 |
| (1,156) | 1:187:J:GLU:CA | 1:169:J:TYR:CE1 | 4 | 0.35 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 3 | 0.35 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 5 | 0.34 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 5 | 0.34 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 3 | 0.34 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 10 | 0.34 |
| (1,2144) | 1:156:L:GLY:CA | 1:160:G:PRO:CD | 2 | 0.34 |
| (1,1500) | 1:165:J:VAL:CB | 1:211:J:LEU:CB | 2 | 0.34 |
| (1,1498) | 1:190:J:LEU:CG | 1:187:J:GLU:CB | 4 | 0.34 |
| (1,1396) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 6 | 0.34 |
| (1,1339) | 1:151:I:LEU:CG | 1:189:I:LEU:CB | 8 | 0.34 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 1 | 0.34 |
| (1,1335) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 6 | 0.34 |
| (1,1203) | 1:190:I:LEU:CD1 | 1:155:I:GLN:CG | 10 | 0.34 |
| (1,1176) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 10 | 0.34 |
| (1,912) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 5 | 0.34 |
| (1,882) | 1:153:H:ILE:CG1 | 1:148:H:THR:CB | 2 | 0.34 |
| (1,721) | 1:191:J:VAL:CG1 | 1:193:J:ASN:CA | 10 | 0.34 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 10 | 0.34 |
| (1,590) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 5 | 0.34 |
| (1,561) | 1:172:K:LEU:CG | 1:153:K:ILE:CB | 9 | 0.34 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 8 | 0.34 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 8 | 0.34 |
| (1,353) | 1:150:I:ILE:CD1 | 1:151:I:LEU:CD1 | 8 | 0.34 |
| (1,95) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 5 | 0.34 |
| (1,43) | 1:165:L:VAL:CG2 | 1:202:L:LEU:CG | 1 | 0.34 |
| (1,43) | 1:165:L:VAL:CG2 | 1:202:L:LEU:CG | 4 | 0.34 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 3 | 0.33 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 3 | 0.33 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22A | 9 | 0.33 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22B | 9 | 0.33 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22C | 9 | 0.33 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 9 | 0.33 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ1 | 10 | 0.33 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ2 | 10 | 0.33 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ3 | 10 | 0.33 |
| (1,2267) | 2:301:H:A1CCY:F33 | 1:226:H:HIS:CA | 9 | 0.33 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 3 | 0.33 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 8 | 0.33 |
| (1,2154) | 1:219:H:GLN:CG | 1:155:G:GLN:CA | 2 | 0.33 |
| (1,1621) | 1:204:G:ALA:CB | 1:206:G:GLY:C | 3 | 0.33 |
| (1,1465) | 1:150:K:ILE:CG2 | 1:153:K:ILE:CG1 | 3 | 0.33 |
| (1,897) | 1:153:K:ILE:CD1 | 1:151:K:LEU:C | 7 | 0.33 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,897) | 1:153:L:ILE:CD1 | 1:151:L:LEU:C | 9 | 0.33 |
| (1,891) | 1:221:L:VAL:CG2 | 1:219:L:GLN:CG | 1 | 0.33 |
| (1,891) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 8 | 0.33 |
| (1,882) | 1:153:H:ILE:CG1 | 1:148:H:THR:CB | 6 | 0.33 |
| (1,667) | 1:191:H:VAL:CG1 | 1:194:H:ALA:C | 3 | 0.33 |
| (1,594) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 7 | 0.33 |
| (1,378) | 1:177:K:ALA:CB | 1:185:K:MET:CA | 9 | 0.33 |
| (1,249) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 6 | 0.33 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 2 | 0.32 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 2 | 0.32 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ1 | 8 | 0.32 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ2 | 8 | 0.32 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ3 | 8 | 0.32 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD2 | 3 | 0.32 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD3 | 3 | 0.32 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 9 | 0.32 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 9 | 0.32 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 9 | 0.32 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 3 | 0.32 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 7 | 0.32 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 3 | 0.32 |
| (1,2144) | 1:156:L:GLY:CA | 1:160:G:PRO:CD | 3 | 0.32 |
| (1,2121) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 6 | 0.32 |
| (1,1818) | 1:191:H:VAL:N | 1:199:H:LYS:CE | 3 | 0.32 |
| (1,1621) | 1:204:L:ALA:CB | 1:206:L:GLY:C | 7 | 0.32 |
| (1,1428) | 1:214:L:MET:CB | 1:205:L:LEU:CA | 1 | 0.32 |
| (1,1335) | 1:217:J:ALA:CB | 1:221:J:VAL:CG2 | 8 | 0.32 |
| (1,1176) | 1:190:J:LEU:CD1 | 1:166:J:ASP:CA | 4 | 0.32 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 1 | 0.32 |
| (1,761) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CG | 6 | 0.32 |
| (1,454) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 1 | 0.32 |
| (1,378) | 1:177:I:ALA:CB | 1:185:I:MET:CA | 5 | 0.32 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 10 | 0.31 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 10 | 0.31 |
| (1,2391) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F33 | 7 | 0.31 |
| (1,1623) | 1:214:I:MET:CB | 1:198:I:CYS:CA | 10 | 0.31 |
| (1,1591) | 1:190:I:LEU:CD1 | 1:194:I:ALA:C | 5 | 0.31 |
| (1,1590) | 1:198:J:CYS:CB | 1:214:J:MET:CA | 7 | 0.31 |
| (1,1505) | 1:172:K:LEU:CG | 1:175:K:GLU:CD | 10 | 0.31 |
| (1,1396) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 10 | 0.31 |
| (1,1288) | 1:201:K:ILE:CG1 | 1:214:K:MET:CA | 4 | 0.31 |
| (1,1046) | 1:238:H:VAL:CG1 | 1:244:H:ILE:CB | 4 | 0.31 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1024) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 4 | 0.31 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 10 | 0.31 |
| (1,662) | 1:150:J:ILE:CG2 | 1:168:J:PHE:C | 2 | 0.31 |
| (1,249) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 8 | 0.31 |
| (1,31) | 1:215:J:MET:CG | 1:219:J:GLN:C | 6 | 0.31 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 1 | 0.3 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 5 | 0.3 |
| (1,1621) | 1:204:G:ALA:CB | 1:206:G:GLY:C | 2 | 0.3 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 3 | 0.3 |
| (1,1396) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 8 | 0.3 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 3 | 0.3 |
| (1,1267) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 1 | 0.3 |
| (1,1191) | 1:171:L:THR:CG2 | 1:175:L:GLU:CA | 6 | 0.3 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 6 | 0.3 |
| (1,1084) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 7 | 0.3 |
| (1,1028) | 1:190:L:LEU:CD1 | 1:169:L:TYR:CB | 7 | 0.3 |
| (1,912) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 1 | 0.3 |
| (1,903) | 1:197:I:ASP:CB | 1:218:I:CYS:CA | 2 | 0.3 |
| (1,897) | 1:153:J:ILE:CD1 | 1:151:J:LEU:C | 1 | 0.3 |
| (1,897) | 1:153:I:ILE:CD1 | 1:151:I:LEU:C | 10 | 0.3 |
| (1,787) | 1:218:I:CYS:CB | 1:197:I:ASP:CB | 6 | 0.3 |
| (1,721) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 1 | 0.3 |
| (1,594) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 6 | 0.3 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 1 | 0.3 |
| (1,475) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 3 | 0.3 |
| (1,107) | 1:150:H:ILE:CA | 1:164:H:TYR:CZ | 1 | 0.3 |
| (1,95) | 1:179:J:GLN:CB | 1:177:J:ALA:CA | 10 | 0.3 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 8 | 0.29 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 8 | 0.29 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 7 | 0.29 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 7 | 0.29 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 7 | 0.29 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 6 | 0.29 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 1 | 0.29 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 4 | 0.29 |
| (1,2152) | 1:219:K:GLN:CG | 1:155:J:GLN:CA | 7 | 0.29 |
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 1 | 0.29 |
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 8 | 0.29 |
| (1,1619) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 1 | 0.29 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 9 | 0.29 |
| (1,1590) | 1:198:I:CYS:CB | 1:214:I:MET:CA | 5 | 0.29 |
| (1,1498) | 1:190:I:LEU:CG | 1:187:I:GLU:CB | 3 | 0.29 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1447) | 1:152:I:ASP:CB | 1:149:I:SER:CB | 5 | 0.29 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 6 | 0.29 |
| (1,939) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 10 | 0.29 |
| (1,667) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 2 | 0.29 |
| (1,667) | 1:191:G:VAL:CG1 | 1:194:G:ALA:C | 10 | 0.29 |
| (1,666) | 1:207:H:PRO:CG | 1:202:H:LEU:CA | 6 | 0.29 |
| (1,454) | 1:201:K:ILE:CG1 | 1:205:K:LEU:CA | 4 | 0.29 |
| (1,249) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 9 | 0.29 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 9 | 0.28 |
| (1,2130) | 1:195:J:ASN:CA | 1:219:K:GLN:CA | 2 | 0.28 |
| (1,1818) | 1:191:I:VAL:N | 1:199:I:LYS:CE | 2 | 0.28 |
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 5 | 0.28 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 7 | 0.28 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 8 | 0.28 |
| (1,1533) | 1:214:I:MET:CG | 1:190:I:LEU:CB | 1 | 0.28 |
| (1,1396) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 4 | 0.28 |
| (1,1337) | 1:185:I:MET:CG | 1:182:I:LYS:CE | 5 | 0.28 |
| (1,1337) | 1:185:I:MET:CG | 1:182:I:LYS:CE | 10 | 0.28 |
| (1,1191) | 1:171:H:THR:CG2 | 1:175:H:GLU:CA | 9 | 0.28 |
| (1,981) | 1:150:J:ILE:CG2 | 1:190:J:LEU:CA | 5 | 0.28 |
| (1,882) | 1:153:K:ILE:CG1 | 1:148:K:THR:CB | 9 | 0.28 |
| (1,696) | 1:151:J:LEU:CG | 1:189:J:LEU:CG | 7 | 0.28 |
| (1,608) | 1:211:L:LEU:CD2 | 1:190:L:LEU:C | 6 | 0.28 |
| (1,590) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 10 | 0.28 |
| (1,454) | 1:201:I:ILE:CG1 | 1:205:I:LEU:CA | 5 | 0.28 |
| (1,434) | 1:230:H:VAL:CG2 | 1:221:H:VAL:CA | 2 | 0.28 |
| (1,249) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 2 | 0.28 |
| (1,104) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 7 | 0.28 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 3 | 0.27 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 3 | 0.27 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 1 | 0.27 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 1 | 0.27 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 1 | 0.27 |
| (1,2393) | 3:301:I:IHP:O35 | 2:301:H:A1CCY:F33 | 5 | 0.27 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 7 | 0.27 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 7 | 0.27 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 7 | 0.27 |
| (1,1624) | 1:150:J:ILE:CD1 | 1:175:J:GLU:CB | 5 | 0.27 |
| (1,1619) | 1:160:I:PRO:CG | 1:161:I:PHE:CG | 5 | 0.27 |
| (1,1619) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 10 | 0.27 |
| (1,1455) | 1:202:K:LEU:CG | 1:161:K:PHE:CB | 9 | 0.27 |
| (1,1447) | 1:152:I:ASP:CB | 1:149:I:SER:CB | 8 | 0.27 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1381) | 1:159:L:GLU:CG | 1:165:L:VAL:CA | 4 | 0.27 |
| (1,1291) | 1:219:K:GLN:CB | 1:160:K:PRO:CA | 7 | 0.27 |
| (1,1203) | 1:190:I:LEU:CD1 | 1:155:I:GLN:CG | 7 | 0.27 |
| (1,1028) | 1:190:G:LEU:CD1 | 1:169:G:TYR:CB | 10 | 0.27 |
| (1,396) | 1:174:H:ALA:CA | 1:148:H:THR:CA | 4 | 0.27 |
| (1,176) | 1:244:J:ILE:CG1 | 1:237:K:GLN:CA | 7 | 0.27 |
| (1,103) | 1:190:H:LEU:CG | 1:164:H:TYR:CB | 6 | 0.27 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 7 | 0.26 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 9 | 0.26 |
| (1,1619) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 2 | 0.26 |
| (1,1218) | 1:202:I:LEU:CD1 | 1:205:I:LEU:CA | 2 | 0.26 |
| (1,981) | 1:150:H:ILE:CG2 | 1:190:H:LEU:CA | 4 | 0.26 |
| (1,903) | 1:197:J:ASP:CB | 1:218:J:CYS:CA | 9 | 0.26 |
| (1,891) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 9 | 0.26 |
| (1,433) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 2 | 0.26 |
| (1,433) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 3 | 0.26 |
| (1,249) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 5 | 0.26 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 1 | 0.25 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 1 | 0.25 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 2 | 0.25 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 1 | 0.25 |
| (1,2286) | 2:301:H:A1CCY:F31 | 1:157:H:PRO:CG | 6 | 0.25 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 8 | 0.25 |
| (1,2226) | 2:301:H:A1CCY:F32 | 1:220:I:GLY:CA | 6 | 0.25 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 3 | 0.25 |
| (1,2215) | 1:225:J:GLY:CA | 1:196:I:PRO:CD | 2 | 0.25 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 8 | 0.25 |
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 4 | 0.25 |
| (1,1544) | 1:214:L:MET:CA | 1:210:L:THR:CB | 2 | 0.25 |
| (1,1428) | 1:214:G:MET:CB | 1:205:G:LEU:CA | 9 | 0.25 |
| (1,1396) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 7 | 0.25 |
| (1,1331) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 5 | 0.25 |
| (1,1282) | 1:242:I:ALA:CB | 1:244:I:ILE:CG1 | 3 | 0.25 |
| (1,1262) | 1:190:I:LEU:CD1 | 1:202:I:LEU:CG | 6 | 0.25 |
| (1,986) | 1:201:K:ILE:CG2 | 1:197:K:ASP:CA | 5 | 0.25 |
| (1,981) | 1:150:J:ILE:CG2 | 1:190:J:LEU:CA | 1 | 0.25 |
| (1,897) | 1:153:L:ILE:CD1 | 1:151:L:LEU:C | 4 | 0.25 |
| (1,761) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CG | 4 | 0.25 |
| (1,721) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 2 | 0.25 |
| (1,666) | 1:207:H:PRO:CG | 1:202:H:LEU:CA | 4 | 0.25 |
| (1,297) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 7 | 0.25 |
| (1,249) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 1 | 0.25 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,103) | 1:190:H:LEU:CG | 1:164:H:TYR:CB | 8 | 0.25 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12A | 6 | 0.24 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12B | 6 | 0.24 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 1 | 0.24 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 1 | 0.24 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 5 | 0.24 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 5 | 0.24 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 5 | 0.24 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 5 | 0.24 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 5 | 0.24 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 1 | 0.24 |
| (1,2360) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:F32 | 5 | 0.24 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ1 | 7 | 0.24 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ2 | 7 | 0.24 |
| (1,2333) | 3:301:I:IHP:P3 | 1:158:J:LYS:HZ3 | 7 | 0.24 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 5 | 0.24 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 5 | 0.24 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 5 | 0.24 |
| (1,2274) | 2:301:H:A1CCY:F32 | 1:226:H:HIS:CD2 | 6 | 0.24 |
| (1,2258) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CA | 1 | 0.24 |
| (1,2255) | 2:301:H:A1CCY:F33 | 1:195:H:ASN:CA | 6 | 0.24 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 9 | 0.24 |
| (1,2232) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CA | 1 | 0.24 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 3 | 0.24 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 9 | 0.24 |
| (1,1477) | 1:193:G:ASN:CB | 1:188:G:THR:C | 8 | 0.24 |
| (1,1428) | 1:214:L:MET:CB | 1:205:L:LEU:CA | 7 | 0.24 |
| (1,1307) | 1:211:L:LEU:CB | 1:212:L:GLU:CD | 5 | 0.24 |
| (1,962) | 1:244:L:ILE:CA | 1:238:L:VAL:CA | 4 | 0.24 |
| (1,721) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 6 | 0.24 |
| (1,563) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 3 | 0.24 |
| (1,475) | 1:153:H:ILE:CD1 | 1:193:H:ASN:CG | 9 | 0.24 |
| (1,433) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 4 | 0.24 |
| (1,396) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 2 | 0.24 |
| (1,284) | 1:150:I:ILE:CD1 | 1:190:I:LEU:CD1 | 9 | 0.24 |
| (1,254) | 1:177:L:ALA:CB | 1:172:L:LEU:CG | 10 | 0.24 |
| (1,107) | 1:150:L:ILE:CA | 1:164:L:TYR:CZ | 10 | 0.24 |
| (1,43) | 1:165:L:VAL:CG2 | 1:202:L:LEU:CG | 7 | 0.24 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 3 | 0.23 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 3 | 0.23 |
| (1,2205) | 1:219:I:GLN:CG | 1:195:H:ASN:CA | 1 | 0.23 |
| (1,2158) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 4 | 0.23 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------------|-------------------|----------|---------------|
| (1,2144) | 1:156:L:GLY:CA | 1:160:G:PRO:CD | 4 | 0.23 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 9 | 0.23 |
| (1,1432) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 3 | 0.23 |
| (1,1396) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 2 | 0.23 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 7 | 0.23 |
| (1,1307) | 1:211:L:LEU:CB | 1:212:L:GLU:CD | 1 | 0.23 |
| (1,1297) | 1:180:L:GLU:CG | 1:184:L:TRP:CA | 5 | 0.23 |
| (1,1070) | 1:150:H:ILE:CD1 | 1:167:H:ARG:CA | 8 | 0.23 |
| (1,959) | 1:158:I:LYS:CD | 1:159:I:GLU:CD | 9 | 0.23 |
| (1,897) | 1:153:L:ILE:CD1 | 1:151:L:LEU:C | 6 | 0.23 |
| (1,882) | 1:153:J:ILE:CG1 | 1:148:J:THR:CB | 4 | 0.23 |
| (1,876) | 1:153:J:ILE:CG2 | 1:164:J:TYR:CA | 2 | 0.23 |
| (1,804) | 1:190:H:LEU:CA | 1:165:H:VAL:CA | 2 | 0.23 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 7 | 0.23 |
| (1,475) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 1 | 0.23 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 3 | 0.23 |
| (1,297) | 1:202:J:LEU:CG | 1:194:J:ALA:CA | 4 | 0.23 |
| (1,103) | 1:190:I:LEU:CG | 1:164:I:TYR:CB | 2 | 0.23 |
| (1,62) | 1:156:I:GLY:CA | 1:164:I:TYR:CA | 3 | 0.23 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 8 | 0.22 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 8 | 0.22 |
| (1,2396) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F33 | 7 | 0.22 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 5 | 0.22 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 6 | 0.22 |
| (1,2282) | 2:301:H:A1CCY:H12A | 1:232:H:ALA:CB | 2 | 0.22 |
| (1,2282) | 2:301:H:A1CCY:H12B | 1:232:H:ALA:CB | 2 | 0.22 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 1 | 0.22 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 1 | 0.22 |
| (1,1590) | 1:198:J:CYS:CB | 1:214:J:MET:CA | 4 | 0.22 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 1 | 0.22 |
| (1,1307) | 1:211:H:LEU:CB | 1:212:H:GLU:CD | 3 | 0.22 |
| (1,1307) | 1:211:G:LEU:CB | 1:212:G:GLU:CD | 4 | 0.22 |
| (1,1191) | 1:171:L:THR:CG2 | 1:175:L:GLU:CA | 2 | 0.22 |
| (1,1147) | 1:153:K:ILE:CB | 1:193:K:ASN:CA | 2 | 0.22 |
| (1,878) | 1:184:G:TRP:CD1 | 1:188:G:THR:C | 5 | 0.22 |
| (1,721) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 3 | 0.22 |
| (1,721) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 8 | 0.22 |
| (1,667) | 1:191:H:VAL:CG1 | 1:194:H:ALA:C | 4 | 0.22 |
| (1,475) | 1:153:H:ILE:CD1 | 1:193:H:ASN:CG | 5 | 0.22 |
| (1,475) | 1:153:J:ILE:CD1 | 1:193:J:ASN:CG | 6 | 0.22 |
| (1,405) | 1:150:K:ILE:CG1 | 1:171:K:THR:CA | 5 | 0.22 |
| (1,297) | 1:202:J:LEU:CG | 1:194:J:ALA:CA | 8 | 0.22 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------------|--------------------|----------|---------------|
| (1,249) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 7 | 0.22 |
| (1,31) | 1:215:I:MET:CG | 1:219:I:GLN:C | 8 | 0.22 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 4 | 0.21 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 4 | 0.21 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 3 | 0.21 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 6 | 0.21 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 6 | 0.21 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 6 | 0.21 |
| (1,2301) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CB | 3 | 0.21 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 3 | 0.21 |
| (1,1591) | 1:190:I:LEU:CD1 | 1:194:I:ALA:C | 8 | 0.21 |
| (1,1590) | 1:198:J:CYS:CB | 1:214:J:MET:CA | 3 | 0.21 |
| (1,1590) | 1:198:I:CYS:CB | 1:214:I:MET:CA | 9 | 0.21 |
| (1,1428) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 8 | 0.21 |
| (1,1176) | 1:190:K:LEU:CD1 | 1:166:K:ASP:CA | 5 | 0.21 |
| (1,1073) | 1:154:K:ARG:CG | 1:151:K:LEU:CA | 8 | 0.21 |
| (1,1028) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 6 | 0.21 |
| (1,903) | 1:197:K:ASP:CB | 1:218:K:CYS:CA | 6 | 0.21 |
| (1,811) | 1:185:G:MET:CE | 1:151:G:LEU:CG | 7 | 0.21 |
| (1,771) | 1:230:J:VAL:CG1 | 1:232:J:ALA:C | 1 | 0.21 |
| (1,667) | 1:191:J:VAL:CG1 | 1:194:J:ALA:C | 5 | 0.21 |
| (1,608) | 1:211:J:LEU:CD2 | 1:190:J:LEU:C | 2 | 0.21 |
| (1,62) | 1:156:H:GLY:CA | 1:164:H:TYR:CA | 4 | 0.21 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 9 | 0.2 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 9 | 0.2 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 6 | 0.2 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 6 | 0.2 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 6 | 0.2 |
| (1,2298) | 2:301:H:A1CCY:F31 | 1:221:H:VAL:CA | 1 | 0.2 |
| (1,2282) | 2:301:H:A1CCY:H12A | 1:232:H:ALA:CB | 8 | 0.2 |
| (1,2282) | 2:301:H:A1CCY:H12B | 1:232:H:ALA:CB | 8 | 0.2 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 4 | 0.2 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 7 | 0.2 |
| (1,2173) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 9 | 0.2 |
| (1,2173) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 9 | 0.2 |
| (1,2173) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 10 | 0.2 |
| (1,2173) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 10 | 0.2 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 3 | 0.2 |
| (1,2162) | 1:162:K:ARG:CG | 1:152:J:ASP:CB | 7 | 0.2 |
| (1,1818) | 1:191:K:VAL:N | 1:199:K:LYS:CE | 5 | 0.2 |
| (1,1661) | 1:150:K:ILE:CG1 | 1:182:K:LYS:CB | 10 | 0.2 |
| (1,1621) | 1:204:H:ALA:CB | 1:206:H:GLY:C | 9 | 0.2 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1621) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 10 | 0.2 |
| (1,1619) | 1:160:J:PRO:CG | 1:161:J:PHE:CG | 6 | 0.2 |
| (1,1591) | 1:190:K:LEU:CD1 | 1:194:K:ALA:C | 2 | 0.2 |
| (1,1331) | 1:205:L:LEU:CD1 | 1:210:L:THR:CA | 4 | 0.2 |
| (1,1297) | 1:180:I:GLU:CG | 1:184:I:TRP:CA | 7 | 0.2 |
| (1,1280) | 1:214:H:MET:CG | 1:207:H:PRO:CA | 8 | 0.2 |
| (1,1280) | 1:214:H:MET:CG | 1:207:H:PRO:CA | 10 | 0.2 |
| (1,1267) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 3 | 0.2 |
| (1,1071) | 1:153:J:ILE:CB | 1:167:J:ARG:CZ | 6 | 0.2 |
| (1,1028) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 1 | 0.2 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 4 | 0.2 |
| (1,914) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 5 | 0.2 |
| (1,903) | 1:197:J:ASP:CB | 1:218:J:CYS:CA | 7 | 0.2 |
| (1,897) | 1:153:K:ILE:CD1 | 1:151:K:LEU:C | 2 | 0.2 |
| (1,897) | 1:153:K:ILE:CD1 | 1:151:K:LEU:C | 8 | 0.2 |
| (1,854) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 8 | 0.2 |
| (1,454) | 1:201:K:ILE:CG1 | 1:205:K:LEU:CA | 9 | 0.2 |
| (1,384) | 1:189:H:LEU:CG | 1:164:H:TYR:CZ | 1 | 0.2 |
| (1,378) | 1:177:L:ALA:CB | 1:185:L:MET:CA | 8 | 0.2 |
| (1,297) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 6 | 0.2 |
| (1,284) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 3 | 0.2 |
| (1,263) | 1:151:K:LEU:CD1 | 1:153:K:ILE:CB | 2 | 0.2 |
| (1,107) | 1:150:I:ILE:CA | 1:164:I:TYR:CZ | 4 | 0.2 |
| (1,62) | 1:156:I:GLY:CA | 1:164:I:TYR:CA | 7 | 0.2 |
| (2,16) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H11 | 9 | 0.19 |
| (1,2310) | 3:301:I:IHP:P5 | 1:158:J:LYS:HA | 6 | 0.19 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 5 | 0.19 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 5 | 0.19 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 4 | 0.19 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 10 | 0.19 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 5 | 0.19 |
| (1,2150) | 1:219:G:GLN:CG | 1:155:L:GLN:CA | 1 | 0.19 |
| (1,2128) | 1:195:H:ASN:CA | 1:219:I:GLN:CA | 5 | 0.19 |
| (1,1533) | 1:214:I:MET:CG | 1:190:I:LEU:CB | 7 | 0.19 |
| (1,1498) | 1:190:J:LEU:CG | 1:187:J:GLU:CB | 10 | 0.19 |
| (1,1030) | 1:148:G:THR:CB | 1:174:G:ALA:C | 6 | 0.19 |
| (1,959) | 1:158:H:LYS:CD | 1:159:H:GLU:CD | 6 | 0.19 |
| (1,939) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 4 | 0.19 |
| (1,914) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 10 | 0.19 |
| (1,903) | 1:197:I:ASP:CB | 1:218:I:CYS:CA | 10 | 0.19 |
| (1,897) | 1:153:K:ILE:CD1 | 1:151:K:LEU:C | 3 | 0.19 |
| (1,876) | 1:153:G:ILE:CG2 | 1:164:G:TYR:CA | 6 | 0.19 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 4 | 0.19 |
| (1,578) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 10 | 0.19 |
| (1,297) | 1:202:H:LEU:CG | 1:194:H:ALA:CA | 10 | 0.19 |
| (1,251) | 1:151:G:LEU:CD1 | 1:150:G:ILE:CG1 | 7 | 0.19 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12A | 7 | 0.18 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12B | 7 | 0.18 |
| (2,20) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H12A | 9 | 0.18 |
| (2,20) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H12B | 9 | 0.18 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 2 | 0.18 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 2 | 0.18 |
| (1,2341) | 3:301:I:IHP:P1 | 1:158:L:LYS:HA | 3 | 0.18 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 10 | 0.18 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 3 | 0.18 |
| (1,2161) | 1:162:L:ARG:CG | 1:152:K:ASP:CB | 1 | 0.18 |
| (1,2152) | 1:219:K:GLN:CG | 1:155:J:GLN:CA | 4 | 0.18 |
| (1,1591) | 1:190:J:LEU:CD1 | 1:194:J:ALA:C | 3 | 0.18 |
| (1,1591) | 1:190:J:LEU:CD1 | 1:194:J:ALA:C | 4 | 0.18 |
| (1,1591) | 1:190:J:LEU:CD1 | 1:194:J:ALA:C | 10 | 0.18 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 8 | 0.18 |
| (1,1428) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 2 | 0.18 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 6 | 0.18 |
| (1,1123) | 1:150:H:ILE:CG2 | 1:184:H:TRP:C | 4 | 0.18 |
| (1,939) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 3 | 0.18 |
| (1,882) | 1:153:L:ILE:CG1 | 1:148:L:THR:CB | 8 | 0.18 |
| (1,783) | 1:148:H:THR:CA | 1:171:H:THR:C | 5 | 0.18 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12A | 2 | 0.17 |
| (2,61) | 3:301:I:IHP:O41 | 2:301:H:A1CCY:H12B | 2 | 0.17 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 4 | 0.17 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 4 | 0.17 |
| (1,2395) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F32 | 2 | 0.17 |
| (1,2391) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F33 | 4 | 0.17 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD2 | 9 | 0.17 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD3 | 9 | 0.17 |
| (1,2273) | 2:301:H:A1CCY:F31 | 1:226:H:HIS:CD2 | 9 | 0.17 |
| (1,2254) | 2:301:H:A1CCY:F32 | 1:195:H:ASN:CA | 8 | 0.17 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 7 | 0.17 |
| (1,2231) | 2:301:H:A1CCY:F31 | 1:227:I:LYS:CA | 5 | 0.17 |
| (1,2216) | 1:225:K:GLY:CA | 1:196:J:PRO:CD | 9 | 0.17 |
| (1,2151) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 10 | 0.17 |
| (1,1565) | 1:234:G:ALA:CB | 1:238:G:VAL:CA | 2 | 0.17 |
| (1,1561) | 1:175:K:GLU:CB | 1:185:K:MET:CB | 9 | 0.17 |
| (1,1491) | 1:160:H:PRO:CD | 1:155:H:GLN:CA | 4 | 0.17 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1396) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 1 | 0.17 |
| (1,1337) | 1:185:L:MET:CG | 1:182:L:LYS:CE | 4 | 0.17 |
| (1,1307) | 1:211:I:LEU:CB | 1:212:I:GLU:CD | 10 | 0.17 |
| (1,1028) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 2 | 0.17 |
| (1,996) | 1:166:K:ASP:CA | 1:169:K:TYR:CZ | 6 | 0.17 |
| (1,959) | 1:158:H:LYS:CD | 1:159:H:GLU:CD | 8 | 0.17 |
| (1,876) | 1:153:K:ILE:CG2 | 1:164:K:TYR:CA | 8 | 0.17 |
| (1,827) | 1:160:H:PRO:CB | 1:161:H:PHE:CD2 | 4 | 0.17 |
| (1,561) | 1:172:H:LEU:CG | 1:153:H:ILE:CB | 5 | 0.17 |
| (1,430) | 1:162:J:ARG:CA | 1:218:J:CYS:CA | 6 | 0.17 |
| (1,297) | 1:202:J:LEU:CG | 1:194:J:ALA:CA | 3 | 0.17 |
| (1,297) | 1:202:J:LEU:CG | 1:194:J:ALA:CA | 5 | 0.17 |
| (1,271) | 1:194:L:ALA:CB | 1:154:L:ARG:CG | 8 | 0.17 |
| (1,251) | 1:151:K:LEU:CD1 | 1:150:K:ILE:CG1 | 2 | 0.17 |
| (1,62) | 1:156:I:GLY:CA | 1:164:I:TYR:CA | 1 | 0.17 |
| (1,31) | 1:215:H:MET:CG | 1:219:H:GLN:C | 1 | 0.17 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9A | 8 | 0.16 |
| (2,54) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H9B | 8 | 0.16 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 10 | 0.16 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 10 | 0.16 |
| (1,2396) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F33 | 10 | 0.16 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD2 | 5 | 0.16 |
| (1,2327) | 3:301:I:IHP:P3 | 1:157:H:PRO:HD3 | 5 | 0.16 |
| (1,2258) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CA | 5 | 0.16 |
| (1,2258) | 2:301:H:A1CCY:F33 | 1:159:H:GLU:CA | 8 | 0.16 |
| (1,2164) | 1:162:I:ARG:CG | 1:152:H:ASP:CB | 9 | 0.16 |
| (1,2160) | 1:223:H:GLY:CA | 1:157:G:PRO:CD | 8 | 0.16 |
| (1,2142) | 1:156:J:GLY:CA | 1:160:K:PRO:CD | 1 | 0.16 |
| (1,2128) | 1:195:H:ASN:CA | 1:219:I:GLN:CA | 2 | 0.16 |
| (1,2128) | 1:195:H:ASN:CA | 1:219:I:GLN:CA | 6 | 0.16 |
| (1,1661) | 1:150:J:ILE:CG1 | 1:182:J:LYS:CB | 5 | 0.16 |
| (1,1457) | 1:165:I:VAL:CG2 | 1:214:I:MET:CA | 10 | 0.16 |
| (1,1432) | 1:153:K:ILE:CG2 | 1:165:K:VAL:C | 2 | 0.16 |
| (1,1339) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 5 | 0.16 |
| (1,1262) | 1:190:I:LEU:CD1 | 1:202:I:LEU:CG | 9 | 0.16 |
| (1,1246) | 1:218:I:CYS:CB | 1:226:I:HIS:CD2 | 7 | 0.16 |
| (1,1147) | 1:153:L:ILE:CB | 1:193:L:ASN:CA | 3 | 0.16 |
| (1,1073) | 1:154:J:ARG:CG | 1:151:J:LEU:CA | 1 | 0.16 |
| (1,854) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 2 | 0.16 |
| (1,854) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 6 | 0.16 |
| (1,843) | 1:215:H:MET:CG | 1:219:H:GLN:CA | 9 | 0.16 |
| (1,833) | 1:235:H:MET:CB | 1:239:H:THR:CA | 7 | 0.16 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,656) | 1:167:I:ARG:CB | 1:159:I:GLU:CG | 9 | 0.16 |
| (1,608) | 1:211:I:LEU:CD2 | 1:190:I:LEU:C | 9 | 0.16 |
| (1,500) | 1:172:I:LEU:CD1 | 1:153:I:ILE:CG1 | 6 | 0.16 |
| (1,144) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 7 | 0.16 |
| (1,62) | 1:156:K:GLY:CA | 1:164:K:TYR:CA | 6 | 0.16 |
| (1,23) | 1:153:K:ILE:CG2 | 1:167:K:ARG:CG | 5 | 0.16 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ1 | 2 | 0.15 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ2 | 2 | 0.15 |
| (1,2334) | 3:301:I:IHP:P3 | 1:158:K:LYS:HZ3 | 2 | 0.15 |
| (1,2299) | 2:301:H:A1CCY:F32 | 1:221:H:VAL:CA | 4 | 0.15 |
| (1,2279) | 2:301:H:A1CCY:H8 | 1:232:H:ALA:CA | 3 | 0.15 |
| (1,2230) | 2:301:H:A1CCY:F33 | 1:223:I:GLY:CA | 1 | 0.15 |
| (1,2173) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 1 | 0.15 |
| (1,2173) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 1 | 0.15 |
| (1,2173) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 4 | 0.15 |
| (1,2173) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 4 | 0.15 |
| (1,2163) | 1:162:J:ARG:CG | 1:152:I:ASP:CB | 6 | 0.15 |
| (1,1591) | 1:190:J:LEU:CD1 | 1:194:J:ALA:C | 1 | 0.15 |
| (1,1590) | 1:198:I:CYS:CB | 1:214:I:MET:CA | 2 | 0.15 |
| (1,1498) | 1:190:J:LEU:CG | 1:187:J:GLU:CB | 2 | 0.15 |
| (1,1498) | 1:190:K:LEU:CG | 1:187:K:GLU:CB | 9 | 0.15 |
| (1,1432) | 1:153:L:ILE:CG2 | 1:165:L:VAL:C | 4 | 0.15 |
| (1,1396) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 3 | 0.15 |
| (1,1351) | 1:162:I:ARG:CG | 1:161:I:PHE:CD1 | 2 | 0.15 |
| (1,1337) | 1:185:H:MET:CG | 1:182:H:LYS:CE | 2 | 0.15 |
| (1,1191) | 1:171:H:THR:CG2 | 1:175:H:GLU:CA | 7 | 0.15 |
| (1,1070) | 1:150:K:ILE:CD1 | 1:167:K:ARG:CA | 2 | 0.15 |
| (1,903) | 1:197:I:ASP:CB | 1:218:I:CYS:CA | 5 | 0.15 |
| (1,903) | 1:197:I:ASP:CB | 1:218:I:CYS:CA | 8 | 0.15 |
| (1,667) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 6 | 0.15 |
| (1,608) | 1:211:J:LEU:CD2 | 1:190:J:LEU:C | 10 | 0.15 |
| (1,454) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 10 | 0.15 |
| (1,433) | 1:187:L:GLU:CB | 1:184:L:TRP:CZ3 | 9 | 0.15 |
| (1,297) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 2 | 0.15 |
| (1,108) | 1:189:I:LEU:CG | 1:153:I:ILE:CA | 5 | 0.15 |
| (1,88) | 1:238:L:VAL:CG1 | 1:235:G:MET:CB | 1 | 0.15 |
| (1,62) | 1:156:G:GLY:CA | 1:164:G:TYR:CA | 5 | 0.15 |
| (1,31) | 1:215:K:MET:CG | 1:219:K:GLN:C | 4 | 0.15 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 3 | 0.14 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 3 | 0.14 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 7 | 0.14 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 7 | 0.14 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12A | 10 | 0.14 |
| (2,59) | 3:301:I:IHP:O31 | 2:301:H:A1CCY:H12B | 10 | 0.14 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12A | 7 | 0.14 |
| (2,18) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:H12B | 7 | 0.14 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22A | 1 | 0.14 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22B | 1 | 0.14 |
| (2,9) | 3:301:I:IHP:O43 | 2:301:H:A1CCY:H22C | 1 | 0.14 |
| (1,2337) | 3:301:I:IHP:P3 | 1:227:I:LYS:HZ1 | 9 | 0.14 |
| (1,2337) | 3:301:I:IHP:P3 | 1:227:I:LYS:HZ2 | 9 | 0.14 |
| (1,2337) | 3:301:I:IHP:P3 | 1:227:I:LYS:HZ3 | 9 | 0.14 |
| (1,2280) | 2:301:H:A1CCY:H9A | 1:232:H:ALA:CA | 4 | 0.14 |
| (1,2280) | 2:301:H:A1CCY:H9B | 1:232:H:ALA:CA | 4 | 0.14 |
| (1,2251) | 2:301:H:A1CCY:F31 | 1:223:H:GLY:CA | 2 | 0.14 |
| (1,2139) | 1:156:G:GLY:CA | 1:160:H:PRO:CD | 10 | 0.14 |
| (1,1590) | 1:198:I:CYS:CB | 1:214:I:MET:CA | 8 | 0.14 |
| (1,1331) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 7 | 0.14 |
| (1,959) | 1:158:H:LYS:CD | 1:159:H:GLU:CD | 7 | 0.14 |
| (1,914) | 1:221:H:VAL:CG1 | 1:223:H:GLY:CA | 4 | 0.14 |
| (1,608) | 1:211:L:LEU:CD2 | 1:190:L:LEU:C | 8 | 0.14 |
| (1,309) | 1:190:I:LEU:CG | 1:193:I:ASN:C | 7 | 0.14 |
| (1,275) | 1:187:I:GLU:CB | 1:183:I:ASN:CB | 6 | 0.14 |
| (1,275) | 1:187:K:GLU:CB | 1:183:K:ASN:CB | 7 | 0.14 |
| (1,61) | 1:150:J:ILE:CG2 | 1:182:J:LYS:C | 10 | 0.14 |
| (1,23) | 1:153:J:ILE:CG2 | 1:167:J:ARG:CG | 4 | 0.14 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9A | 4 | 0.13 |
| (2,11) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H9B | 4 | 0.13 |
| (1,2320) | 3:301:I:IHP:P6 | 1:227:J:LYS:HZ1 | 6 | 0.13 |
| (1,2320) | 3:301:I:IHP:P6 | 1:227:J:LYS:HZ2 | 6 | 0.13 |
| (1,2320) | 3:301:I:IHP:P6 | 1:227:J:LYS:HZ3 | 6 | 0.13 |
| (1,2293) | 2:301:H:A1CCY:F32 | 1:222:H:GLY:CA | 2 | 0.13 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 10 | 0.13 |
| (1,2230) | 2:301:H:A1CCY:F33 | 1:223:I:GLY:CA | 7 | 0.13 |
| (1,2223) | 2:301:H:A1CCY:F32 | 1:227:I:LYS:CD | 6 | 0.13 |
| (1,2215) | 1:225:J:GLY:CA | 1:196:I:PRO:CD | 10 | 0.13 |
| (1,2070) | 1:240:K:ASN:N | 1:237:K:GLN:CB | 8 | 0.13 |
| (1,1525) | 1:211:J:LEU:CD1 | 1:213:J:GLU:C | 8 | 0.13 |
| (1,1487) | 1:153:J:ILE:CG1 | 1:193:J:ASN:CB | 6 | 0.13 |
| (1,1395) | 1:211:K:LEU:CD2 | 1:209:K:ALA:CA | 8 | 0.13 |
| (1,1331) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 3 | 0.13 |
| (1,1307) | 1:211:H:LEU:CB | 1:212:H:GLU:CD | 7 | 0.13 |
| (1,1291) | 1:219:H:GLN:CB | 1:160:H:PRO:CA | 6 | 0.13 |
| (1,1246) | 1:218:I:CYS:CB | 1:226:I:HIS:CD2 | 2 | 0.13 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1218) | 1:202:J:LEU:CD1 | 1:205:J:LEU:CA | 7 | 0.13 |
| (1,1063) | 1:190:H:LEU:CD1 | 1:161:H:PHE:CA | 1 | 0.13 |
| (1,1063) | 1:190:H:LEU:CD1 | 1:161:H:PHE:CA | 3 | 0.13 |
| (1,929) | 1:201:I:ILE:CA | 1:226:I:HIS:CE1 | 4 | 0.13 |
| (1,811) | 1:185:G:MET:CE | 1:151:G:LEU:CG | 6 | 0.13 |
| (1,804) | 1:190:H:LEU:CA | 1:165:H:VAL:CA | 4 | 0.13 |
| (1,703) | 1:205:I:LEU:CG | 1:218:I:CYS:CA | 6 | 0.13 |
| (1,667) | 1:191:J:VAL:CG1 | 1:194:J:ALA:C | 7 | 0.13 |
| (1,666) | 1:207:H:PRO:CG | 1:202:H:LEU:CA | 3 | 0.13 |
| (1,294) | 1:152:L:ASP:CB | 1:148:L:THR:CB | 6 | 0.13 |
| (1,61) | 1:150:L:ILE:CG2 | 1:182:L:LYS:C | 7 | 0.13 |
| (1,23) | 1:153:J:ILE:CG2 | 1:167:J:ARG:CG | 8 | 0.13 |
| (1,23) | 1:153:J:ILE:CG2 | 1:167:J:ARG:CG | 10 | 0.13 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22A | 10 | 0.12 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22B | 10 | 0.12 |
| (2,5) | 3:301:I:IHP:O23 | 2:301:H:A1CCY:H22C | 10 | 0.12 |
| (2,1) | 2:301:H:A1CCY:H27 | 1:197:H:ASP:N | 10 | 0.12 |
| (1,2396) | 3:301:I:IHP:O45 | 2:301:H:A1CCY:F33 | 3 | 0.12 |
| (1,2391) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F33 | 10 | 0.12 |
| (1,2390) | 3:301:I:IHP:O25 | 2:301:H:A1CCY:F32 | 2 | 0.12 |
| (1,2360) | 3:301:I:IHP:O33 | 2:301:H:A1CCY:F32 | 3 | 0.12 |
| (1,2259) | 2:301:H:A1CCY:F31 | 1:197:H:ASP:CA | 4 | 0.12 |
| (1,2254) | 2:301:H:A1CCY:F32 | 1:195:H:ASN:CA | 2 | 0.12 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 5 | 0.12 |
| (1,2229) | 2:301:H:A1CCY:F32 | 1:223:I:GLY:CA | 9 | 0.12 |
| (1,2206) | 1:219:H:GLN:CG | 1:195:G:ASN:CA | 2 | 0.12 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 10 | 0.12 |
| (1,1591) | 1:190:K:LEU:CD1 | 1:194:K:ALA:C | 6 | 0.12 |
| (1,1561) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 3 | 0.12 |
| (1,1544) | 1:214:I:MET:CA | 1:210:I:THR:CB | 5 | 0.12 |
| (1,1531) | 1:148:I:THR:CA | 1:174:I:ALA:C | 7 | 0.12 |
| (1,1498) | 1:190:K:LEU:CG | 1:187:K:GLU:CB | 7 | 0.12 |
| (1,1267) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 10 | 0.12 |
| (1,1063) | 1:190:H:LEU:CD1 | 1:161:H:PHE:CA | 2 | 0.12 |
| (1,1028) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 9 | 0.12 |
| (1,939) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 2 | 0.12 |
| (1,827) | 1:160:I:PRO:CB | 1:161:I:PHE:CD2 | 9 | 0.12 |
| (1,561) | 1:172:H:LEU:CG | 1:153:H:ILE:CB | 3 | 0.12 |
| (1,455) | 1:230:L:VAL:CG1 | 1:233:L:GLU:CD | 6 | 0.12 |
| (1,453) | 1:201:H:ILE:CD1 | 1:161:H:PHE:CD1 | 4 | 0.12 |
| (1,414) | 1:171:G:THR:CA | 1:168:G:PHE:CG | 2 | 0.12 |
| (1,403) | 1:189:G:LEU:CG | 1:151:G:LEU:CB | 9 | 0.12 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|--------------------|-----------------|----------|---------------|
| (1,158) | 1:153:K:ILE:CG1 | 1:148:K:THR:CA | 9 | 0.12 |
| (1,114) | 1:198:I:CYS:CB | 1:214:I:MET:CB | 8 | 0.12 |
| (1,103) | 1:190:H:LEU:CG | 1:164:H:TYR:CB | 9 | 0.12 |
| (1,62) | 1:156:G:GLY:CA | 1:164:G:TYR:CA | 10 | 0.12 |
| (1,40) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 1 | 0.12 |
| (1,23) | 1:153:K:ILE:CG2 | 1:167:K:ARG:CG | 6 | 0.12 |
| (1,2293) | 2:301:H:A1CCY:F32 | 1:222:H:GLY:CA | 10 | 0.11 |
| (1,2282) | 2:301:H:A1CCY:H12A | 1:232:H:ALA:CB | 6 | 0.11 |
| (1,2282) | 2:301:H:A1CCY:H12B | 1:232:H:ALA:CB | 6 | 0.11 |
| (1,2234) | 2:301:H:A1CCY:F31 | 1:226:I:HIS:CA | 3 | 0.11 |
| (1,2153) | 1:219:J:GLN:CG | 1:155:I:GLN:CA | 8 | 0.11 |
| (1,2132) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 5 | 0.11 |
| (1,1791) | 1:194:L:ALA:N | 1:153:L:ILE:CG2 | 3 | 0.11 |
| (1,1432) | 1:153:K:ILE:CG2 | 1:165:K:VAL:C | 5 | 0.11 |
| (1,1395) | 1:211:I:LEU:CD2 | 1:209:I:ALA:CA | 6 | 0.11 |
| (1,1073) | 1:154:I:ARG:CG | 1:151:I:LEU:CA | 2 | 0.11 |
| (1,1063) | 1:190:H:LEU:CD1 | 1:161:H:PHE:CA | 10 | 0.11 |
| (1,986) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CA | 3 | 0.11 |
| (1,959) | 1:158:H:LYS:CD | 1:159:H:GLU:CD | 4 | 0.11 |
| (1,914) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 7 | 0.11 |
| (1,892) | 1:197:L:ASP:CB | 1:222:L:GLY:C | 3 | 0.11 |
| (1,804) | 1:190:I:LEU:CA | 1:165:I:VAL:CA | 8 | 0.11 |
| (1,797) | 1:238:K:VAL:CG2 | 1:243:K:THR:CA | 2 | 0.11 |
| (1,787) | 1:218:I:CYS:CB | 1:197:I:ASP:CB | 2 | 0.11 |
| (1,667) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 1 | 0.11 |
| (1,641) | 1:217:K:ALA:CB | 1:213:K:GLU:CG | 7 | 0.11 |
| (1,534) | 1:211:L:LEU:CD2 | 1:190:L:LEU:CA | 4 | 0.11 |
| (1,414) | 1:171:G:THR:CA | 1:168:G:PHE:CG | 9 | 0.11 |
| (1,378) | 1:177:L:ALA:CB | 1:185:L:MET:CA | 3 | 0.11 |
| (1,313) | 1:190:J:LEU:CD1 | 1:169:J:TYR:CD2 | 5 | 0.11 |
| (1,271) | 1:194:G:ALA:CB | 1:154:G:ARG:CG | 7 | 0.11 |
| (1,251) | 1:151:G:LEU:CD1 | 1:150:G:ILE:CG1 | 1 | 0.11 |
| (1,151) | 1:156:G:GLY:CA | 1:160:G:PRO:C | 10 | 0.11 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ1 | 1 | 0.1 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ2 | 1 | 0.1 |
| (1,2319) | 3:301:I:IHP:P6 | 1:227:I:LYS:HZ3 | 1 | 0.1 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ1 | 2 | 0.1 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ2 | 2 | 0.1 |
| (1,2316) | 3:301:I:IHP:P6 | 1:158:L:LYS:HZ3 | 2 | 0.1 |
| (1,2242) | 2:301:H:A1CCY:H12A | 1:232:I:ALA:CA | 10 | 0.1 |
| (1,2242) | 2:301:H:A1CCY:H12B | 1:232:I:ALA:CA | 10 | 0.1 |
| (1,2157) | 1:223:K:GLY:CA | 1:157:J:PRO:CD | 1 | 0.1 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1661) | 1:150:H:ILE:CG1 | 1:175:H:GLU:CB | 6 | 0.1 |
| (1,1565) | 1:234:J:ALA:CB | 1:238:J:VAL:CA | 3 | 0.1 |
| (1,1246) | 1:218:H:CYS:CB | 1:226:H:HIS:CD2 | 10 | 0.1 |
| (1,878) | 1:184:G:TRP:CD1 | 1:188:G:THR:C | 3 | 0.1 |
| (1,703) | 1:205:K:LEU:CG | 1:218:K:CYS:CA | 1 | 0.1 |
| (1,667) | 1:191:L:VAL:CG1 | 1:194:L:ALA:C | 9 | 0.1 |
| (1,656) | 1:167:K:ARG:CB | 1:159:K:GLU:CG | 2 | 0.1 |
| (1,475) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 10 | 0.1 |
| (1,405) | 1:150:I:ILE:CG1 | 1:171:I:THR:CA | 10 | 0.1 |
| (1,284) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 6 | 0.1 |
| (1,103) | 1:190:I:LEU:CG | 1:164:I:TYR:CB | 1 | 0.1 |

10 Dihedral-angle violation analysis [i](#)

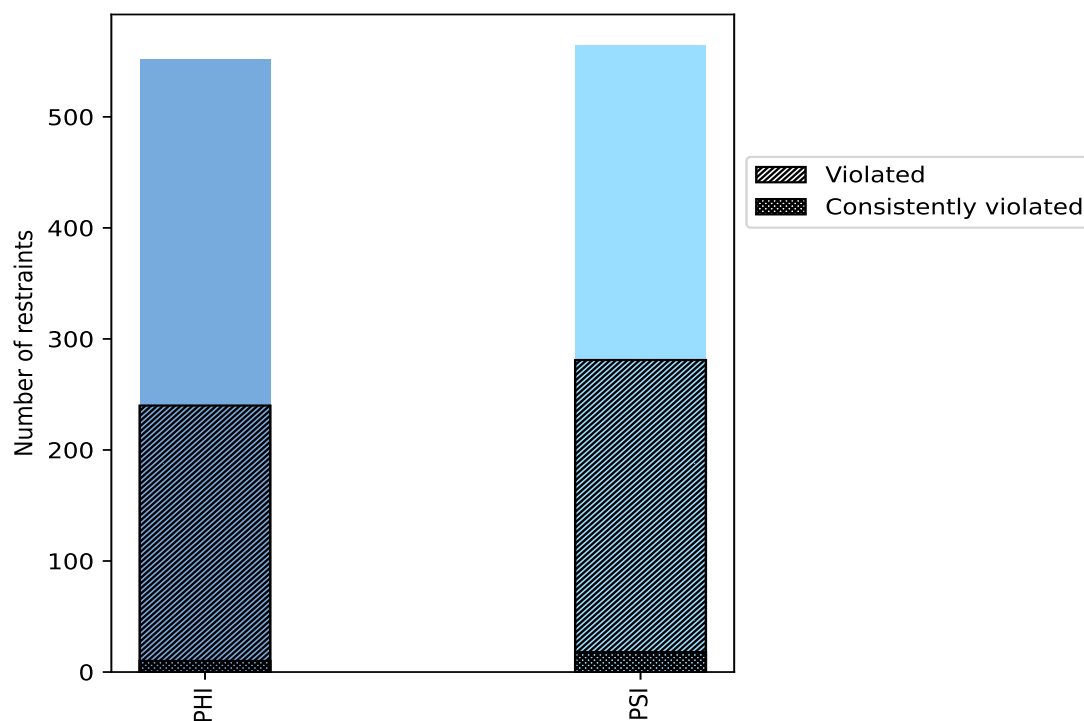
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 552 | 49.5 | 240 | 43.5 | 21.5 | 10 | 1.8 | 0.9 |
| PSI | 564 | 50.5 | 281 | 49.8 | 25.2 | 18 | 3.2 | 1.6 |
| Total | 1116 | 100.0 | 521 | 46.7 | 46.7 | 28 | 2.5 | 2.5 |

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



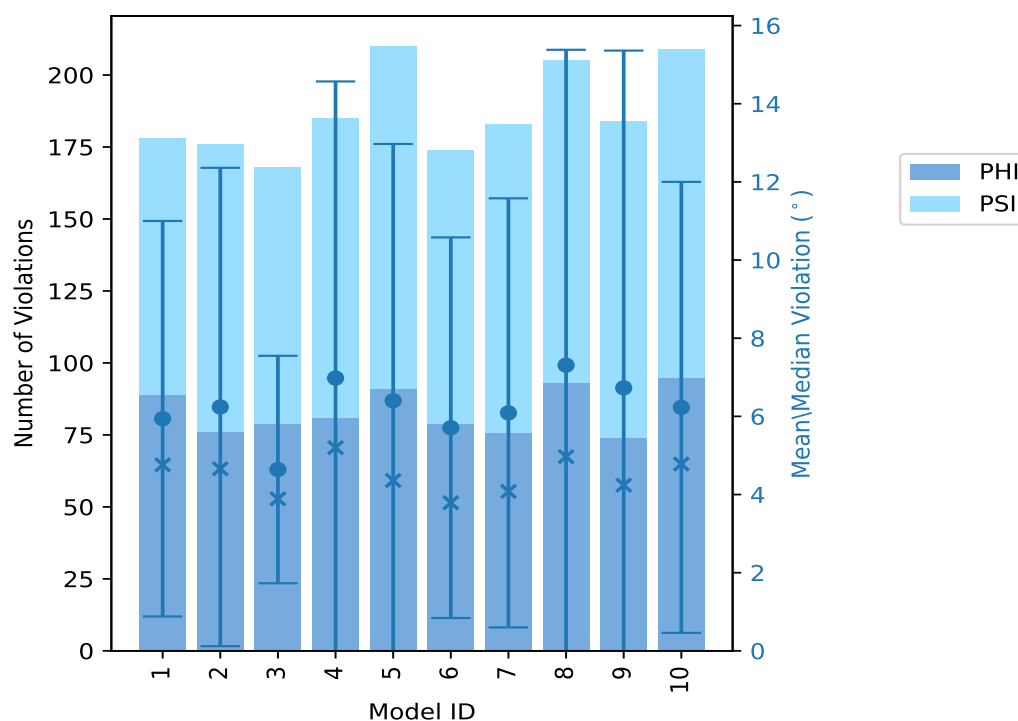
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 89 | 89 | 178 | 5.94 | 36.98 | 5.06 | 4.76 |
| 2 | 76 | 100 | 176 | 6.24 | 39.18 | 6.12 | 4.66 |
| 3 | 79 | 89 | 168 | 4.64 | 14.33 | 2.91 | 3.89 |
| 4 | 81 | 104 | 185 | 6.98 | 55.38 | 7.59 | 5.2 |
| 5 | 91 | 119 | 210 | 6.4 | 38.99 | 6.57 | 4.36 |
| 6 | 79 | 95 | 174 | 5.71 | 21.45 | 4.87 | 3.79 |
| 7 | 76 | 107 | 183 | 6.09 | 35.1 | 5.49 | 4.08 |
| 8 | 93 | 112 | 205 | 7.31 | 54.52 | 8.07 | 4.97 |
| 9 | 74 | 110 | 184 | 6.73 | 72.7 | 8.63 | 4.24 |
| 10 | 95 | 114 | 209 | 6.23 | 51.39 | 5.77 | 4.78 |

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

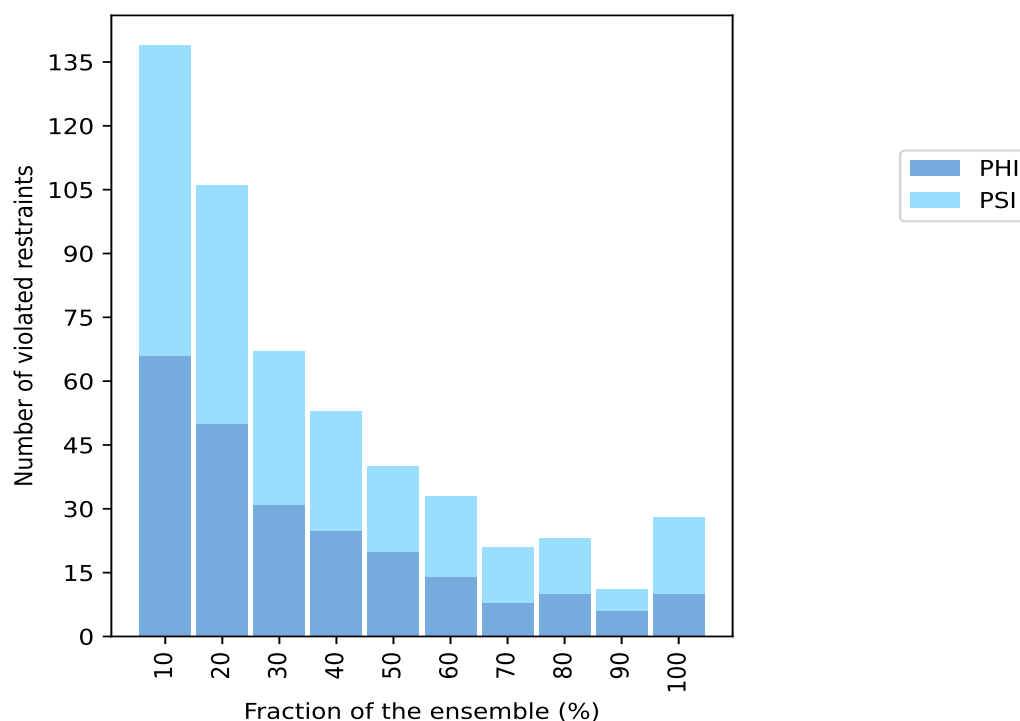
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 66 | 73 | 139 | 1 | 10.0 |
| 50 | 56 | 106 | 2 | 20.0 |
| 31 | 36 | 67 | 3 | 30.0 |
| 25 | 28 | 53 | 4 | 40.0 |
| 20 | 20 | 40 | 5 | 50.0 |
| 14 | 19 | 33 | 6 | 60.0 |
| 8 | 13 | 21 | 7 | 70.0 |
| 10 | 13 | 23 | 8 | 80.0 |
| 6 | 5 | 11 | 9 | 90.0 |
| 10 | 18 | 28 | 10 | 100.0 |

¹ Number of models with violations

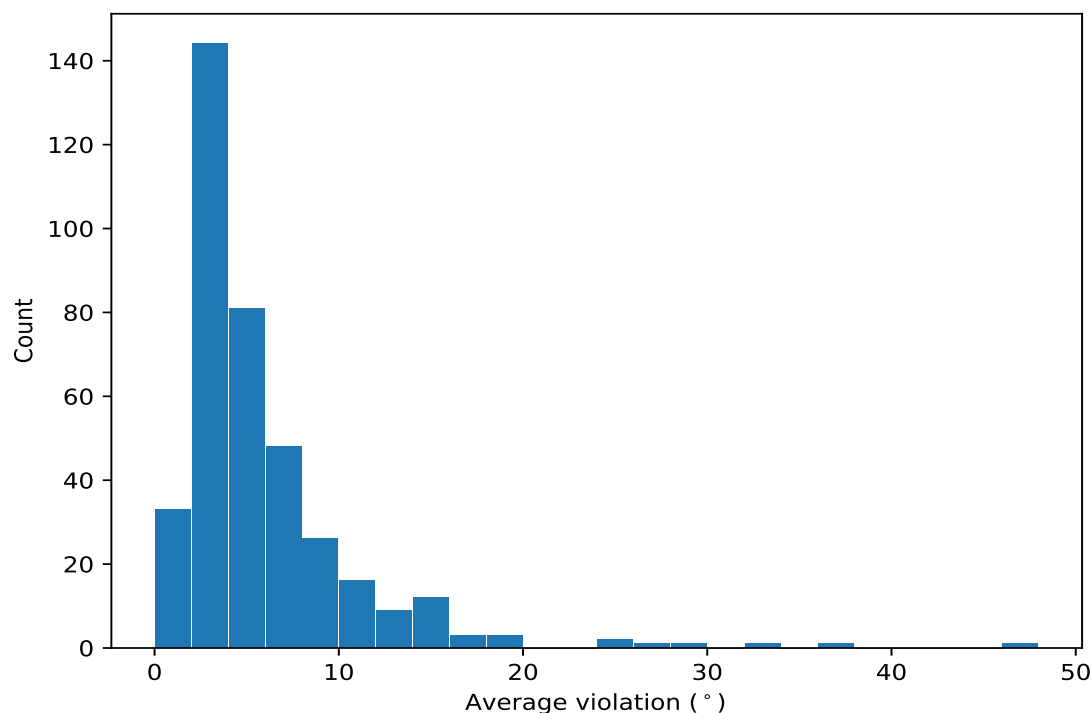
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 10 | 15.29 | 3.61 | 14.82 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 10 | 14.75 | 2.78 | 14.9 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 10 | 11.33 | 4.02 | 11.11 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 10 | 11.15 | 2.65 | 12.24 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 10 | 10.26 | 3.59 | 9.5 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 10 | 10.16 | 0.69 | 10.07 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 10 | 9.82 | 2.3 | 9.28 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 10 | 9.09 | 1.45 | 9.09 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 10 | 8.8 | 2.02 | 8.64 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 10 | 8.32 | 4.82 | 7.66 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 10 | 8.24 | 2.78 | 8.01 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 10 | 8.05 | 1.74 | 8.18 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 10 | 7.75 | 2.53 | 8.72 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 10 | 7.73 | 1.52 | 7.93 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 10 | 6.78 | 1.31 | 6.64 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 10 | 6.6 | 1.35 | 6.72 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 10 | 6.49 | 2.41 | 6.16 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 10 | 6.39 | 2.12 | 6.93 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 10 | 6.32 | 1.44 | 6.14 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 10 | 6.31 | 2.42 | 6.69 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 10 | 6.31 | 2.12 | 6.85 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 10 | 6.24 | 2.96 | 6.82 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 10 | 5.77 | 2.92 | 4.8 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 10 | 5.54 | 2.05 | 5.97 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 10 | 5.32 | 2.39 | 5.28 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 10 | 4.72 | 2.26 | 4.88 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 10 | 4.54 | 1.79 | 4.14 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 10 | 4.2 | 1.49 | 4.24 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 9 | 12.19 | 7.17 | 8.7 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 9 | 12.09 | 7.89 | 9.28 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 9 | 11.68 | 6.83 | 10.14 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 9 | 8.09 | 4.58 | 7.78 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 9 | 7.97 | 2.79 | 7.77 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 9 | 7.92 | 3.64 | 8.36 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 9 | 6.2 | 3.04 | 6.39 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 9 | 6.1 | 1.62 | 5.96 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 9 | 5.38 | 2.77 | 4.44 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 9 | 3.29 | 1.25 | 2.9 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 9 | 3.23 | 1.84 | 2.73 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 8 | 14.55 | 8.66 | 13.93 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 8 | 13.87 | 8.48 | 14.65 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 8 | 12.33 | 3.18 | 11.74 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 8 | 12.13 | 11.12 | 8.74 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 8 | 11.61 | 8.71 | 8.77 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 8 | 9.17 | 5.49 | 8.46 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 8 | 8.82 | 4.2 | 8.19 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 8 | 8.42 | 7.29 | 5.82 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 8 | 7.99 | 1.61 | 8.3 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 8 | 7.64 | 3.54 | 7.8 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 8 | 7.49 | 2.89 | 6.96 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 8 | 7.43 | 3.65 | 7.89 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 8 | 7.08 | 2.75 | 6.94 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 8 | 6.26 | 2.9 | 6.27 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 8 | 5.92 | 4.54 | 3.99 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 8 | 4.55 | 1.75 | 4.54 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 8 | 4.27 | 1.4 | 4.44 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 8 | 4.26 | 2.28 | 3.96 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 8 | 4.04 | 0.66 | 3.94 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 8 | 3.97 | 0.73 | 3.98 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 8 | 3.67 | 1.74 | 3.61 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 8 | 3.66 | 1.63 | 3.72 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 8 | 2.74 | 1.41 | 2.26 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 7 | 15.38 | 12.22 | 11.9 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 7 | 14.18 | 4.46 | 15.9 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 7 | 8.4 | 2.36 | 8.87 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 7 | 8.0 | 1.6 | 7.37 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 7 | 7.71 | 2.21 | 8.2 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 7 | 7.58 | 3.9 | 8.78 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 7 | 5.47 | 2.62 | 5.78 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 7 | 5.43 | 1.7 | 5.61 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 7 | 5.36 | 2.07 | 5.0 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 7 | 4.98 | 3.08 | 4.25 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 7 | 4.95 | 2.5 | 4.64 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 7 | 4.63 | 1.6 | 4.75 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 7 | 4.54 | 1.64 | 5.13 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 7 | 4.32 | 3.12 | 2.73 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 7 | 3.75 | 1.42 | 3.67 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 7 | 3.68 | 2.05 | 4.0 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 7 | 3.26 | 0.79 | 3.7 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 7 | 3.14 | 0.96 | 2.54 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 7 | 2.54 | 1.49 | 1.99 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 7 | 2.37 | 0.86 | 2.77 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 7 | 2.21 | 0.64 | 2.01 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 6 | 15.35 | 9.91 | 13.71 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 6 | 14.38 | 11.66 | 13.78 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 6 | 12.3 | 4.96 | 13.85 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 6 | 11.59 | 6.29 | 11.85 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 6 | 11.44 | 13.83 | 3.76 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 6 | 10.43 | 5.87 | 8.75 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 6 | 10.38 | 10.75 | 4.59 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 6 | 9.08 | 4.39 | 8.14 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 6 | 8.38 | 6.97 | 4.86 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 6 | 8.13 | 2.69 | 9.21 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 6 | 7.68 | 8.68 | 4.8 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 6 | 7.09 | 4.9 | 5.62 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 6 | 6.95 | 3.75 | 5.56 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 6 | 6.68 | 3.44 | 6.75 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 6 | 6.51 | 2.8 | 6.06 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 6 | 6.33 | 3.73 | 5.06 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 6 | 6.05 | 2.5 | 6.29 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 6 | 5.71 | 2.37 | 6.02 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 6 | 5.66 | 2.29 | 5.84 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 6 | 5.63 | 2.71 | 4.85 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 6 | 5.52 | 2.61 | 5.22 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 6 | 4.84 | 2.15 | 4.77 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 6 | 4.68 | 1.96 | 4.24 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 6 | 4.35 | 2.34 | 3.34 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 6 | 3.72 | 1.37 | 4.0 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 6 | 3.55 | 2.54 | 2.38 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 6 | 3.41 | 2.2 | 2.26 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 6 | 3.14 | 1.33 | 3.24 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 6 | 3.07 | 1.31 | 2.74 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 6 | 2.57 | 0.7 | 2.43 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 6 | 2.51 | 1.52 | 1.79 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 6 | 2.25 | 1.14 | 1.74 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 6 | 1.96 | 0.56 | 1.91 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 5 | 27.82 | 21.14 | 32.31 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 5 | 18.39 | 11.71 | 17.62 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 5 | 18.22 | 10.95 | 16.77 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 5 | 15.22 | 7.08 | 18.77 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 5 | 14.7 | 5.79 | 17.4 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 5 | 12.87 | 11.87 | 4.37 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 5 | 11.85 | 5.33 | 12.57 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 5 | 11.84 | 5.69 | 11.24 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 5 | 11.73 | 9.05 | 6.26 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 5 | 9.45 | 9.61 | 5.82 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 5 | 9.28 | 4.33 | 8.77 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 5 | 9.06 | 0.85 | 8.94 |
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 5 | 7.39 | 2.22 | 8.26 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 5 | 6.96 | 9.54 | 2.19 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 5 | 6.7 | 1.81 | 7.69 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 5 | 6.32 | 1.91 | 6.68 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 5 | 6.12 | 1.44 | 5.5 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 5 | 5.98 | 4.49 | 4.65 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 5 | 5.8 | 1.4 | 6.12 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 5 | 5.33 | 3.12 | 6.67 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 5 | 5.26 | 2.33 | 5.49 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 5 | 4.92 | 4.66 | 3.12 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 5 | 4.85 | 1.79 | 5.19 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 5 | 4.4 | 2.26 | 5.04 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 5 | 3.96 | 1.77 | 3.91 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 5 | 3.96 | 1.84 | 3.38 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 5 | 3.71 | 2.6 | 3.14 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 5 | 3.45 | 3.23 | 2.1 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 5 | 3.33 | 0.94 | 3.16 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 5 | 3.17 | 2.16 | 2.33 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 5 | 3.11 | 1.97 | 2.03 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 5 | 2.91 | 1.51 | 3.07 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 5 | 2.87 | 0.94 | 2.74 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 5 | 2.73 | 1.56 | 2.29 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 5 | 2.57 | 1.29 | 1.99 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 5 | 2.54 | 0.42 | 2.79 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 5 | 2.15 | 0.66 | 2.1 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 5 | 1.87 | 0.77 | 1.45 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 5 | 1.84 | 0.69 | 1.64 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 5 | 1.68 | 0.45 | 1.76 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 4 | 37.85 | 22.57 | 40.82 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 4 | 25.64 | 19.6 | 22.98 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 4 | 19.5 | 10.05 | 23.62 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 4 | 17.56 | 6.54 | 19.3 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 4 | 16.22 | 5.38 | 16.94 |
| (1,1106) | 1:241:H:THR:C | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 4 | 14.98 | 14.24 | 9.1 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 4 | 14.69 | 9.17 | 14.76 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 4 | 14.27 | 8.34 | 15.26 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 4 | 13.26 | 9.64 | 11.5 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 4 | 8.42 | 2.14 | 8.21 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,1105) | 1:241:G:THR:C | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 4 | 7.82 | 6.79 | 5.48 |
| (1,1008) | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1:239:L:THR:N | 4 | 7.22 | 3.02 | 6.57 |
| (1,1070) | 1:174:H:ALA:C | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 4 | 7.2 | 5.24 | 6.28 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 4 | 5.93 | 0.94 | 5.6 |
| (1,1083) | 1:175:I:GLU:C | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 4 | 5.92 | 2.03 | 5.45 |
| (1,847) | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 1:226:G:HIS:N | 4 | 5.92 | 1.48 | 6.68 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 4 | 5.82 | 0.71 | 5.6 |
| (1,152) | 1:161:H:PHE:N | 1:161:H:PHE:CA | 1:161:H:PHE:C | 1:162:H:ARG:N | 4 | 5.45 | 3.55 | 4.46 |
| (1,1007) | 1:238:K:VAL:N | 1:238:K:VAL:CA | 1:238:K:VAL:C | 1:239:K:THR:N | 4 | 5.04 | 2.87 | 3.78 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 4 | 5.01 | 2.82 | 5.24 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 4 | 4.73 | 2.71 | 4.46 |
| (1,1089) | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 1:177:I:ALA:N | 4 | 4.66 | 4.22 | 2.79 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 4 | 4.43 | 2.16 | 4.66 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 4 | 4.38 | 2.17 | 4.64 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 4 | 4.18 | 1.71 | 4.93 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 4 | 4.11 | 3.04 | 3.12 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 4 | 4.08 | 1.89 | 3.7 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 4 | 4.08 | 1.23 | 3.92 |
| (1,485) | 1:190:K:LEU:C | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 4 | 3.77 | 1.74 | 3.27 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 4 | 3.71 | 2.45 | 3.36 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 4 | 3.38 | 1.7 | 2.86 |
| (1,297) | 1:173:I:ARG:N | 1:173:I:ARG:CA | 1:173:I:ARG:C | 1:174:I:ALA:N | 4 | 3.3 | 1.28 | 3.51 |
| (1,745) | 1:215:G:MET:C | 1:216:G:THR:N | 1:216:G:THR:CA | 1:216:G:THR:C | 4 | 3.26 | 1.63 | 3.18 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 4 | 3.17 | 1.2 | 3.58 |
| (1,783) | 1:218:I:CYS:C | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 4 | 3.13 | 1.29 | 3.0 |
| (1,744) | 1:215:L:MET:N | 1:215:L:MET:CA | 1:215:L:MET:C | 1:216:L:THR:N | 4 | 3.06 | 1.07 | 3.6 |
| (1,1085) | 1:175:K:GLU:C | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 4 | 2.96 | 1.33 | 2.63 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 4 | 2.88 | 1.72 | 2.6 |
| (1,252) | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 1:170:L:LYS:N | 4 | 2.84 | 0.67 | 3.08 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 4 | 2.78 | 1.45 | 2.8 |
| (1,468) | 1:189:L:LEU:N | 1:189:L:LEU:CA | 1:189:L:LEU:C | 1:190:L:LEU:N | 4 | 2.69 | 0.71 | 2.4 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 4 | 2.65 | 1.1 | 2.42 |
| (1,465) | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1:190:I:LEU:N | 4 | 2.64 | 1.03 | 2.22 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 4 | 2.47 | 1.3 | 1.82 |
| (1,180) | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1:164:L:TYR:N | 4 | 2.41 | 1.09 | 2.04 |
| (1,657) | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 1:209:I:ALA:N | 4 | 2.1 | 0.54 | 2.0 |
| (1,1086) | 1:175:L:GLU:C | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 4 | 2.07 | 1.09 | 1.66 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 4 | 2.06 | 0.34 | 2.18 |
| (1,1081) | 1:175:G:GLU:C | 1:176:G:GLN:N | 1:176:G:GLN:CA | 1:176:G:GLN:C | 4 | 2.04 | 0.8 | 1.85 |
| (1,103) | 1:157:G:PRO:N | 1:157:G:PRO:CA | 1:157:G:PRO:C | 1:158:G:LYS:N | 4 | 1.98 | 0.42 | 2.03 |
| (1,695) | 1:211:K:LEU:N | 1:211:K:LEU:CA | 1:211:K:LEU:C | 1:212:K:GLU:N | 4 | 1.8 | 0.54 | 1.8 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 4 | 1.72 | 0.61 | 1.46 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 4 | 1.53 | 0.2 | 1.46 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 3 | 46.5 | 3.68 | 45.57 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 3 | 29.94 | 30.49 | 13.36 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 3 | 17.85 | 8.54 | 23.14 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 3 | 12.59 | 6.89 | 17.0 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 3 | 11.5 | 5.71 | 8.51 |
| (1,1006) | 1:238:J:VAL:N | 1:238:J:VAL:CA | 1:238:J:VAL:C | 1:239:J:THR:N | 3 | 9.23 | 5.86 | 6.5 |
| (1,1003) | 1:238:G:VAL:N | 1:238:G:VAL:CA | 1:238:G:VAL:C | 1:239:G:THR:N | 3 | 9.01 | 5.1 | 5.61 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 3 | 8.63 | 4.78 | 9.44 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|-------|
| (1,801) | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1:221:I:VAL:N | 3 | 7.32 | 2.46 | 8.15 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 3 | 7.13 | 5.87 | 4.96 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 3 | 6.99 | 0.33 | 6.9 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 3 | 6.84 | 3.66 | 7.22 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 3 | 6.25 | 3.3 | 6.52 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 3 | 6.23 | 1.48 | 7.17 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 3 | 5.95 | 1.54 | 6.83 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 3 | 5.94 | 3.79 | 3.64 |
| (1,1004) | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1:239:H:THR:N | 3 | 5.76 | 2.08 | 6.03 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 3 | 5.7 | 3.1 | 7.12 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 3 | 5.24 | 0.6 | 5.5 |
| (1,502) | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 1:193:J:ASN:N | 3 | 5.11 | 1.37 | 4.33 |
| (1,818) | 1:222:H:GLY:N | 1:222:H:GLY:CA | 1:222:H:GLY:C | 1:223:H:GLY:N | 3 | 5.0 | 2.56 | 5.68 |
| (1,11) | 1:145:K:GLY:C | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 3 | 4.91 | 2.0 | 6.29 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 3 | 4.87 | 2.66 | 5.12 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 3 | 4.85 | 1.5 | 5.06 |
| (1,35) | 1:147:K:PRO:C | 1:148:K:THR:N | 1:148:K:THR:CA | 1:148:K:THR:C | 3 | 4.81 | 1.43 | 4.52 |
| (1,989) | 1:236:K:SER:C | 1:237:K:GLN:N | 1:237:K:GLN:CA | 1:237:K:GLN:C | 3 | 4.79 | 0.89 | 4.21 |
| (1,459) | 1:188:I:THR:C | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 3 | 4.67 | 2.82 | 2.78 |
| (1,467) | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 1:190:K:LEU:N | 3 | 4.46 | 1.05 | 4.65 |
| (1,375) | 1:181:I:VAL:C | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 3 | 4.43 | 3.43 | 2.53 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 3 | 4.25 | 1.86 | 4.76 |
| (1,646) | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 1:206:J:GLY:N | 3 | 4.1 | 0.67 | 3.9 |
| (1,21) | 1:146:I:SER:C | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 3 | 3.96 | 1.35 | 4.9 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 3 | 3.84 | 1.46 | 3.08 |
| (1,246) | 1:168:L:PHE:C | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 3 | 3.8 | 1.85 | 4.4 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 3 | 3.71 | 0.18 | 3.61 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 3 | 3.64 | 1.71 | 3.53 |
| (1,987) | 1:236:I:SER:C | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 3 | 3.63 | 1.17 | 3.1 |
| (1,190) | 1:164:J:TYR:N | 1:164:J:TYR:CA | 1:164:J:TYR:C | 1:165:J:VAL:N | 3 | 3.53 | 1.9 | 3.6 |
| (1,10) | 1:145:J:GLY:C | 1:146:J:SER:N | 1:146:J:SER:CA | 1:146:J:SER:C | 3 | 3.45 | 1.3 | 2.81 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 3 | 3.28 | 1.64 | 2.58 |
| (1,153) | 1:161:I:PHE:N | 1:161:I:PHE:CA | 1:161:I:PHE:C | 1:162:I:ARG:N | 3 | 3.2 | 1.69 | 2.85 |
| (1,8) | 1:145:H:GLY:C | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 3 | 3.12 | 1.63 | 2.12 |
| (1,238) | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 1:169:J:TYR:N | 3 | 3.11 | 1.22 | 3.6 |
| (1,1051) | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1:244:G:ILE:N | 3 | 3.08 | 1.65 | 2.21 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 3 | 2.96 | 1.26 | 2.09 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 3 | 2.91 | 1.88 | 1.88 |
| (1,165) | 1:162:I:ARG:N | 1:162:I:ARG:CA | 1:162:I:ARG:C | 1:163:I:ASP:N | 3 | 2.66 | 0.92 | 2.99 |
| (1,1092) | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 1:177:L:ALA:N | 3 | 2.65 | 0.63 | 2.61 |
| (1,456) | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 1:189:L:LEU:N | 3 | 2.55 | 0.99 | 2.44 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 3 | 2.51 | 0.87 | 2.71 |
| (1,15) | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 1:147:I:PRO:N | 3 | 2.45 | 0.89 | 2.28 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 3 | 2.38 | 0.61 | 2.46 |
| (1,251) | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 1:170:K:LYS:N | 3 | 2.37 | 0.42 | 2.14 |
| (1,622) | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 1:204:J:ALA:N | 3 | 2.26 | 0.65 | 2.19 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 3 | 2.24 | 0.26 | 2.25 |
| (1,162) | 1:161:L:PHE:C | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 3 | 2.22 | 0.9 | 2.0 |
| (1,248) | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 1:170:H:LYS:N | 3 | 2.07 | 0.38 | 2.05 |
| (1,486) | 1:190:L:LEU:C | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 3 | 2.07 | 0.28 | 1.88 |
| (1,439) | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 1:188:G:THR:N | 3 | 2.04 | 0.4 | 2.01 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|-------|
| (1,452) | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1:189:H:LEU:N | 3 | 2.04 | 0.65 | 1.67 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 3 | 2.0 | 0.69 | 1.62 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 3 | 1.93 | 0.94 | 1.56 |
| (1,552) | 1:197:L:ASP:N | 1:197:L:ASP:CA | 1:197:L:ASP:C | 1:198:L:CYS:N | 3 | 1.87 | 0.19 | 1.9 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 3 | 1.87 | 0.57 | 1.71 |
| (1,770) | 1:217:H:ALA:C | 1:218:H:CYS:N | 1:218:H:CYS:CA | 1:218:H:CYS:C | 3 | 1.86 | 1.12 | 1.09 |
| (1,591) | 1:200:I:THR:C | 1:201:I:ILE:N | 1:201:I:ILE:CA | 1:201:I:ILE:C | 3 | 1.74 | 0.54 | 1.44 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 3 | 1.44 | 0.29 | 1.34 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 2 | 32.2 | 15.2 | 32.2 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 2 | 25.39 | 12.71 | 25.39 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 2 | 11.12 | 9.05 | 11.12 |
| (1,861) | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 1:227:I:LYS:N | 2 | 10.34 | 1.56 | 10.34 |
| (1,855) | 1:225:I:GLY:C | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 2 | 9.54 | 2.81 | 9.54 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 2 | 9.32 | 0.35 | 9.32 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 2 | 8.48 | 2.8 | 8.48 |
| (1,1069) | 1:174:G:ALA:C | 1:175:G:GLU:N | 1:175:G:GLU:CA | 1:175:G:GLU:C | 2 | 8.03 | 0.44 | 8.03 |
| (1,953) | 1:233:K:GLU:C | 1:234:K:ALA:N | 1:234:K:ALA:CA | 1:234:K:ALA:C | 2 | 7.5 | 2.32 | 7.5 |
| (1,372) | 1:181:L:VAL:N | 1:181:L:VAL:CA | 1:181:L:VAL:C | 1:182:L:LYS:N | 2 | 6.88 | 2.18 | 6.88 |
| (1,822) | 1:222:L:GLY:N | 1:222:L:GLY:CA | 1:222:L:GLY:C | 1:223:L:GLY:N | 2 | 6.68 | 0.66 | 6.68 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 2 | 6.39 | 2.98 | 6.39 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 2 | 6.06 | 1.96 | 6.06 |
| (1,186) | 1:163:L:ASP:C | 1:164:L:TYR:N | 1:164:L:TYR:CA | 1:164:L:TYR:C | 2 | 5.61 | 3.11 | 5.61 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 2 | 5.56 | 0.29 | 5.56 |
| (1,1084) | 1:175:J:GLU:C | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 2 | 5.5 | 0.2 | 5.5 |
| (1,842) | 1:224:H:PRO:C | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 2 | 5.47 | 4.18 | 5.47 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 2 | 5.4 | 3.44 | 5.4 |
| (1,369) | 1:181:I:VAL:N | 1:181:I:VAL:CA | 1:181:I:VAL:C | 1:182:I:LYS:N | 2 | 5.17 | 1.04 | 5.17 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 2 | 5.13 | 3.25 | 5.13 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 2 | 5.03 | 3.38 | 5.03 |
| (1,419) | 1:185:K:MET:N | 1:185:K:MET:CA | 1:185:K:MET:C | 1:186:K:THR:N | 2 | 4.9 | 2.08 | 4.9 |
| (1,992) | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 1:238:H:VAL:N | 2 | 4.5 | 1.27 | 4.5 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 2 | 4.31 | 1.27 | 4.31 |
| (1,22) | 1:146:J:SER:C | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 2 | 4.2 | 1.38 | 4.2 |
| (1,31) | 1:147:G:PRO:C | 1:148:G:THR:N | 1:148:G:THR:CA | 1:148:G:THR:C | 2 | 4.2 | 0.34 | 4.2 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 2 | 4.16 | 0.22 | 4.16 |
| (1,99) | 1:156:I:GLY:C | 1:157:I:PRO:N | 1:157:I:PRO:CA | 1:157:I:PRO:C | 2 | 4.14 | 2.62 | 4.14 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 2 | 3.99 | 1.09 | 3.99 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 2 | 3.96 | 1.82 | 3.96 |
| (1,1076) | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 1:176:H:GLN:N | 2 | 3.96 | 0.58 | 3.96 |
| (1,443) | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 1:188:K:THR:N | 2 | 3.9 | 1.93 | 3.9 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 2 | 3.84 | 2.0 | 3.84 |
| (1,644) | 1:205:H:LEU:N | 1:205:H:LEU:CA | 1:205:H:LEU:C | 1:206:H:GLY:N | 2 | 3.83 | 0.85 | 3.83 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 2 | 3.74 | 1.18 | 3.74 |
| (1,977) | 1:235:K:MET:C | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 2 | 3.72 | 2.48 | 3.72 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 2 | 3.7 | 0.5 | 3.7 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 2 | 3.67 | 1.05 | 3.67 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 2 | 3.6 | 1.6 | 3.6 |
| (1,17) | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 1:147:K:PRO:N | 2 | 3.51 | 1.9 | 3.51 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 2 | 3.5 | 0.09 | 3.5 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 2 | 3.48 | 1.48 | 3.48 |
| (1,789) | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 1:220:I:GLY:N | 2 | 3.46 | 1.5 | 3.46 |

Continued on next page.

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|-------|
| (1,1005) | 1:238:I:VAL:N | 1:238:I:VAL:CA | 1:238:I:VAL:C | 1:239:I:THR:N | 2 | 3.46 | 0.32 | 3.46 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 2 | 3.23 | 1.67 | 3.23 |
| (1,247) | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 1:170:G:LYS:N | 2 | 3.19 | 0.58 | 3.19 |
| (1,617) | 1:202:K:LEU:C | 1:203:K:LYS:N | 1:203:K:LYS:CA | 1:203:K:LYS:C | 2 | 3.19 | 0.56 | 3.19 |
| (1,249) | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 1:170:I:LYS:N | 2 | 3.18 | 0.7 | 3.18 |
| (1,616) | 1:202:J:LEU:C | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 2 | 3.09 | 0.46 | 3.09 |
| (1,867) | 1:226:I:HIS:C | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 2 | 3.06 | 1.19 | 3.06 |
| (1,731) | 1:214:K:MET:N | 1:214:K:MET:CA | 1:214:K:MET:C | 1:215:K:MET:N | 2 | 3.02 | 1.88 | 3.02 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 2 | 3.02 | 0.38 | 3.02 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 2 | 3.0 | 1.88 | 3.0 |
| (1,668) | 1:209:H:ALA:N | 1:209:H:ALA:CA | 1:209:H:ALA:C | 1:210:H:THR:N | 2 | 2.94 | 0.38 | 2.94 |
| (1,1090) | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 1:177:J:ALA:N | 2 | 2.92 | 0.0 | 2.92 |
| (1,732) | 1:214:L:MET:N | 1:214:L:MET:CA | 1:214:L:MET:C | 1:215:L:MET:N | 2 | 2.87 | 1.51 | 2.87 |
| (1,23) | 1:146:K:SER:C | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 2 | 2.84 | 0.17 | 2.84 |
| (1,132) | 1:159:L:GLU:N | 1:159:L:GLU:CA | 1:159:L:GLU:C | 1:160:L:PRO:N | 2 | 2.8 | 0.72 | 2.8 |
| (1,302) | 1:173:H:ARG:C | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 2 | 2.78 | 0.72 | 2.78 |
| (1,13) | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 1:147:G:PRO:N | 2 | 2.76 | 0.84 | 2.76 |
| (1,14) | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 1:147:H:PRO:N | 2 | 2.74 | 0.12 | 2.74 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 2 | 2.73 | 0.51 | 2.73 |
| (1,7) | 1:145:G:GLY:C | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 2 | 2.68 | 0.62 | 2.68 |
| (1,710) | 1:212:H:GLU:C | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 2 | 2.55 | 0.53 | 2.55 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 2 | 2.5 | 1.08 | 2.5 |
| (1,25) | 1:147:G:PRO:N | 1:147:G:PRO:CA | 1:147:G:PRO:C | 1:148:G:THR:N | 2 | 2.46 | 0.58 | 2.46 |
| (1,241) | 1:168:G:PHE:C | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 2 | 2.45 | 0.48 | 2.45 |
| (1,812) | 1:221:H:VAL:N | 1:221:H:VAL:CA | 1:221:H:VAL:C | 1:222:H:GLY:N | 2 | 2.41 | 1.38 | 2.41 |
| (1,930) | 1:231:L:LEU:C | 1:232:L:ALA:N | 1:232:L:ALA:CA | 1:232:L:ALA:C | 2 | 2.41 | 0.41 | 2.41 |
| (1,696) | 1:211:L:LEU:N | 1:211:L:LEU:CA | 1:211:L:LEU:C | 1:212:L:GLU:N | 2 | 2.4 | 0.05 | 2.4 |
| (1,941) | 1:232:K:ALA:C | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 2 | 2.38 | 0.36 | 2.38 |
| (1,466) | 1:189:J:LEU:N | 1:189:J:LEU:CA | 1:189:J:LEU:C | 1:190:J:LEU:N | 2 | 2.31 | 1.17 | 2.31 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 2 | 2.26 | 0.34 | 2.26 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 2 | 2.25 | 0.27 | 2.25 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 2 | 2.22 | 0.23 | 2.22 |
| (1,933) | 1:232:I:ALA:N | 1:232:I:ALA:CA | 1:232:I:ALA:C | 1:233:I:GLU:N | 2 | 2.22 | 0.29 | 2.22 |
| (1,166) | 1:162:J:ARG:N | 1:162:J:ARG:CA | 1:162:J:ARG:C | 1:163:J:ASP:N | 2 | 2.2 | 0.37 | 2.2 |
| (1,228) | 1:167:L:ARG:N | 1:167:L:ARG:CA | 1:167:L:ARG:C | 1:168:L:PHE:N | 2 | 2.14 | 0.44 | 2.14 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 2 | 2.14 | 0.86 | 2.14 |
| (1,347) | 1:179:K:GLN:N | 1:179:K:GLN:CA | 1:179:K:GLN:C | 1:180:K:GLU:N | 2 | 2.14 | 0.97 | 2.14 |
| (1,718) | 1:213:J:GLU:N | 1:213:J:GLU:CA | 1:213:J:GLU:C | 1:214:J:MET:N | 2 | 2.12 | 0.8 | 2.12 |
| (1,12) | 1:145:L:GLY:C | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 2 | 2.12 | 0.38 | 2.12 |
| (1,885) | 1:228:I:ALA:N | 1:228:I:ALA:CA | 1:228:I:ALA:C | 1:229:I:ARG:N | 2 | 2.11 | 0.54 | 2.11 |
| (1,585) | 1:200:I:THR:N | 1:200:I:THR:CA | 1:200:I:THR:C | 1:201:I:ILE:N | 2 | 2.1 | 0.31 | 2.1 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 2 | 2.06 | 0.7 | 2.06 |
| (1,628) | 1:203:J:LYS:C | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 2 | 2.03 | 0.7 | 2.03 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 2 | 2.0 | 0.88 | 2.0 |
| (1,414) | 1:184:L:TRP:C | 1:185:L:MET:N | 1:185:L:MET:CA | 1:185:L:MET:C | 2 | 1.96 | 0.38 | 1.96 |
| (1,276) | 1:171:L:THR:N | 1:171:L:THR:CA | 1:171:L:THR:C | 1:172:L:LEU:N | 2 | 1.94 | 0.86 | 1.94 |
| (1,171) | 1:162:I:ARG:C | 1:163:I:ASP:N | 1:163:I:ASP:CA | 1:163:I:ASP:C | 2 | 1.92 | 0.54 | 1.92 |
| (1,791) | 1:219:K:GLN:N | 1:219:K:GLN:CA | 1:219:K:GLN:C | 1:220:K:GLY:N | 2 | 1.92 | 0.59 | 1.92 |
| (1,954) | 1:233:L:GLU:C | 1:234:L:ALA:N | 1:234:L:ALA:CA | 1:234:L:ALA:C | 2 | 1.88 | 0.19 | 1.88 |
| (1,306) | 1:173:L:ARG:C | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 2 | 1.87 | 0.36 | 1.87 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 2 | 1.78 | 0.47 | 1.78 |

Continued on next page.

Continued from previous page...

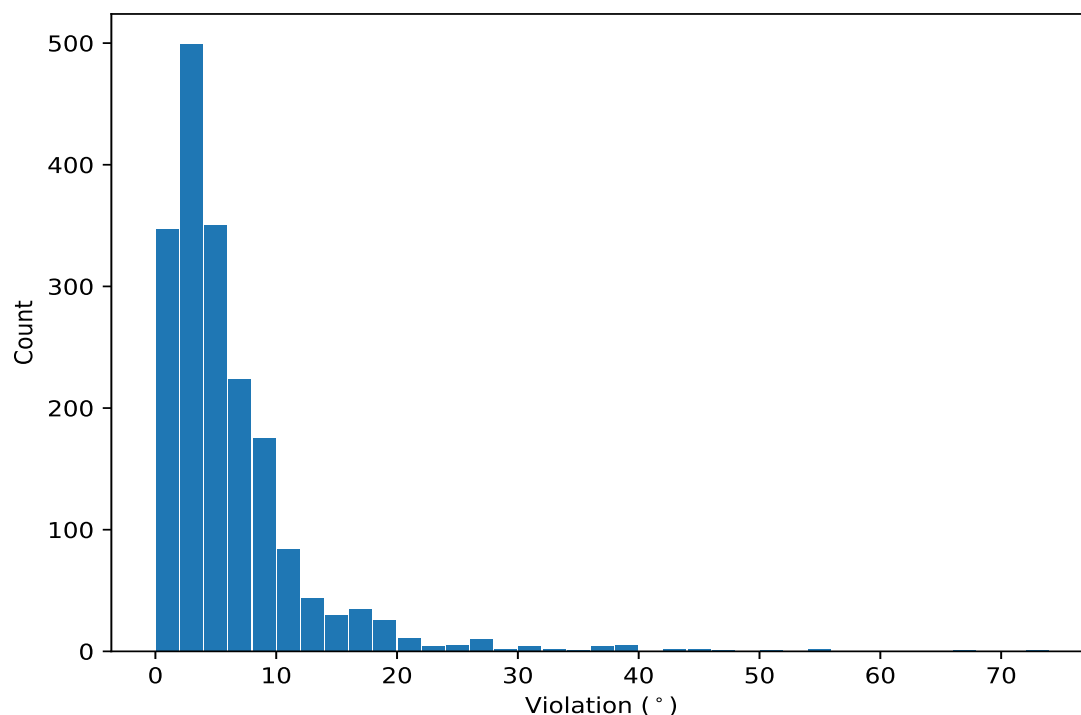
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Media |
|----------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|-------|
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 2 | 1.73 | 0.44 | 1.73 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 2 | 1.68 | 0.06 | 1.68 |
| (1,418) | 1:185:J:MET:N | 1:185:J:MET:CA | 1:185:J:MET:C | 1:186:J:THR:N | 2 | 1.65 | 0.0 | 1.65 |
| (1,938) | 1:232:H:ALA:C | 1:233:H:GLU:N | 1:233:H:GLU:CA | 1:233:H:GLU:C | 2 | 1.62 | 0.6 | 1.62 |
| (1,866) | 1:226:H:HIS:C | 1:227:H:LYS:N | 1:227:H:LYS:CA | 1:227:H:LYS:C | 2 | 1.55 | 0.01 | 1.55 |
| (1,399) | 1:183:I:ASN:C | 1:184:I:TRP:N | 1:184:I:TRP:CA | 1:184:I:TRP:C | 2 | 1.49 | 0.21 | 1.49 |
| (1,18) | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 1:147:L:PRO:N | 2 | 1.42 | 0.09 | 1.42 |
| (1,996) | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 1:238:L:VAL:N | 2 | 1.4 | 0.24 | 1.4 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 2 | 1.27 | 0.11 | 1.27 |
| (1,650) | 1:207:H:PRO:C | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 2 | 1.25 | 0.19 | 1.25 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 2 | 1.19 | 0.17 | 1.19 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 2 | 1.18 | 0.17 | 1.18 |

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [\(i\)](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 9 | 72.7 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 9 | 66.48 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 4 | 55.38 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 8 | 54.52 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 10 | 51.39 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 8 | 47.41 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 8 | 45.57 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 4 | 45.3 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 8 | 42.58 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 4 | 42.53 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 2 | 39.18 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 4 | 39.06 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 5 | 38.99 |
| (1,1106) | 1:241:H:THR:C | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 5 | 38.56 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 9 | 38.1 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 5 | 37.61 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 5 | 37.33 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1 | 36.98 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 2 | 36.83 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 7 | 35.1 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 2 | 32.48 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 10 | 32.31 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 7 | 31.75 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 2 | 30.68 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 8 | 30.43 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 9 | 30.24 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 5 | 28.74 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 1 | 28.1 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 8 | 27.81 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 10 | 27.73 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 8 | 27.57 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 8 | 27.48 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 10 | 27.34 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 2 | 27.3 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1 | 27.28 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 5 | 26.79 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 2 | 26.6 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 8 | 26.5 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 9 | 25.98 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 9 | 24.69 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 8 | 24.6 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 1 | 24.56 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 8 | 24.46 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 4 | 23.9 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 4 | 23.2 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 4 | 23.14 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 8 | 22.4 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 8 | 21.96 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 7 | 21.89 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 9 | 21.71 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 6 | 21.45 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 7 | 20.97 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 5 | 20.91 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 4 | 20.82 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1 | 20.68 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 4 | 20.3 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 8 | 20.24 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 5 | 20.17 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 5 | 19.97 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 4 | 19.91 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 7 | 19.65 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 10 | 19.5 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 4 | 19.5 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 9 | 19.5 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 4 | 19.49 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 10 | 19.41 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 6 | 19.36 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 5 | 19.36 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 6 | 19.33 |
| (1,1105) | 1:241:G:THR:C | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 5 | 19.15 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 8 | 18.92 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 7 | 18.84 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 9 | 18.77 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 7 | 18.5 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 6 | 18.42 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 10 | 18.39 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 8 | 18.38 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 4 | 18.36 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 6 | 18.32 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 8 | 18.24 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 5 | 18.19 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 9 | 18.17 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 6 | 18.12 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 5 | 18.01 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 8 | 17.97 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 8 | 17.91 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1 | 17.91 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 6 | 17.9 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 4 | 17.82 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 4 | 17.81 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 6 | 17.73 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 6 | 17.67 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 7 | 17.62 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 10 | 17.59 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 5 | 17.51 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 10 | 17.4 |
| (1,1006) | 1:238:J:VAL:N | 1:238:J:VAL:CA | 1:238:J:VAL:C | 1:239:J:THR:N | 9 | 17.37 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 7 | 17.29 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 10 | 17.2 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 7 | 17.17 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 2 | 17.17 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 7 | 17.14 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 7 | 17.11 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 9 | 17.09 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 6 | 17.04 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 1 | 17.04 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 4 | 17.0 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 4 | 17.0 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 2 | 16.77 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 6 | 16.77 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 7 | 16.58 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 4 | 16.48 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 2 | 16.48 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 7 | 16.39 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 6 | 16.32 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 6 | 16.23 |
| (1,1003) | 1:238:G:VAL:N | 1:238:G:VAL:CA | 1:238:G:VAL:C | 1:239:G:THR:N | 8 | 16.22 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 7 | 16.18 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 7 | 16.01 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 1 | 15.9 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 7 | 15.9 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 10 | 15.86 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 6 | 15.76 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 5 | 15.63 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 8 | 15.58 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 8 | 15.57 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 6 | 15.45 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 6 | 15.34 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 5 | 15.28 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 5 | 15.19 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 1 | 15.18 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 6 | 15.18 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 2 | 15.16 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 7 | 15.02 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 9 | 14.98 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 9 | 14.77 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 9 | 14.77 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 6 | 14.67 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 2 | 14.66 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 5 | 14.63 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 6 | 14.51 |
| (1,288) | 1:172:L:LEU:N | 1:172:L:LEU:CA | 1:172:L:LEU:C | 1:173:L:ARG:N | 5 | 14.47 |
| (1,1070) | 1:174:H:ALA:C | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 10 | 14.42 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 8 | 14.35 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 3 | 14.33 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 10 | 14.24 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 2 | 14.06 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 8 | 14.03 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 5 | 14.01 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 2 | 13.92 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 8 | 13.89 |
| (1,1106) | 1:241:H:THR:C | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 10 | 13.88 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 7 | 13.88 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 2 | 13.81 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 10 | 13.53 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 9 | 13.46 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 10 | 13.43 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 4 | 13.38 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 9 | 13.36 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1 | 13.36 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 7 | 13.24 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 7 | 13.19 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 2 | 13.16 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 2 | 13.13 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 9 | 13.06 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 5 | 13.04 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 10 | 13.03 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 8 | 13.02 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1 | 12.97 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 5 | 12.95 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 5 | 12.91 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 6 | 12.78 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 4 | 12.75 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 6 | 12.73 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 9 | 12.7 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 1 | 12.68 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 3 | 12.66 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 2 | 12.6 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 4 | 12.58 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 5 | 12.57 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 10 | 12.47 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 10 | 12.46 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 3 | 12.45 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 3 | 12.38 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 9 | 12.36 |
| (1,855) | 1:225:I:GLY:C | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 8 | 12.35 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 6 | 12.31 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 4 | 12.29 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 4 | 12.28 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 6 | 12.25 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 1 | 12.23 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 9 | 12.15 |
| (1,1008) | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1:239:L:THR:N | 8 | 12.04 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 9 | 11.97 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 5 | 11.97 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 2 | 11.93 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 2 | 11.9 |
| (1,861) | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 1:227:I:LYS:N | 9 | 11.9 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 9 | 11.89 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1 | 11.84 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1089) | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 1:177:I:ALA:N | 5 | 11.8 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 10 | 11.75 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 4 | 11.69 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 9 | 11.66 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 8 | 11.61 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 10 | 11.57 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 5 | 11.56 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 5 | 11.55 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 6 | 11.51 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 8 | 11.48 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 1 | 11.43 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 10 | 11.38 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 10 | 11.37 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 3 | 11.33 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 8 | 11.31 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 8 | 11.31 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 10 | 11.29 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 5 | 11.29 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 6 | 11.29 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1 | 11.28 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 7 | 11.27 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 2 | 11.24 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 7 | 11.24 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 7 | 11.23 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 9 | 11.21 |
| (1,152) | 1:161:H:PHE:N | 1:161:H:PHE:CA | 1:161:H:PHE:C | 1:162:H:ARG:N | 4 | 11.17 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 5 | 11.13 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 10 | 11.13 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 2 | 11.09 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 4 | 11.05 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 10 | 11.02 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 6 | 10.91 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 3 | 10.9 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 2 | 10.87 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 9 | 10.86 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 7 | 10.84 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 2 | 10.82 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 3 | 10.8 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 2 | 10.8 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 7 | 10.78 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 1 | 10.75 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 10 | 10.74 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 8 | 10.73 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 8 | 10.72 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 5 | 10.72 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 6 | 10.61 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 9 | 10.56 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 9 | 10.55 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 6 | 10.55 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 5 | 10.54 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 9 | 10.53 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 7 | 10.51 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 5 | 10.47 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 1 | 10.46 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 3 | 10.4 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 5 | 10.38 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 2 | 10.37 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 3 | 10.35 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 7 | 10.33 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 3 | 10.32 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 9 | 10.28 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 2 | 10.27 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 3 | 10.26 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 9 | 10.24 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 9 | 10.22 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1 | 10.18 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 5 | 10.16 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 8 | 10.14 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 4 | 10.13 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 9 | 10.12 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 7 | 10.11 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 2 | 10.08 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 7 | 10.08 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 4 | 10.08 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 4 | 10.05 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 10 | 10.04 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 5 | 10.04 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 9 | 9.96 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 6 | 9.96 |
| (1,1070) | 1:174:H:ALA:C | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 5 | 9.95 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 5 | 9.94 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 8 | 9.93 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 3 | 9.92 |
| (1,1007) | 1:238:K:VAL:N | 1:238:K:VAL:CA | 1:238:K:VAL:C | 1:239:K:THR:N | 10 | 9.91 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 10 | 9.88 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 9 | 9.88 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 7 | 9.86 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 10 | 9.85 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 5 | 9.84 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 4 | 9.84 |
| (1,801) | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1:221:I:VAL:N | 8 | 9.83 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 1 | 9.83 |
| (1,953) | 1:233:K:GLU:C | 1:234:K:ALA:N | 1:234:K:ALA:CA | 1:234:K:ALA:C | 9 | 9.81 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 6 | 9.81 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 9 | 9.79 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 8 | 9.78 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 4 | 9.75 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 6 | 9.75 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 4 | 9.74 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 3 | 9.72 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 3 | 9.72 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 9 | 9.69 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1 | 9.69 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 9 | 9.69 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 10 | 9.68 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 7 | 9.67 |
| (1,842) | 1:224:H:PRO:C | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 6 | 9.65 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 5 | 9.64 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 3 | 9.6 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 1 | 9.54 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 2 | 9.53 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 3 | 9.49 |
| (1,158) | 1:161:H:PHE:C | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 4 | 9.46 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 2 | 9.44 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 5 | 9.43 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 9 | 9.42 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 9 | 9.41 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 7 | 9.38 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 4 | 9.37 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 10 | 9.37 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 2 | 9.29 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 8 | 9.29 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 9 | 9.28 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 8 | 9.27 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 3 | 9.27 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 6 | 9.25 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 2 | 9.24 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 1 | 9.24 |
| (1,375) | 1:181:I:VAL:C | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 4 | 9.24 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 7 | 9.17 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 8 | 9.16 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 4 | 9.16 |
| (1,1083) | 1:175:I:GLU:C | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 10 | 9.14 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 3 | 9.14 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 1 | 9.14 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 7 | 9.11 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 8 | 9.11 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 1 | 9.1 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 5 | 9.09 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 2 | 9.09 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 4 | 9.09 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 7 | 9.09 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 9 | 9.08 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 1 | 9.07 |
| (1,372) | 1:181:L:VAL:N | 1:181:L:VAL:CA | 1:181:L:VAL:C | 1:182:L:LYS:N | 7 | 9.07 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1 | 9.06 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 7 | 9.05 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 3 | 9.05 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 1 | 9.02 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 8 | 9.01 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 8 | 9.01 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 7 | 9.0 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 5 | 8.97 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 9 | 8.96 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 1 | 8.96 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 3 | 8.95 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 10 | 8.94 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 4 | 8.93 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 10 | 8.93 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 6 | 8.92 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 5 | 8.88 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 1 | 8.87 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 4 | 8.87 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 3 | 8.84 |
| (1,1074) | 1:174:L:ALA:C | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 10 | 8.83 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 6 | 8.82 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 7 | 8.81 |
| (1,861) | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 1:227:I:LYS:N | 8 | 8.79 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 6 | 8.78 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 2 | 8.78 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 9 | 8.77 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1 | 8.77 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 2 | 8.75 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 7 | 8.73 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 10 | 8.73 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 10 | 8.72 |
| (1,186) | 1:163:L:ASP:C | 1:164:L:TYR:N | 1:164:L:TYR:CA | 1:164:L:TYR:C | 1 | 8.72 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 6 | 8.72 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 4 | 8.71 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 5 | 8.71 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 1 | 8.7 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 4 | 8.69 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 2 | 8.68 |
| (1,459) | 1:188:I:THR:C | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 4 | 8.66 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 1 | 8.65 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 1 | 8.63 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 8 | 8.63 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 5 | 8.62 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 1 | 8.59 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 2 | 8.58 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 10 | 8.58 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 8 | 8.57 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 2 | 8.55 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 1 | 8.54 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 8 | 8.53 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 1 | 8.51 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 10 | 8.51 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 5 | 8.49 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 10 | 8.48 |
| (1,1069) | 1:174:G:ALA:C | 1:175:G:GLU:N | 1:175:G:GLU:CA | 1:175:G:GLU:C | 10 | 8.47 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 10 | 8.45 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 8 | 8.42 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 1 | 8.42 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 5 | 8.41 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 1 | 8.41 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 5 | 8.41 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 8 | 8.38 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 10 | 8.36 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 10 | 8.36 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 5 | 8.34 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 7 | 8.33 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 3 | 8.29 |
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 5 | 8.27 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 6 | 8.27 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 5 | 8.26 |
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 8 | 8.26 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 4 | 8.25 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 10 | 8.24 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 4 | 8.22 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 8 | 8.22 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 1 | 8.2 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 4 | 8.19 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 5 | 8.18 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 10 | 8.17 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 1 | 8.17 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 9 | 8.17 |
| (1,1004) | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1:239:H:THR:N | 4 | 8.16 |
| (1,801) | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1:221:I:VAL:N | 2 | 8.15 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 3 | 8.15 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 10 | 8.14 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 6 | 8.14 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 2 | 8.14 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 10 | 8.14 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 7 | 8.13 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 2 | 8.13 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 2 | 8.12 |
| (1,1059) | 1:243:I:THR:C | 1:244:I:ILE:N | 1:244:I:ILE:CA | 1:244:I:ILE:C | 4 | 8.12 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 4 | 8.12 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 5 | 8.11 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 5 | 8.1 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 8 | 8.09 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 10 | 8.09 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 5 | 8.06 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 1 | 8.06 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 7 | 8.06 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 8 | 8.05 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 10 | 8.03 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 10 | 8.03 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 10 | 8.03 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 8 | 8.02 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 8 | 8.02 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 10 | 8.0 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 10 | 7.99 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 5 | 7.98 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 5 | 7.97 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 4 | 7.96 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 9 | 7.95 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 10 | 7.95 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 4 | 7.92 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 2 | 7.92 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 10 | 7.92 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 9 | 7.9 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 7 | 7.9 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 10 | 7.9 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 9 | 7.88 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 10 | 7.87 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 4 | 7.86 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 9 | 7.81 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 10 | 7.8 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 6 | 7.79 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 4 | 7.78 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 3 | 7.78 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 7 | 7.78 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 1 | 7.77 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 10 | 7.77 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 5 | 7.76 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 4 | 7.75 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 10 | 7.75 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 1 | 7.74 |
| (1,818) | 1:222:H:GLY:N | 1:222:H:GLY:CA | 1:222:H:GLY:C | 1:223:H:GLY:N | 6 | 7.74 |
| (1,315) | 1:176:I:GLN:C | 1:177:I:ALA:N | 1:177:I:ALA:CA | 1:177:I:ALA:C | 1 | 7.73 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 2 | 7.73 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 10 | 7.71 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 6 | 7.71 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 2 | 7.7 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 6 | 7.69 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 4 | 7.68 |
| (1,471) | 1:189:I:LEU:C | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 6 | 7.68 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 3 | 7.67 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 3 | 7.65 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 7 | 7.64 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 4 | 7.63 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 2 | 7.61 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 3 | 7.61 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 2 | 7.6 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 8 | 7.6 |
| (1,1069) | 1:174:G:ALA:C | 1:175:G:GLU:N | 1:175:G:GLU:CA | 1:175:G:GLU:C | 5 | 7.59 |
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 3 | 7.56 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 1 | 7.51 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 4 | 7.51 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 7 | 7.49 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 1 | 7.48 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 2 | 7.47 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 5 | 7.47 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 9 | 7.46 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 6 | 7.46 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 3 | 7.45 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 5 | 7.45 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 4 | 7.43 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1 | 7.42 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 8 | 7.42 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 10 | 7.42 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 7 | 7.41 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 7 | 7.4 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 10 | 7.4 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 8 | 7.39 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 4 | 7.38 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 1 | 7.38 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 9 | 7.38 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 3 | 7.37 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 7 | 7.37 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 4 | 7.36 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 8 | 7.36 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 3 | 7.35 |
| (1,822) | 1:222:L:GLY:N | 1:222:L:GLY:CA | 1:222:L:GLY:C | 1:223:L:GLY:N | 10 | 7.34 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 4 | 7.33 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 3 | 7.32 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 1 | 7.31 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 8 | 7.29 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 2 | 7.29 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 8 | 7.28 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 4 | 7.28 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 3 | 7.26 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 1 | 7.23 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 9 | 7.23 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 10 | 7.22 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 7 | 7.22 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 10 | 7.21 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 6 | 7.19 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 2 | 7.17 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 1 | 7.17 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 1 | 7.17 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 4 | 7.15 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 8 | 7.15 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 10 | 7.14 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 7 | 7.13 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 5 | 7.13 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 10 | 7.12 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 10 | 7.12 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 9 | 7.09 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 10 | 7.08 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 1 | 7.07 |
| (1,924) | 1:231:L:LEU:N | 1:231:L:LEU:CA | 1:231:L:LEU:C | 1:232:L:ALA:N | 10 | 7.05 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 2 | 7.05 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 8 | 7.04 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 1 | 7.04 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 2 | 7.04 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 10 | 7.03 |
| (1,502) | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 1:193:J:ASN:N | 8 | 7.03 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 3 | 7.02 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 5 | 7.02 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 4 | 7.01 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 4 | 7.0 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 7 | 7.0 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 2 | 6.99 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 9 | 6.98 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 2 | 6.98 |
| (1,419) | 1:185:K:MET:N | 1:185:K:MET:CA | 1:185:K:MET:C | 1:186:K:THR:N | 1 | 6.98 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 4 | 6.98 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 8 | 6.96 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 10 | 6.96 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 5 | 6.94 |
| (1,847) | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 1:226:G:HIS:N | 2 | 6.94 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 1 | 6.91 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 3 | 6.9 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 7 | 6.9 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 9 | 6.87 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 2 | 6.87 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 8 | 6.86 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 9 | 6.85 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 10 | 6.83 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 10 | 6.81 |
| (1,847) | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 1:226:G:HIS:N | 9 | 6.81 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 5 | 6.78 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 4 | 6.78 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 6 | 6.78 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 7 | 6.77 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 3 | 6.77 |
| (1,1008) | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1:239:L:THR:N | 7 | 6.76 |
| (1,99) | 1:156:I:GLY:C | 1:157:I:PRO:N | 1:157:I:PRO:CA | 1:157:I:PRO:C | 5 | 6.76 |
| (1,855) | 1:225:I:GLY:C | 1:226:I:HIS:N | 1:226:I:HIS:CA | 1:226:I:HIS:C | 2 | 6.73 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 4 | 6.72 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 5 | 6.71 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1 | 6.7 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 1 | 6.69 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 4 | 6.69 |
| (1,35) | 1:147:K:PRO:C | 1:148:K:THR:N | 1:148:K:THR:CA | 1:148:K:THR:C | 10 | 6.69 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 4 | 6.68 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 2 | 6.68 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 2 | 6.67 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 1 | 6.67 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 3 | 6.66 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1 | 6.65 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 7 | 6.64 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 1 | 6.64 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 3 | 6.63 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 8 | 6.63 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 6 | 6.63 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 2 | 6.58 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 4 | 6.58 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 6 | 6.57 |
| (1,991) | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 1:238:G:VAL:N | 3 | 6.56 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 4 | 6.54 |
| (1,847) | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 1:226:G:HIS:N | 8 | 6.54 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 8 | 6.53 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 2 | 6.53 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 10 | 6.52 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 7 | 6.52 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 10 | 6.51 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 9 | 6.5 |
| (1,1006) | 1:238:J:VAL:N | 1:238:J:VAL:CA | 1:238:J:VAL:C | 1:239:J:THR:N | 8 | 6.5 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 1 | 6.5 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 1 | 6.49 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 10 | 6.48 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 3 | 6.47 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 10 | 6.47 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 4 | 6.44 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 5 | 6.43 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 4 | 6.42 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 6 | 6.42 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 3 | 6.41 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 9 | 6.39 |
| (1,1008) | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1:239:L:THR:N | 4 | 6.38 |
| (1,485) | 1:190:K:LEU:C | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 9 | 6.38 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 3 | 6.36 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 5 | 6.36 |
| (1,11) | 1:145:K:GLY:C | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 3 | 6.36 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 2 | 6.35 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 3 | 6.35 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 10 | 6.34 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 6 | 6.33 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 8 | 6.32 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 4 | 6.32 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 10 | 6.31 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 4 | 6.29 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 3 | 6.29 |
| (1,11) | 1:145:K:GLY:C | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 8 | 6.29 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 2 | 6.27 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 7 | 6.26 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 5 | 6.23 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 4 | 6.21 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 3 | 6.21 |
| (1,369) | 1:181:I:VAL:N | 1:181:I:VAL:CA | 1:181:I:VAL:C | 1:182:I:LYS:N | 7 | 6.21 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 7 | 6.21 |
| (1,977) | 1:235:K:MET:C | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 10 | 6.2 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 6 | 6.2 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 2 | 6.2 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 4 | 6.18 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1 | 6.16 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 6 | 6.12 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 9 | 6.11 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 8 | 6.09 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 3 | 6.08 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 9 | 6.08 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 8 | 6.07 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 6 | 6.06 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 10 | 6.06 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 9 | 6.06 |
| (1,989) | 1:236:K:SER:C | 1:237:K:GLN:N | 1:237:K:GLN:CA | 1:237:K:GLN:C | 7 | 6.05 |
| (1,978) | 1:235:L:MET:C | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 4 | 6.05 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 5 | 6.05 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 8 | 6.04 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 2 | 6.03 |
| (1,1004) | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1:239:H:THR:N | 8 | 6.03 |
| (1,822) | 1:222:L:GLY:N | 1:222:L:GLY:CA | 1:222:L:GLY:C | 1:223:L:GLY:N | 5 | 6.01 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 1 | 6.0 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 5 | 5.99 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 2 | 5.98 |
| (1,1105) | 1:241:G:THR:C | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 10 | 5.96 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 2 | 5.96 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 8 | 5.96 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 5 | 5.95 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 2 | 5.94 |
| (1,1083) | 1:175:I:GLU:C | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 8 | 5.92 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 7 | 5.92 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 9 | 5.91 |
| (1,854) | 1:225:H:GLY:C | 1:226:H:HIS:N | 1:226:H:HIS:CA | 1:226:H:HIS:C | 4 | 5.88 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1 | 5.88 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 7 | 5.88 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 10 | 5.88 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 9 | 5.87 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 2 | 5.87 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 7 | 5.87 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 3 | 5.86 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 9 | 5.86 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 5 | 5.86 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 6 | 5.85 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 7 | 5.84 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 4 | 5.84 |
| (1,443) | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 1:188:K:THR:N | 5 | 5.83 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 8 | 5.82 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 9 | 5.82 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 6 | 5.82 |
| (1,190) | 1:164:J:TYR:N | 1:164:J:TYR:CA | 1:164:J:TYR:C | 1:165:J:VAL:N | 8 | 5.82 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 10 | 5.81 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1 | 5.81 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 2 | 5.8 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 10 | 5.8 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 9 | 5.8 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1 | 5.79 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 3 | 5.79 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 10 | 5.79 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 5 | 5.79 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 9 | 5.79 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 2 | 5.78 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 8 | 5.78 |
| (1,838) | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 1:225:J:GLY:N | 5 | 5.78 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 3 | 5.78 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 9 | 5.78 |
| (1,992) | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 1:238:H:VAL:N | 7 | 5.77 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 7 | 5.76 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 3 | 5.75 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 4 | 5.75 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 6 | 5.73 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 6 | 5.72 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 8 | 5.72 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 2 | 5.71 |
| (1,737) | 1:214:K:MET:C | 1:215:K:MET:N | 1:215:K:MET:CA | 1:215:K:MET:C | 8 | 5.71 |
| (1,246) | 1:168:L:PHE:C | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 7 | 5.71 |
| (1,1084) | 1:175:J:GLU:C | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 8 | 5.69 |
| (1,818) | 1:222:H:GLY:N | 1:222:H:GLY:CA | 1:222:H:GLY:C | 1:223:H:GLY:N | 4 | 5.68 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 7 | 5.68 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 9 | 5.67 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 9 | 5.66 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 2 | 5.64 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 1 | 5.64 |
| (1,467) | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 1:190:K:LEU:N | 3 | 5.63 |
| (1,1003) | 1:238:G:VAL:N | 1:238:G:VAL:CA | 1:238:G:VAL:C | 1:239:G:THR:N | 10 | 5.61 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 8 | 5.61 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 3 | 5.6 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 5 | 5.6 |
| (1,294) | 1:172:L:LEU:C | 1:173:L:ARG:N | 1:173:L:ARG:CA | 1:173:L:ARG:C | 5 | 5.6 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 1 | 5.59 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 8 | 5.58 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 10 | 5.58 |
| (1,22) | 1:146:J:SER:C | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 8 | 5.58 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 1 | 5.57 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1 | 5.57 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 5 | 5.56 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1 | 5.55 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 5 | 5.55 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 8 | 5.55 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 4 | 5.54 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 7 | 5.51 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 4 | 5.5 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 7 | 5.5 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 9 | 5.5 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 5 | 5.5 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 4 | 5.5 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 7 | 5.49 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 1 | 5.49 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 5 | 5.49 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 4 | 5.49 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 9 | 5.47 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 1 | 5.47 |
| (1,1065) | 1:244:I:ILE:N | 1:244:I:ILE:CA | 1:244:I:ILE:C | 1:245:I:MET:N | 2 | 5.46 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 8 | 5.45 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 8 | 5.44 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 6 | 5.43 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 7 | 5.42 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 1 | 5.42 |
| (1,153) | 1:161:I:PHE:N | 1:161:I:PHE:CA | 1:161:I:PHE:C | 1:162:I:ARG:N | 8 | 5.42 |
| (1,8) | 1:145:H:GLY:C | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 8 | 5.42 |
| (1,152) | 1:161:H:PHE:N | 1:161:H:PHE:CA | 1:161:H:PHE:C | 1:162:H:ARG:N | 8 | 5.4 |
| (1,17) | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 1:147:K:PRO:N | 7 | 5.4 |
| (1,1051) | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1:244:G:ILE:N | 10 | 5.39 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 1 | 5.38 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 9 | 5.37 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 9 | 5.37 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 4 | 5.36 |
| (1,745) | 1:215:G:MET:C | 1:216:G:THR:N | 1:216:G:THR:CA | 1:216:G:THR:C | 8 | 5.36 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 5 | 5.36 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 8 | 5.35 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 4 | 5.35 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 3 | 5.35 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 8 | 5.34 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 8 | 5.34 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 4 | 5.32 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 2 | 5.31 |
| (1,1084) | 1:175:J:GLU:C | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 2 | 5.3 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 5 | 5.3 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 2 | 5.29 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 2 | 5.26 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 10 | 5.26 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 7 | 5.26 |
| (1,10) | 1:145:J:GLY:C | 1:146:J:SER:N | 1:146:J:SER:CA | 1:146:J:SER:C | 8 | 5.26 |
| (1,987) | 1:236:I:SER:C | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 1 | 5.25 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 6 | 5.25 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 4 | 5.25 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 1 | 5.24 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 4 | 5.24 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 8 | 5.23 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 3 | 5.23 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 6 | 5.23 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 9 | 5.21 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 9 | 5.21 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 8 | 5.21 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 10 | 5.2 |
| (1,1003) | 1:238:G:VAL:N | 1:238:G:VAL:CA | 1:238:G:VAL:C | 1:239:G:THR:N | 4 | 5.2 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 3 | 5.19 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 5 | 5.19 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 4 | 5.19 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,953) | 1:233:K:GLU:C | 1:234:K:ALA:N | 1:234:K:ALA:CA | 1:234:K:ALA:C | 3 | 5.18 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 6 | 5.16 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 5 | 5.16 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1 | 5.16 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 4 | 5.16 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 7 | 5.14 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 9 | 5.13 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 7 | 5.13 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 1 | 5.12 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 5 | 5.12 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 7 | 5.12 |
| (1,1085) | 1:175:K:GLU:C | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 4 | 5.11 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 3 | 5.1 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 7 | 5.1 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 3 | 5.1 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 4 | 5.09 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 5 | 5.08 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 10 | 5.07 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 6 | 5.07 |
| (1,783) | 1:218:I:CYS:C | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 1 | 5.07 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 10 | 5.07 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 8 | 5.06 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 7 | 5.06 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 6 | 5.06 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 6 | 5.05 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 5 | 5.04 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 9 | 5.04 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 4 | 5.04 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 2 | 5.04 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 7 | 5.02 |
| (1,1105) | 1:241:G:THR:C | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 3 | 5.01 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 7 | 5.0 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 3 | 5.0 |
| (1,646) | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 1:206:J:GLY:N | 6 | 5.0 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 2 | 5.0 |
| (1,1083) | 1:175:I:GLU:C | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 5 | 4.98 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 2 | 4.98 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 1 | 4.97 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 2 | 4.97 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 8 | 4.97 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 10 | 4.97 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 5 | 4.97 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 1 | 4.97 |
| (1,789) | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 1:220:I:GLY:N | 2 | 4.96 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 5 | 4.96 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 6 | 4.96 |
| (1,413) | 1:184:K:TRP:C | 1:185:K:MET:N | 1:185:K:MET:CA | 1:185:K:MET:C | 9 | 4.95 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 3 | 4.94 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 10 | 4.93 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 2 | 4.93 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 8 | 4.92 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,21) | 1:146:I:SER:C | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 6 | 4.92 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 3 | 4.91 |
| (1,869) | 1:226:K:HIS:C | 1:227:K:LYS:N | 1:227:K:LYS:CA | 1:227:K:LYS:C | 9 | 4.9 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 6 | 4.9 |
| (1,731) | 1:214:K:MET:N | 1:214:K:MET:CA | 1:214:K:MET:C | 1:215:K:MET:N | 8 | 4.9 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 4 | 4.9 |
| (1,21) | 1:146:I:SER:C | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 3 | 4.9 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 4 | 4.89 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 10 | 4.88 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 9 | 4.87 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 5 | 4.85 |
| (1,557) | 1:197:K:ASP:C | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 3 | 4.85 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 9 | 4.84 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 2 | 4.84 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 5 | 4.84 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1 | 4.84 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 6 | 4.83 |
| (1,9) | 1:145:I:GLY:C | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 1 | 4.82 |
| (1,999) | 1:237:I:GLN:C | 1:238:I:VAL:N | 1:238:I:VAL:CA | 1:238:I:VAL:C | 10 | 4.81 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 7 | 4.81 |
| (1,160) | 1:161:J:PHE:C | 1:162:J:ARG:N | 1:162:J:ARG:CA | 1:162:J:ARG:C | 9 | 4.81 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 10 | 4.8 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 6 | 4.79 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 10 | 4.78 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 10 | 4.78 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 1 | 4.77 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 10 | 4.76 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 1 | 4.76 |
| (1,1107) | 1:241:I:THR:C | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 3 | 4.75 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 3 | 4.75 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 6 | 4.75 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 2 | 4.75 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 1 | 4.72 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 2 | 4.7 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 1 | 4.7 |
| (1,372) | 1:181:L:VAL:N | 1:181:L:VAL:CA | 1:181:L:VAL:C | 1:182:L:LYS:N | 1 | 4.7 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 2 | 4.7 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 4 | 4.68 |
| (1,644) | 1:205:H:LEU:N | 1:205:H:LEU:CA | 1:205:H:LEU:C | 1:206:H:GLY:N | 8 | 4.68 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 1 | 4.68 |
| (1,514) | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 1:194:J:ALA:N | 5 | 4.68 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 2 | 4.68 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 3 | 4.67 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 3 | 4.66 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 8 | 4.65 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 2 | 4.65 |
| (1,467) | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 1:190:K:LEU:N | 2 | 4.65 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 1 | 4.64 |
| (1,297) | 1:173:I:ARG:N | 1:173:I:ARG:CA | 1:173:I:ARG:C | 1:174:I:ALA:N | 5 | 4.64 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 2 | 4.64 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 3 | 4.63 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 8 | 4.63 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 6 | 4.62 |
| (1,536) | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1:197:H:ASP:N | 10 | 4.62 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 3 | 4.61 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 8 | 4.61 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 7 | 4.6 |
| (1,561) | 1:198:I:CYS:N | 1:198:I:CYS:CA | 1:198:I:CYS:C | 1:199:I:LYS:N | 4 | 4.59 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 7 | 4.57 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 1 | 4.57 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 8 | 4.57 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 8 | 4.55 |
| (1,1076) | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 1:176:H:GLN:N | 10 | 4.54 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 3 | 4.54 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 5 | 4.54 |
| (1,31) | 1:147:G:PRO:C | 1:148:G:THR:N | 1:148:G:THR:CA | 1:148:G:THR:C | 10 | 4.54 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 8 | 4.53 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 4 | 4.52 |
| (1,35) | 1:147:K:PRO:C | 1:148:K:THR:N | 1:148:K:THR:CA | 1:148:K:THR:C | 1 | 4.52 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 10 | 4.46 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 2 | 4.45 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 9 | 4.44 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 3 | 4.44 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 5 | 4.43 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 6 | 4.43 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 3 | 4.42 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 5 | 4.42 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 10 | 4.41 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 5 | 4.41 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 6 | 4.4 |
| (1,297) | 1:173:I:ARG:N | 1:173:I:ARG:CA | 1:173:I:ARG:C | 1:174:I:ALA:N | 6 | 4.4 |
| (1,246) | 1:168:L:PHE:C | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 6 | 4.4 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 10 | 4.39 |
| (1,732) | 1:214:L:MET:N | 1:214:L:MET:CA | 1:214:L:MET:C | 1:215:L:MET:N | 5 | 4.38 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 8 | 4.38 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 9 | 4.38 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 7 | 4.37 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 1 | 4.37 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 3 | 4.37 |
| (1,465) | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1:190:I:LEU:N | 5 | 4.36 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1 | 4.36 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 5 | 4.35 |
| (1,485) | 1:190:K:LEU:C | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 8 | 4.35 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 5 | 4.35 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 6 | 4.34 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 9 | 4.34 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 4 | 4.34 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 3 | 4.33 |
| (1,1106) | 1:241:H:THR:C | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 3 | 4.33 |
| (1,502) | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 1:193:J:ASN:N | 3 | 4.33 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 9 | 4.32 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 3 | 4.31 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 6 | 4.31 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 5 | 4.31 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 4 | 4.3 |
| (1,1007) | 1:238:K:VAL:N | 1:238:K:VAL:CA | 1:238:K:VAL:C | 1:239:K:THR:N | 4 | 4.3 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 4 | 4.3 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 2 | 4.3 |
| (1,238) | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 1:169:J:TYR:N | 8 | 4.3 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 8 | 4.3 |
| (1,745) | 1:215:G:MET:C | 1:216:G:THR:N | 1:216:G:THR:CA | 1:216:G:THR:C | 10 | 4.29 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 7 | 4.28 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 8 | 4.28 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 10 | 4.28 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 7 | 4.28 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 6 | 4.27 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 10 | 4.27 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 3 | 4.25 |
| (1,867) | 1:226:I:HIS:C | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 9 | 4.25 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 4 | 4.25 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 2 | 4.24 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1 | 4.23 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 9 | 4.23 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 3 | 4.23 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 10 | 4.22 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 5 | 4.22 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 8 | 4.22 |
| (1,989) | 1:236:K:SER:C | 1:237:K:GLN:N | 1:237:K:GLN:CA | 1:237:K:GLN:C | 4 | 4.21 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 1 | 4.21 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 10 | 4.21 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 5 | 4.21 |
| (1,180) | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1:164:L:TYR:N | 4 | 4.2 |
| (1,914) | 1:230:H:VAL:C | 1:231:H:LEU:N | 1:231:H:LEU:CA | 1:231:H:LEU:C | 9 | 4.17 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 6 | 4.15 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 5 | 4.14 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 3 | 4.14 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 7 | 4.13 |
| (1,659) | 1:208:K:GLY:N | 1:208:K:GLY:CA | 1:208:K:GLY:C | 1:209:K:ALA:N | 8 | 4.13 |
| (1,369) | 1:181:I:VAL:N | 1:181:I:VAL:CA | 1:181:I:VAL:C | 1:182:I:LYS:N | 10 | 4.13 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 1 | 4.12 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 9 | 4.11 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 10 | 4.11 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 6 | 4.11 |
| (1,989) | 1:236:K:SER:C | 1:237:K:GLN:N | 1:237:K:GLN:CA | 1:237:K:GLN:C | 6 | 4.1 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 4 | 4.1 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 8 | 4.09 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 5 | 4.09 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 9 | 4.08 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 7 | 4.08 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 7 | 4.08 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 9 | 4.07 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 8 | 4.07 |
| (1,734) | 1:214:H:MET:C | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 7 | 4.07 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 9 | 4.07 |
| (1,970) | 1:235:J:MET:N | 1:235:J:MET:CA | 1:235:J:MET:C | 1:236:J:SER:N | 5 | 4.06 |
| (1,239) | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 1:169:K:TYR:N | 6 | 4.05 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 10 | 4.04 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 1 | 4.03 |
| (1,1055) | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 1:244:K:ILE:N | 5 | 4.02 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 8 | 4.02 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 8 | 4.02 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 2 | 4.02 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 6 | 4.0 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 10 | 3.99 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 10 | 3.99 |
| (1,1068) | 1:244:L:ILE:N | 1:244:L:ILE:CA | 1:244:L:ILE:C | 1:245:L:MET:N | 2 | 3.98 |
| (1,801) | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1:221:I:VAL:N | 1 | 3.98 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 10 | 3.97 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 7 | 3.97 |
| (1,502) | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 1:193:J:ASN:N | 7 | 3.97 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 1 | 3.96 |
| (1,948) | 1:233:L:GLU:N | 1:233:L:GLU:CA | 1:233:L:GLU:C | 1:234:L:ALA:N | 8 | 3.94 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 1 | 3.94 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 7 | 3.94 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 4 | 3.92 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 4 | 3.92 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 3 | 3.92 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 10 | 3.92 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 7 | 3.91 |
| (1,1086) | 1:175:L:GLU:C | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 8 | 3.9 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 3 | 3.9 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 10 | 3.9 |
| (1,646) | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 1:206:J:GLY:N | 7 | 3.9 |
| (1,249) | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 1:170:I:LYS:N | 8 | 3.89 |
| (1,993) | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 1:238:I:VAL:N | 3 | 3.88 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 6 | 3.87 |
| (1,468) | 1:189:L:LEU:N | 1:189:L:LEU:CA | 1:189:L:LEU:C | 1:190:L:LEU:N | 9 | 3.87 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 9 | 3.87 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 9 | 3.87 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 2 | 3.86 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 2 | 3.85 |
| (1,31) | 1:147:G:PRO:C | 1:148:G:THR:N | 1:148:G:THR:CA | 1:148:G:THR:C | 5 | 3.85 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 8 | 3.83 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 6 | 3.83 |
| (1,744) | 1:215:L:MET:N | 1:215:L:MET:CA | 1:215:L:MET:C | 1:216:L:THR:N | 5 | 3.82 |
| (1,1006) | 1:238:J:VAL:N | 1:238:J:VAL:CA | 1:238:J:VAL:C | 1:239:J:THR:N | 10 | 3.81 |
| (1,456) | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 1:189:L:LEU:N | 8 | 3.81 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 3 | 3.8 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 8 | 3.8 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 1 | 3.8 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 5 | 3.79 |
| (1,812) | 1:221:H:VAL:N | 1:221:H:VAL:CA | 1:221:H:VAL:C | 1:222:H:GLY:N | 4 | 3.79 |
| (1,365) | 1:180:K:GLU:C | 1:181:K:VAL:N | 1:181:K:VAL:CA | 1:181:K:VAL:C | 8 | 3.79 |
| (1,1089) | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 1:177:I:ALA:N | 2 | 3.78 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1005) | 1:238:I:VAL:N | 1:238:I:VAL:CA | 1:238:I:VAL:C | 1:239:I:THR:N | 8 | 3.78 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 5 | 3.78 |
| (1,254) | 1:169:H:TYR:C | 1:170:H:LYS:N | 1:170:H:LYS:CA | 1:170:H:LYS:C | 3 | 3.77 |
| (1,247) | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 1:170:G:LYS:N | 8 | 3.77 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 3 | 3.76 |
| (1,617) | 1:202:K:LEU:C | 1:203:K:LYS:N | 1:203:K:LYS:CA | 1:203:K:LYS:C | 6 | 3.75 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 5 | 3.75 |
| (1,69) | 1:153:I:ILE:N | 1:153:I:ILE:CA | 1:153:I:ILE:C | 1:154:I:ARG:N | 10 | 3.74 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 1 | 3.73 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 5 | 3.73 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 2 | 3.73 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 2 | 3.71 |
| (1,1008) | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1:239:L:THR:N | 10 | 3.71 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 8 | 3.7 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1 | 3.7 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 7 | 3.69 |
| (1,844) | 1:224:J:PRO:C | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 8 | 3.69 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 6 | 3.67 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 7 | 3.67 |
| (1,736) | 1:214:J:MET:C | 1:215:J:MET:N | 1:215:J:MET:CA | 1:215:J:MET:C | 9 | 3.67 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 9 | 3.67 |
| (1,1083) | 1:175:I:GLU:C | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 3 | 3.65 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 2 | 3.65 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 9 | 3.65 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 3 | 3.64 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 4 | 3.64 |
| (1,744) | 1:215:L:MET:N | 1:215:L:MET:CA | 1:215:L:MET:C | 1:216:L:THR:N | 3 | 3.64 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 5 | 3.64 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 7 | 3.63 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 9 | 3.63 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 8 | 3.62 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1 | 3.62 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 2 | 3.62 |
| (1,15) | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 1:147:I:PRO:N | 2 | 3.62 |
| (1,841) | 1:224:G:PRO:C | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 8 | 3.61 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 2 | 3.61 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 7 | 3.6 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 2 | 3.6 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 3 | 3.6 |
| (1,238) | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 1:169:J:TYR:N | 2 | 3.6 |
| (1,190) | 1:164:J:TYR:N | 1:164:J:TYR:CA | 1:164:J:TYR:C | 1:165:J:VAL:N | 6 | 3.6 |
| (1,55) | 1:151:G:LEU:N | 1:151:G:LEU:CA | 1:151:G:LEU:C | 1:152:G:ASP:N | 9 | 3.6 |
| (1,13) | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 1:147:G:PRO:N | 5 | 3.6 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 3 | 3.59 |
| (1,165) | 1:162:I:ARG:N | 1:162:I:ARG:CA | 1:162:I:ARG:C | 1:163:I:ASP:N | 10 | 3.59 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 1 | 3.58 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 5 | 3.58 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 8 | 3.58 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 7 | 3.57 |
| (1,744) | 1:215:L:MET:N | 1:215:L:MET:CA | 1:215:L:MET:C | 1:216:L:THR:N | 9 | 3.57 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 10 | 3.57 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 3 | 3.57 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 7 | 3.56 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 3 | 3.55 |
| (1,616) | 1:202:J:LEU:C | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 10 | 3.55 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 6 | 3.55 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 3 | 3.54 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 7 | 3.54 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 7 | 3.54 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 2 | 3.53 |
| (1,152) | 1:161:H:PHE:N | 1:161:H:PHE:CA | 1:161:H:PHE:C | 1:162:H:ARG:N | 6 | 3.53 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 6 | 3.53 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 9 | 3.53 |
| (1,132) | 1:159:L:GLU:N | 1:159:L:GLU:CA | 1:159:L:GLU:C | 1:160:L:PRO:N | 8 | 3.52 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 9 | 3.5 |
| (1,302) | 1:173:H:ARG:C | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 3 | 3.49 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 7 | 3.49 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 8 | 3.49 |
| (1,466) | 1:189:J:LEU:N | 1:189:J:LEU:CA | 1:189:J:LEU:C | 1:190:J:LEU:N | 8 | 3.48 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 6 | 3.47 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 6 | 3.47 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 6 | 3.46 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 7 | 3.45 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 5 | 3.45 |
| (1,1092) | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 1:177:L:ALA:N | 7 | 3.44 |
| (1,770) | 1:217:H:ALA:C | 1:218:H:CYS:N | 1:218:H:CYS:CA | 1:218:H:CYS:C | 7 | 3.44 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 10 | 3.44 |
| (1,252) | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 1:170:L:LYS:N | 7 | 3.44 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 5 | 3.44 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 10 | 3.44 |
| (1,1052) | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 1:244:H:ILE:N | 10 | 3.43 |
| (1,119) | 1:158:K:LYS:N | 1:158:K:LYS:CA | 1:158:K:LYS:C | 1:159:K:GLU:N | 5 | 3.43 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 10 | 3.41 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 4 | 3.41 |
| (1,162) | 1:161:L:PHE:C | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 9 | 3.41 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 4 | 3.41 |
| (1,24) | 1:146:L:SER:C | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 3 | 3.41 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 2 | 3.4 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 8 | 3.39 |
| (1,646) | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 1:206:J:GLY:N | 3 | 3.39 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 1 | 3.38 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 8 | 3.38 |
| (1,743) | 1:215:K:MET:N | 1:215:K:MET:CA | 1:215:K:MET:C | 1:216:K:THR:N | 3 | 3.38 |
| (1,1076) | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 1:176:H:GLN:N | 5 | 3.37 |
| (1,847) | 1:225:G:GLY:N | 1:225:G:GLY:CA | 1:225:G:GLY:C | 1:226:G:HIS:N | 6 | 3.37 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1 | 3.37 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 2 | 3.37 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 4 | 3.36 |
| (1,252) | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 1:170:L:LYS:N | 6 | 3.36 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 7 | 3.35 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 3 | 3.35 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 3 | 3.34 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1081) | 1:175:G:GLU:C | 1:176:G:GLN:N | 1:176:G:GLN:CA | 1:176:G:GLN:C | 10 | 3.32 |
| (1,668) | 1:209:H:ALA:N | 1:209:H:ALA:CA | 1:209:H:ALA:C | 1:210:H:THR:N | 10 | 3.32 |
| (1,164) | 1:162:H:ARG:N | 1:162:H:ARG:CA | 1:162:H:ARG:C | 1:163:H:ASP:N | 3 | 3.32 |
| (1,7) | 1:145:G:GLY:C | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 8 | 3.31 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 5 | 3.3 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 10 | 3.29 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 10 | 3.29 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 5 | 3.29 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 10 | 3.29 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 5 | 3.28 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1 | 3.27 |
| (1,1007) | 1:238:K:VAL:N | 1:238:K:VAL:CA | 1:238:K:VAL:C | 1:239:K:THR:N | 2 | 3.27 |
| (1,729) | 1:214:I:MET:N | 1:214:I:MET:CA | 1:214:I:MET:C | 1:215:I:MET:N | 9 | 3.27 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 4 | 3.26 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 4 | 3.26 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 5 | 3.24 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 8 | 3.24 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 7 | 3.24 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 6 | 3.23 |
| (1,992) | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 1:238:H:VAL:N | 9 | 3.23 |
| (1,35) | 1:147:K:PRO:C | 1:148:K:THR:N | 1:148:K:THR:CA | 1:148:K:THR:C | 5 | 3.23 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 7 | 3.22 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 7 | 3.22 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 9 | 3.22 |
| (1,84) | 1:154:L:ARG:N | 1:154:L:ARG:CA | 1:154:L:ARG:C | 1:155:L:GLN:N | 6 | 3.22 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 6 | 3.21 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 7 | 3.2 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 10 | 3.2 |
| (1,783) | 1:218:I:CYS:C | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 4 | 3.18 |
| (1,273) | 1:171:I:THR:N | 1:171:I:THR:CA | 1:171:I:THR:C | 1:172:I:LEU:N | 4 | 3.18 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 6 | 3.16 |
| (1,470) | 1:189:H:LEU:C | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 10 | 3.16 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 10 | 3.16 |
| (1,1106) | 1:241:H:THR:C | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1 | 3.14 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 2 | 3.14 |
| (1,1005) | 1:238:I:VAL:N | 1:238:I:VAL:CA | 1:238:I:VAL:C | 1:239:I:THR:N | 4 | 3.13 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 1 | 3.13 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 1 | 3.13 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 3 | 3.13 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1 | 3.12 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 7 | 3.12 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 2 | 3.11 |
| (1,347) | 1:179:K:GLN:N | 1:179:K:GLN:CA | 1:179:K:GLN:C | 1:180:K:GLU:N | 10 | 3.11 |
| (1,987) | 1:236:I:SER:C | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 2 | 3.1 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 3 | 3.1 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 6 | 3.1 |
| (1,622) | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 1:204:J:ALA:N | 1 | 3.09 |
| (1,467) | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 1:190:K:LEU:N | 7 | 3.09 |
| (1,1004) | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1:239:H:THR:N | 2 | 3.08 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 10 | 3.08 |
| (1,710) | 1:212:H:GLU:C | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 4 | 3.08 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 6 | 3.08 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 5 | 3.08 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 3 | 3.07 |
| (1,997) | 1:237:G:GLN:C | 1:238:G:VAL:N | 1:238:G:VAL:CA | 1:238:G:VAL:C | 3 | 3.07 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 3 | 3.07 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 2 | 3.05 |
| (1,323) | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 1:178:K:SER:N | 5 | 3.05 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 8 | 3.05 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 5 | 3.05 |
| (1,25) | 1:147:G:PRO:N | 1:147:G:PRO:CA | 1:147:G:PRO:C | 1:148:G:THR:N | 5 | 3.05 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 2 | 3.04 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 7 | 3.04 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 5 | 3.03 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 1 | 3.01 |
| (1,23) | 1:146:K:SER:C | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 2 | 3.01 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 8 | 3.0 |
| (1,165) | 1:162:I:ARG:N | 1:162:I:ARG:CA | 1:162:I:ARG:C | 1:163:I:ASP:N | 4 | 2.99 |
| (1,644) | 1:205:H:LEU:N | 1:205:H:LEU:CA | 1:205:H:LEU:C | 1:206:H:GLY:N | 2 | 2.98 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 6 | 2.98 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 3 | 2.98 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 2 | 2.97 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 6 | 2.96 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 8 | 2.96 |
| (1,452) | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1:189:H:LEU:N | 6 | 2.96 |
| (1,251) | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 1:170:K:LYS:N | 1 | 2.96 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 3 | 2.95 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 6 | 2.94 |
| (1,718) | 1:213:J:GLU:N | 1:213:J:GLU:CA | 1:213:J:GLU:C | 1:214:J:MET:N | 4 | 2.93 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 1 | 2.93 |
| (1,241) | 1:168:G:PHE:C | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 2 | 2.93 |
| (1,1090) | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 1:177:J:ALA:N | 8 | 2.92 |
| (1,1062) | 1:243:L:THR:C | 1:244:L:ILE:N | 1:244:L:ILE:CA | 1:244:L:ILE:C | 7 | 2.92 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 10 | 2.92 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 8 | 2.92 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 8 | 2.92 |
| (1,1090) | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 1:177:J:ALA:N | 2 | 2.91 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 8 | 2.91 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 5 | 2.9 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 7 | 2.9 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 4 | 2.9 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 5 | 2.9 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1 | 2.89 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 8 | 2.89 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 1 | 2.89 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 3 | 2.88 |
| (1,371) | 1:181:K:VAL:N | 1:181:K:VAL:CA | 1:181:K:VAL:C | 1:182:K:LYS:N | 8 | 2.88 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 6 | 2.88 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 7 | 2.87 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 10 | 2.86 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 9 | 2.86 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 10 | 2.86 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,153) | 1:161:I:PHE:N | 1:161:I:PHE:CA | 1:161:I:PHE:C | 1:162:I:ARG:N | 4 | 2.85 |
| (1,14) | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 1:147:H:PRO:N | 2 | 2.85 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 9 | 2.84 |
| (1,461) | 1:188:K:THR:C | 1:189:K:LEU:N | 1:189:K:LEU:CA | 1:189:K:LEU:C | 7 | 2.84 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 7 | 2.83 |
| (1,930) | 1:231:L:LEU:C | 1:232:L:ALA:N | 1:232:L:ALA:CA | 1:232:L:ALA:C | 7 | 2.82 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 6 | 2.82 |
| (1,419) | 1:185:K:MET:N | 1:185:K:MET:CA | 1:185:K:MET:C | 1:186:K:THR:N | 5 | 2.82 |
| (1,22) | 1:146:J:SER:C | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 6 | 2.82 |
| (1,783) | 1:218:I:CYS:C | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 9 | 2.81 |
| (1,657) | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 1:209:I:ALA:N | 10 | 2.81 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 1 | 2.81 |
| (1,10) | 1:145:J:GLY:C | 1:146:J:SER:N | 1:146:J:SER:CA | 1:146:J:SER:C | 2 | 2.81 |
| (1,276) | 1:171:L:THR:N | 1:171:L:THR:CA | 1:171:L:THR:C | 1:172:L:LEU:N | 2 | 2.8 |
| (1,252) | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 1:170:L:LYS:N | 4 | 2.8 |
| (1,1085) | 1:175:K:GLU:C | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 3 | 2.79 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 3 | 2.79 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 8 | 2.79 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 5 | 2.79 |
| (1,750) | 1:215:L:MET:C | 1:216:L:THR:N | 1:216:L:THR:CA | 1:216:L:THR:C | 9 | 2.79 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 9 | 2.79 |
| (1,333) | 1:178:I:SER:N | 1:178:I:SER:CA | 1:178:I:SER:C | 1:179:I:GLN:N | 1 | 2.79 |
| (1,694) | 1:211:J:LEU:N | 1:211:J:LEU:CA | 1:211:J:LEU:C | 1:212:J:GLU:N | 6 | 2.78 |
| (1,459) | 1:188:I:THR:C | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 8 | 2.78 |
| (1,335) | 1:178:K:SER:N | 1:178:K:SER:CA | 1:178:K:SER:C | 1:179:K:GLN:N | 5 | 2.78 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 9 | 2.78 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 7 | 2.77 |
| (1,777) | 1:218:I:CYS:N | 1:218:I:CYS:CA | 1:218:I:CYS:C | 1:219:I:GLN:N | 1 | 2.77 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 7 | 2.77 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 2 | 2.76 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 8 | 2.76 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 1 | 2.76 |
| (1,941) | 1:232:K:ALA:C | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1 | 2.75 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 1 | 2.75 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 3 | 2.75 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 6 | 2.75 |
| (1,1110) | 1:241:L:THR:C | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1 | 2.74 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 10 | 2.74 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 1 | 2.74 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 8 | 2.74 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 9 | 2.74 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 6 | 2.74 |
| (1,628) | 1:203:J:LYS:C | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 3 | 2.73 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 9 | 2.73 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 3 | 2.73 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 6 | 2.73 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 2 | 2.73 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 6 | 2.72 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 10 | 2.71 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 10 | 2.7 |
| (1,785) | 1:218:K:CYS:C | 1:219:K:GLN:N | 1:219:K:GLN:CA | 1:219:K:GLN:C | 9 | 2.7 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 5 | 2.7 |
| (1,1007) | 1:238:K:VAL:N | 1:238:K:VAL:CA | 1:238:K:VAL:C | 1:239:K:THR:N | 8 | 2.69 |
| (1,490) | 1:191:J:VAL:N | 1:191:J:VAL:CA | 1:191:J:VAL:C | 1:192:J:GLN:N | 4 | 2.68 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 6 | 2.67 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 1 | 2.67 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 8 | 2.67 |
| (1,23) | 1:146:K:SER:C | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 6 | 2.66 |
| (1,885) | 1:228:I:ALA:N | 1:228:I:ALA:CA | 1:228:I:ALA:C | 1:229:I:ARG:N | 5 | 2.65 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 3 | 2.65 |
| (1,468) | 1:189:L:LEU:N | 1:189:L:LEU:CA | 1:189:L:LEU:C | 1:190:L:LEU:N | 7 | 2.65 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 6 | 2.65 |
| (1,224) | 1:167:H:ARG:N | 1:167:H:ARG:CA | 1:167:H:ARG:C | 1:168:H:PHE:N | 8 | 2.65 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 7 | 2.65 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 9 | 2.65 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 2 | 2.64 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 6 | 2.64 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 3 | 2.64 |
| (1,617) | 1:202:K:LEU:C | 1:203:K:LYS:N | 1:203:K:LYS:CA | 1:203:K:LYS:C | 9 | 2.63 |
| (1,616) | 1:202:J:LEU:C | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 1 | 2.63 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 8 | 2.63 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 9 | 2.62 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 7 | 2.62 |
| (1,297) | 1:173:I:ARG:N | 1:173:I:ARG:CA | 1:173:I:ARG:C | 1:174:I:ALA:N | 8 | 2.62 |
| (1,275) | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 1:172:K:LEU:N | 4 | 2.62 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 6 | 2.62 |
| (1,14) | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 1:147:H:PRO:N | 7 | 2.62 |
| (1,1092) | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 1:177:L:ALA:N | 9 | 2.61 |
| (1,1070) | 1:174:H:ALA:C | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 9 | 2.61 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 6 | 2.61 |
| (1,247) | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 1:170:G:LYS:N | 2 | 2.61 |
| (1,19) | 1:146:G:SER:C | 1:147:G:PRO:N | 1:147:G:PRO:CA | 1:147:G:PRO:C | 1 | 2.61 |
| (1,929) | 1:231:K:LEU:C | 1:232:K:ALA:N | 1:232:K:ALA:CA | 1:232:K:ALA:C | 9 | 2.6 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 9 | 2.6 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 7 | 2.6 |
| (1,1060) | 1:243:J:THR:C | 1:244:J:ILE:N | 1:244:J:ILE:CA | 1:244:J:ILE:C | 4 | 2.59 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 6 | 2.59 |
| (1,135) | 1:159:I:GLU:C | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 10 | 2.59 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 5 | 2.59 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 3 | 2.58 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 3 | 2.58 |
| (1,359) | 1:180:K:GLU:N | 1:180:K:GLU:CA | 1:180:K:GLU:C | 1:181:K:VAL:N | 9 | 2.58 |
| (1,228) | 1:167:L:ARG:N | 1:167:L:ARG:CA | 1:167:L:ARG:C | 1:168:L:PHE:N | 10 | 2.58 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 5 | 2.57 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 10 | 2.57 |
| (1,668) | 1:209:H:ALA:N | 1:209:H:ALA:CA | 1:209:H:ALA:C | 1:210:H:THR:N | 7 | 2.57 |
| (1,459) | 1:188:I:THR:C | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1 | 2.57 |
| (1,166) | 1:162:J:ARG:N | 1:162:J:ARG:CA | 1:162:J:ARG:C | 1:163:J:ASP:N | 2 | 2.57 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 5 | 2.57 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 3 | 2.57 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 6 | 2.56 |
| (1,144) | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 1:161:L:PHE:N | 3 | 2.56 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 4 | 2.56 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 5 | 2.55 |
| (1,987) | 1:236:I:SER:C | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 3 | 2.54 |
| (1,439) | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 1:188:G:THR:N | 4 | 2.54 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 9 | 2.54 |
| (1,248) | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 1:170:H:LYS:N | 9 | 2.54 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 9 | 2.53 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 4 | 2.53 |
| (1,375) | 1:181:I:VAL:C | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 10 | 2.53 |
| (1,465) | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1:190:I:LEU:N | 10 | 2.52 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 2 | 2.52 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 10 | 2.52 |
| (1,933) | 1:232:I:ALA:N | 1:232:I:ALA:CA | 1:232:I:ALA:C | 1:233:I:GLU:N | 4 | 2.51 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 9 | 2.51 |
| (1,791) | 1:219:K:GLN:N | 1:219:K:GLN:CA | 1:219:K:GLN:C | 1:220:K:GLY:N | 2 | 2.51 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 2 | 2.5 |
| (1,591) | 1:200:I:THR:C | 1:201:I:ILE:N | 1:201:I:ILE:CA | 1:201:I:ILE:C | 10 | 2.5 |
| (1,186) | 1:163:L:ASP:C | 1:164:L:TYR:N | 1:164:L:TYR:CA | 1:164:L:TYR:C | 8 | 2.5 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1 | 2.5 |
| (1,12) | 1:145:L:GLY:C | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 4 | 2.5 |
| (1,879) | 1:227:I:LYS:C | 1:228:I:ALA:N | 1:228:I:ALA:CA | 1:228:I:ALA:C | 8 | 2.49 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 7 | 2.49 |
| (1,695) | 1:211:K:LEU:N | 1:211:K:LEU:CA | 1:211:K:LEU:C | 1:212:K:GLU:N | 3 | 2.49 |
| (1,103) | 1:157:G:PRO:N | 1:157:G:PRO:CA | 1:157:G:PRO:C | 1:158:G:LYS:N | 8 | 2.49 |
| (1,249) | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 1:170:I:LYS:N | 7 | 2.48 |
| (1,1085) | 1:175:K:GLU:C | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1 | 2.47 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 3 | 2.46 |
| (1,486) | 1:190:L:LEU:C | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 3 | 2.46 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 9 | 2.46 |
| (1,171) | 1:162:I:ARG:C | 1:163:I:ASP:N | 1:163:I:ASP:CA | 1:163:I:ASP:C | 8 | 2.46 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 6 | 2.46 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 5 | 2.45 |
| (1,696) | 1:211:L:LEU:N | 1:211:L:LEU:CA | 1:211:L:LEU:C | 1:212:L:GLU:N | 7 | 2.45 |
| (1,456) | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 1:189:L:LEU:N | 1 | 2.44 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 4 | 2.43 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 5 | 2.43 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 2 | 2.43 |
| (1,657) | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 1:209:I:ALA:N | 6 | 2.42 |
| (1,170) | 1:162:H:ARG:C | 1:163:H:ASP:N | 1:163:H:ASP:CA | 1:163:H:ASP:C | 6 | 2.42 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 6 | 2.41 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 10 | 2.41 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 1 | 2.41 |
| (1,585) | 1:200:I:THR:N | 1:200:I:THR:CA | 1:200:I:THR:C | 1:201:I:ILE:N | 9 | 2.41 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 4 | 2.39 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 9 | 2.39 |
| (1,330) | 1:177:L:ALA:C | 1:178:L:SER:N | 1:178:L:SER:CA | 1:178:L:SER:C | 5 | 2.38 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 2 | 2.36 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 10 | 2.36 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 9 | 2.35 |
| (1,696) | 1:211:L:LEU:N | 1:211:L:LEU:CA | 1:211:L:LEU:C | 1:212:L:GLU:N | 4 | 2.35 |
| (1,414) | 1:184:L:TRP:C | 1:185:L:MET:N | 1:185:L:MET:CA | 1:185:L:MET:C | 2 | 2.34 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 3 | 2.34 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 2 | 2.33 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 4 | 2.33 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 1 | 2.32 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 2 | 2.31 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 3 | 2.31 |
| (1,180) | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1:164:L:TYR:N | 5 | 2.3 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 7 | 2.29 |
| (1,10) | 1:145:J:GLY:C | 1:146:J:SER:N | 1:146:J:SER:CA | 1:146:J:SER:C | 6 | 2.29 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 8 | 2.28 |
| (1,15) | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 1:147:I:PRO:N | 7 | 2.28 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 8 | 2.27 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 9 | 2.25 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 9 | 2.25 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 2 | 2.25 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 6 | 2.24 |
| (1,938) | 1:232:H:ALA:C | 1:233:H:GLU:N | 1:233:H:GLU:CA | 1:233:H:GLU:C | 7 | 2.23 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 9 | 2.23 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 10 | 2.22 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 7 | 2.22 |
| (1,575) | 1:199:K:LYS:N | 1:199:K:LYS:CA | 1:199:K:LYS:C | 1:200:K:THR:N | 5 | 2.22 |
| (1,306) | 1:173:L:ARG:C | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 10 | 2.22 |
| (1,284) | 1:172:H:LEU:N | 1:172:H:LEU:CA | 1:172:H:LEU:C | 1:173:H:ARG:N | 4 | 2.22 |
| (1,103) | 1:157:G:PRO:N | 1:157:G:PRO:CA | 1:157:G:PRO:C | 1:158:G:LYS:N | 1 | 2.22 |
| (1,1051) | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1:244:G:ILE:N | 2 | 2.21 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 8 | 2.2 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 1 | 2.19 |
| (1,622) | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 1:204:J:ALA:N | 6 | 2.19 |
| (1,485) | 1:190:K:LEU:C | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 6 | 2.19 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 9 | 2.18 |
| (1,968) | 1:235:H:MET:N | 1:235:H:MET:CA | 1:235:H:MET:C | 1:236:H:SER:N | 4 | 2.18 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 1 | 2.18 |
| (1,485) | 1:190:K:LEU:C | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 7 | 2.18 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 7 | 2.17 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 10 | 2.17 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 7 | 2.16 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 3 | 2.15 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1 | 2.15 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 5 | 2.15 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 9 | 2.15 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 4 | 2.15 |
| (1,141) | 1:160:I:PRO:N | 1:160:I:PRO:CA | 1:160:I:PRO:C | 1:161:I:PHE:N | 3 | 2.15 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 8 | 2.15 |
| (1,876) | 1:227:L:LYS:N | 1:227:L:LYS:CA | 1:227:L:LYS:C | 1:228:L:ALA:N | 5 | 2.14 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 7 | 2.14 |
| (1,468) | 1:189:L:LEU:N | 1:189:L:LEU:CA | 1:189:L:LEU:C | 1:190:L:LEU:N | 5 | 2.14 |
| (1,251) | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 1:170:K:LYS:N | 10 | 2.14 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 6 | 2.14 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 8 | 2.13 |
| (1,183) | 1:163:I:ASP:C | 1:164:I:TYR:N | 1:164:I:TYR:CA | 1:164:I:TYR:C | 8 | 2.13 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 5 | 2.12 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 1 | 2.12 |
| (1,8) | 1:145:H:GLY:C | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 1 | 2.12 |
| (1,537) | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 1:197:I:ASP:N | 3 | 2.11 |
| (1,468) | 1:189:L:LEU:N | 1:189:L:LEU:CA | 1:189:L:LEU:C | 1:190:L:LEU:N | 3 | 2.11 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 8 | 2.1 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 1 | 2.1 |
| (1,695) | 1:211:K:LEU:N | 1:211:K:LEU:CA | 1:211:K:LEU:C | 1:212:K:GLU:N | 4 | 2.1 |
| (1,417) | 1:185:I:MET:N | 1:185:I:MET:CA | 1:185:I:MET:C | 1:186:I:THR:N | 7 | 2.1 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 9 | 2.1 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 5 | 2.09 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 6 | 2.09 |
| (1,552) | 1:197:L:ASP:N | 1:197:L:ASP:CA | 1:197:L:ASP:C | 1:198:L:CYS:N | 4 | 2.09 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 3 | 2.09 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 7 | 2.09 |
| (1,11) | 1:145:K:GLY:C | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 6 | 2.09 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 7 | 2.08 |
| (1,745) | 1:215:G:MET:C | 1:216:G:THR:N | 1:216:G:THR:CA | 1:216:G:THR:C | 5 | 2.08 |
| (1,132) | 1:159:L:GLU:N | 1:159:L:GLU:CA | 1:159:L:GLU:C | 1:160:L:PRO:N | 1 | 2.08 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 10 | 2.08 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 9 | 2.08 |
| (1,954) | 1:233:L:GLU:C | 1:234:L:ALA:N | 1:234:L:ALA:CA | 1:234:L:ALA:C | 4 | 2.07 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 6 | 2.07 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 6 | 2.07 |
| (1,302) | 1:173:H:ARG:C | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1 | 2.06 |
| (1,7) | 1:145:G:GLY:C | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 4 | 2.06 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 10 | 2.05 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 3 | 2.05 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 2 | 2.05 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 7 | 2.05 |
| (1,405) | 1:184:I:TRP:N | 1:184:I:TRP:CA | 1:184:I:TRP:C | 1:185:I:MET:N | 4 | 2.05 |
| (1,248) | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 1:170:H:LYS:N | 1 | 2.05 |
| (1,21) | 1:146:I:SER:C | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 7 | 2.05 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 7 | 2.04 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 9 | 2.03 |
| (1,941) | 1:232:K:ALA:C | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 6 | 2.02 |
| (1,710) | 1:212:H:GLU:C | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 8 | 2.02 |
| (1,251) | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 1:170:K:LYS:N | 5 | 2.02 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 8 | 2.01 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 6 | 2.01 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 3 | 2.01 |
| (1,439) | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 1:188:G:THR:N | 5 | 2.01 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 7 | 2.01 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 8 | 2.01 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 10 | 2.01 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 4 | 2.01 |
| (1,1082) | 1:175:H:GLU:C | 1:176:H:GLN:N | 1:176:H:GLN:CA | 1:176:H:GLN:C | 1 | 2.0 |
| (1,930) | 1:231:L:LEU:C | 1:232:L:ALA:N | 1:232:L:ALA:CA | 1:232:L:ALA:C | 6 | 2.0 |
| (1,162) | 1:161:L:PHE:C | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 2 | 2.0 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 2 | 2.0 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 4 | 2.0 |
| (1,964) | 1:234:J:ALA:C | 1:235:J:MET:N | 1:235:J:MET:CA | 1:235:J:MET:C | 5 | 1.99 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 5 | 1.99 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 8 | 1.99 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 4 | 1.99 |
| (1,660) | 1:208:L:GLY:N | 1:208:L:GLY:CA | 1:208:L:GLY:C | 1:209:L:ALA:N | 5 | 1.99 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 6 | 1.99 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 2 | 1.99 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 5 | 1.98 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 4 | 1.98 |
| (1,4) | 1:144:J:GLY:C | 1:145:J:GLY:N | 1:145:J:GLY:CA | 1:145:J:GLY:C | 7 | 1.98 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 2 | 1.97 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 5 | 1.97 |
| (1,443) | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 1:188:K:THR:N | 6 | 1.97 |
| (1,241) | 1:168:G:PHE:C | 1:169:G:TYR:N | 1:169:G:TYR:CA | 1:169:G:TYR:C | 6 | 1.97 |
| (1,809) | 1:220:K:GLY:C | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 9 | 1.96 |
| (1,789) | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 1:220:I:GLY:N | 4 | 1.96 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 6 | 1.96 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 2 | 1.95 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 5 | 1.95 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 9 | 1.94 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 4 | 1.94 |
| (1,933) | 1:232:I:ALA:N | 1:232:I:ALA:CA | 1:232:I:ALA:C | 1:233:I:GLU:N | 5 | 1.93 |
| (1,465) | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1:190:I:LEU:N | 2 | 1.93 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 2 | 1.93 |
| (1,13) | 1:146:G:SER:N | 1:146:G:SER:CA | 1:146:G:SER:C | 1:147:G:PRO:N | 10 | 1.93 |
| (1,1101) | 1:207:I:PRO:N | 1:207:I:PRO:CA | 1:207:I:PRO:C | 1:208:I:GLY:N | 3 | 1.92 |
| (1,962) | 1:234:H:ALA:C | 1:235:H:MET:N | 1:235:H:MET:CA | 1:235:H:MET:C | 5 | 1.92 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 10 | 1.92 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 5 | 1.92 |
| (1,850) | 1:225:J:GLY:N | 1:225:J:GLY:CA | 1:225:J:GLY:C | 1:226:J:HIS:N | 9 | 1.91 |
| (1,552) | 1:197:L:ASP:N | 1:197:L:ASP:CA | 1:197:L:ASP:C | 1:198:L:CYS:N | 5 | 1.9 |
| (1,159) | 1:161:I:PHE:C | 1:162:I:ARG:N | 1:162:I:ARG:CA | 1:162:I:ARG:C | 1 | 1.9 |
| (1,1092) | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 1:177:L:ALA:N | 2 | 1.89 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 10 | 1.89 |
| (1,388) | 1:182:J:LYS:C | 1:183:J:ASN:N | 1:183:J:ASN:CA | 1:183:J:ASN:C | 6 | 1.89 |
| (1,285) | 1:172:I:LEU:N | 1:172:I:LEU:CA | 1:172:I:LEU:C | 1:173:I:ARG:N | 5 | 1.89 |
| (1,486) | 1:190:L:LEU:C | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 4 | 1.88 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 3 | 1.88 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 6 | 1.88 |
| (1,25) | 1:147:G:PRO:N | 1:147:G:PRO:CA | 1:147:G:PRO:C | 1:148:G:THR:N | 1 | 1.88 |
| (1,867) | 1:226:I:HIS:C | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 8 | 1.87 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 4 | 1.86 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 1 | 1.86 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 5 | 1.86 |
| (1,486) | 1:190:L:LEU:C | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 10 | 1.86 |
| (1,1081) | 1:175:G:GLU:C | 1:176:G:GLN:N | 1:176:G:GLN:CA | 1:176:G:GLN:C | 1 | 1.85 |
| (1,1081) | 1:175:G:GLU:C | 1:176:G:GLN:N | 1:176:G:GLN:CA | 1:176:G:GLN:C | 9 | 1.85 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 1 | 1.85 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 10 | 1.85 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 10 | 1.84 |
| (1,848) | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 1:226:H:HIS:N | 7 | 1.84 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 5 | 1.84 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 7 | 1.84 |
| (1,103) | 1:157:G:PRO:N | 1:157:G:PRO:CA | 1:157:G:PRO:C | 1:158:G:LYS:N | 9 | 1.84 |
| (1,166) | 1:162:J:ARG:N | 1:162:J:ARG:CA | 1:162:J:ARG:C | 1:163:J:ASP:N | 4 | 1.83 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 5 | 1.83 |
| (1,788) | 1:219:H:GLN:N | 1:219:H:GLN:CA | 1:219:H:GLN:C | 1:220:H:GLY:N | 2 | 1.82 |
| (1,1070) | 1:174:H:ALA:C | 1:175:H:GLU:N | 1:175:H:GLU:CA | 1:175:H:GLU:C | 2 | 1.81 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 8 | 1.81 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 2 | 1.81 |
| (1,110) | 1:157:H:PRO:C | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 5 | 1.81 |
| (1,8) | 1:145:H:GLY:C | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 6 | 1.81 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 8 | 1.8 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 3 | 1.8 |
| (1,1089) | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 1:177:I:ALA:N | 8 | 1.8 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 9 | 1.8 |
| (1,691) | 1:211:G:LEU:N | 1:211:G:LEU:CA | 1:211:G:LEU:C | 1:212:G:GLU:N | 3 | 1.8 |
| (1,585) | 1:200:I:THR:N | 1:200:I:THR:CA | 1:200:I:THR:C | 1:201:I:ILE:N | 8 | 1.79 |
| (1,180) | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1:164:L:TYR:N | 2 | 1.79 |
| (1,806) | 1:220:H:GLY:C | 1:221:H:VAL:N | 1:221:H:VAL:CA | 1:221:H:VAL:C | 6 | 1.78 |
| (1,726) | 1:213:L:GLU:C | 1:214:L:MET:N | 1:214:L:MET:CA | 1:214:L:MET:C | 1 | 1.78 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 9 | 1.78 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 9 | 1.78 |
| (1,1086) | 1:175:L:GLU:C | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 4 | 1.77 |
| (1,773) | 1:217:K:ALA:C | 1:218:K:CYS:N | 1:218:K:CYS:CA | 1:218:K:CYS:C | 6 | 1.77 |
| (1,651) | 1:207:I:PRO:C | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 10 | 1.77 |
| (1,465) | 1:189:I:LEU:N | 1:189:I:LEU:CA | 1:189:I:LEU:C | 1:190:I:LEU:N | 9 | 1.77 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 3 | 1.77 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 4 | 1.76 |
| (1,252) | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 1:170:L:LYS:N | 1 | 1.76 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 3 | 1.75 |
| (1,817) | 1:222:G:GLY:N | 1:222:G:GLY:CA | 1:222:G:GLY:C | 1:223:G:GLY:N | 9 | 1.75 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 6 | 1.75 |
| (1,334) | 1:178:J:SER:N | 1:178:J:SER:CA | 1:178:J:SER:C | 1:179:J:GLN:N | 7 | 1.75 |
| (1,846) | 1:224:L:PRO:C | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 2 | 1.74 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 3 | 1.74 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 2 | 1.74 |
| (1,272) | 1:171:H:THR:N | 1:171:H:THR:CA | 1:171:H:THR:C | 1:172:H:LEU:N | 9 | 1.73 |
| (1,12) | 1:145:L:GLY:C | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 5 | 1.73 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 3 | 1.72 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 7 | 1.72 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 2 | 1.72 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 7 | 1.72 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 5 | 1.71 |
| (1,228) | 1:167:L:ARG:N | 1:167:L:ARG:CA | 1:167:L:ARG:C | 1:168:L:PHE:N | 2 | 1.71 |
| (1,152) | 1:161:H:PHE:N | 1:161:H:PHE:CA | 1:161:H:PHE:C | 1:162:H:ARG:N | 7 | 1.71 |
| (1,807) | 1:220:I:GLY:C | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 7 | 1.7 |
| (1,399) | 1:183:I:ASN:C | 1:184:I:TRP:N | 1:184:I:TRP:CA | 1:184:I:TRP:C | 6 | 1.7 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 4 | 1.69 |
| (1,954) | 1:233:L:GLU:C | 1:234:L:ALA:N | 1:234:L:ALA:CA | 1:234:L:ALA:C | 10 | 1.68 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 3 | 1.68 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 9 | 1.68 |
| (1,452) | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1:189:H:LEU:N | 7 | 1.67 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 5 | 1.66 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 7 | 1.66 |
| (1,233) | 1:167:K:ARG:C | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 6 | 1.66 |
| (1,418) | 1:185:J:MET:N | 1:185:J:MET:CA | 1:185:J:MET:C | 1:186:J:THR:N | 6 | 1.65 |
| (1,418) | 1:185:J:MET:N | 1:185:J:MET:CA | 1:185:J:MET:C | 1:186:J:THR:N | 7 | 1.65 |
| (1,244) | 1:168:J:PHE:C | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 9 | 1.65 |
| (1,1061) | 1:243:K:THR:C | 1:244:K:ILE:N | 1:244:K:ILE:CA | 1:244:K:ILE:C | 4 | 1.64 |
| (1,996) | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 1:238:L:VAL:N | 3 | 1.64 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 6 | 1.64 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1 | 1.64 |
| (1,792) | 1:219:L:GLN:N | 1:219:L:GLN:CA | 1:219:L:GLN:C | 1:220:L:GLY:N | 5 | 1.64 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 6 | 1.64 |
| (1,106) | 1:157:J:PRO:N | 1:157:J:PRO:CA | 1:157:J:PRO:C | 1:158:J:LYS:N | 2 | 1.64 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 10 | 1.64 |
| (1,1051) | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1:244:G:ILE:N | 5 | 1.63 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 6 | 1.63 |
| (1,552) | 1:197:L:ASP:N | 1:197:L:ASP:CA | 1:197:L:ASP:C | 1:198:L:CYS:N | 10 | 1.63 |
| (1,492) | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 1:192:L:GLN:N | 3 | 1.63 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 10 | 1.63 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 5 | 1.63 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 4 | 1.62 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 9 | 1.62 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 8 | 1.62 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 2 | 1.61 |
| (1,248) | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 1:170:H:LYS:N | 2 | 1.61 |
| (1,131) | 1:159:K:GLU:N | 1:159:K:GLU:CA | 1:159:K:GLU:C | 1:160:K:PRO:N | 10 | 1.61 |
| (1,17) | 1:146:K:SER:N | 1:146:K:SER:CA | 1:146:K:SER:C | 1:147:K:PRO:N | 5 | 1.61 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 6 | 1.6 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 2 | 1.6 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 5 | 1.6 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 4 | 1.6 |
| (1,657) | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 1:209:I:ALA:N | 2 | 1.58 |
| (1,657) | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 1:209:I:ALA:N | 8 | 1.58 |
| (1,885) | 1:228:I:ALA:N | 1:228:I:ALA:CA | 1:228:I:ALA:C | 1:229:I:ARG:N | 6 | 1.57 |
| (1,818) | 1:222:H:GLY:N | 1:222:H:GLY:CA | 1:222:H:GLY:C | 1:223:H:GLY:N | 8 | 1.57 |
| (1,488) | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1:192:H:GLN:N | 6 | 1.57 |
| (1,439) | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 1:188:G:THR:N | 1 | 1.57 |
| (1,414) | 1:184:L:TRP:C | 1:185:L:MET:N | 1:185:L:MET:CA | 1:185:L:MET:C | 1 | 1.57 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 8 | 1.57 |
| (1,866) | 1:226:H:HIS:C | 1:227:H:LYS:N | 1:227:H:LYS:CA | 1:227:H:LYS:C | 6 | 1.56 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 10 | 1.56 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 3 | 1.56 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 7 | 1.56 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 8 | 1.56 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 2 | 1.56 |
| (1,1086) | 1:175:L:GLU:C | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 3 | 1.55 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 9 | 1.55 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 5 | 1.55 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 8 | 1.55 |
| (1,636) | 1:204:L:ALA:N | 1:204:L:ALA:CA | 1:204:L:ALA:C | 1:205:L:LEU:N | 9 | 1.55 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 5 | 1.55 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,303) | 1:173:I:ARG:C | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 10 | 1.55 |
| (1,297) | 1:173:I:ARG:N | 1:173:I:ARG:CA | 1:173:I:ARG:C | 1:174:I:ALA:N | 2 | 1.55 |
| (1,139) | 1:160:G:PRO:N | 1:160:G:PRO:CA | 1:160:G:PRO:C | 1:161:G:PHE:N | 6 | 1.55 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 7 | 1.55 |
| (1,866) | 1:226:H:HIS:C | 1:227:H:LYS:N | 1:227:H:LYS:CA | 1:227:H:LYS:C | 5 | 1.54 |
| (1,821) | 1:222:K:GLY:N | 1:222:K:GLY:CA | 1:222:K:GLY:C | 1:223:K:GLY:N | 4 | 1.54 |
| (1,300) | 1:173:L:ARG:N | 1:173:L:ARG:CA | 1:173:L:ARG:C | 1:174:L:ALA:N | 5 | 1.54 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 3 | 1.53 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 2 | 1.53 |
| (1,375) | 1:181:I:VAL:C | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1 | 1.52 |
| (1,99) | 1:156:I:GLY:C | 1:157:I:PRO:N | 1:157:I:PRO:CA | 1:157:I:PRO:C | 10 | 1.52 |
| (1,622) | 1:203:J:LYS:N | 1:203:J:LYS:CA | 1:203:J:LYS:C | 1:204:J:ALA:N | 9 | 1.51 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 3 | 1.51 |
| (1,306) | 1:173:L:ARG:C | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 5 | 1.51 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 1 | 1.51 |
| (1,18) | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 1:147:L:PRO:N | 10 | 1.51 |
| (1,695) | 1:211:K:LEU:N | 1:211:K:LEU:CA | 1:211:K:LEU:C | 1:212:K:GLU:N | 5 | 1.5 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 5 | 1.5 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 10 | 1.49 |
| (1,452) | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1:189:H:LEU:N | 8 | 1.49 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 9 | 1.49 |
| (1,1085) | 1:175:K:GLU:C | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 8 | 1.48 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 6 | 1.48 |
| (1,655) | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 1:209:G:ALA:N | 4 | 1.47 |
| (1,402) | 1:183:L:ASN:C | 1:184:L:TRP:N | 1:184:L:TRP:CA | 1:184:L:TRP:C | 5 | 1.47 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 3 | 1.47 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 2 | 1.47 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 9 | 1.47 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 6 | 1.45 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 4 | 1.45 |
| (1,783) | 1:218:I:CYS:C | 1:219:I:GLN:N | 1:219:I:GLN:CA | 1:219:I:GLN:C | 5 | 1.45 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 1 | 1.45 |
| (1,650) | 1:207:H:PRO:C | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 6 | 1.45 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 4 | 1.45 |
| (1,15) | 1:146:I:SER:N | 1:146:I:SER:CA | 1:146:I:SER:C | 1:147:I:PRO:N | 10 | 1.45 |
| (1,591) | 1:200:I:THR:C | 1:201:I:ILE:N | 1:201:I:ILE:CA | 1:201:I:ILE:C | 8 | 1.44 |
| (1,238) | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 1:169:J:TYR:N | 9 | 1.44 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 10 | 1.44 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 4 | 1.43 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 5 | 1.43 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 8 | 1.43 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 10 | 1.42 |
| (1,384) | 1:182:L:LYS:N | 1:182:L:LYS:CA | 1:182:L:LYS:C | 1:183:L:ASN:N | 5 | 1.42 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 7 | 1.42 |
| (1,874) | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 1:228:J:ALA:N | 6 | 1.41 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 10 | 1.41 |
| (1,549) | 1:197:I:ASP:N | 1:197:I:ASP:CA | 1:197:I:ASP:C | 1:198:I:CYS:N | 5 | 1.41 |
| (1,440) | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 1:188:H:THR:N | 8 | 1.41 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 8 | 1.4 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 6 | 1.4 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 4 | 1.4 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 3 | 1.4 |
| (1,165) | 1:162:I:ARG:N | 1:162:I:ARG:CA | 1:162:I:ARG:C | 1:163:I:ASP:N | 3 | 1.4 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 8 | 1.39 |
| (1,456) | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 1:189:L:LEU:N | 3 | 1.39 |
| (1,171) | 1:162:I:ARG:C | 1:163:I:ASP:N | 1:163:I:ASP:CA | 1:163:I:ASP:C | 3 | 1.39 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 9 | 1.38 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 7 | 1.37 |
| (1,1109) | 1:241:K:THR:C | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 4 | 1.36 |
| (1,732) | 1:214:L:MET:N | 1:214:L:MET:CA | 1:214:L:MET:C | 1:215:L:MET:N | 8 | 1.36 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 5 | 1.36 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 1 | 1.36 |
| (1,481) | 1:190:G:LEU:C | 1:191:G:VAL:N | 1:191:G:VAL:CA | 1:191:G:VAL:C | 1 | 1.36 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 4 | 1.36 |
| (1,103) | 1:157:G:PRO:N | 1:157:G:PRO:CA | 1:157:G:PRO:C | 1:158:G:LYS:N | 7 | 1.36 |
| (1,1) | 1:144:G:GLY:C | 1:145:G:GLY:N | 1:145:G:GLY:CA | 1:145:G:GLY:C | 9 | 1.36 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 4 | 1.34 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 2 | 1.34 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 6 | 1.34 |
| (1,180) | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 1:164:L:TYR:N | 9 | 1.34 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 10 | 1.34 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 6 | 1.33 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 3 | 1.33 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 3 | 1.33 |
| (1,628) | 1:203:J:LYS:C | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 7 | 1.33 |
| (1,432) | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 1:187:L:GLU:N | 7 | 1.33 |
| (1,153) | 1:161:I:PHE:N | 1:161:I:PHE:CA | 1:161:I:PHE:C | 1:162:I:ARG:N | 10 | 1.33 |
| (1,18) | 1:146:L:SER:N | 1:146:L:SER:CA | 1:146:L:SER:C | 1:147:L:PRO:N | 5 | 1.33 |
| (1,791) | 1:219:K:GLN:N | 1:219:K:GLN:CA | 1:219:K:GLN:C | 1:220:K:GLY:N | 9 | 1.32 |
| (1,745) | 1:215:G:MET:C | 1:216:G:THR:N | 1:216:G:THR:CA | 1:216:G:THR:C | 4 | 1.32 |
| (1,718) | 1:213:J:GLU:N | 1:213:J:GLU:CA | 1:213:J:GLU:C | 1:214:J:MET:N | 8 | 1.32 |
| (1,428) | 1:186:H:THR:N | 1:186:H:THR:CA | 1:186:H:THR:C | 1:187:H:GLU:N | 3 | 1.32 |
| (1,234) | 1:167:L:ARG:C | 1:168:L:PHE:N | 1:168:L:PHE:CA | 1:168:L:PHE:C | 8 | 1.32 |
| (1,2) | 1:144:H:GLY:C | 1:145:H:GLY:N | 1:145:H:GLY:CA | 1:145:H:GLY:C | 8 | 1.32 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 2 | 1.31 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 1 | 1.3 |
| (1,269) | 1:170:K:LYS:C | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 5 | 1.3 |
| (1,108) | 1:157:L:PRO:N | 1:157:L:PRO:CA | 1:157:L:PRO:C | 1:158:L:LYS:N | 1 | 1.3 |
| (1,1091) | 1:176:K:GLN:N | 1:176:K:GLN:CA | 1:176:K:GLN:C | 1:177:K:ALA:N | 8 | 1.29 |
| (1,928) | 1:231:J:LEU:C | 1:232:J:ALA:N | 1:232:J:ALA:CA | 1:232:J:ALA:C | 10 | 1.29 |
| (1,842) | 1:224:H:PRO:C | 1:225:H:GLY:N | 1:225:H:GLY:CA | 1:225:H:GLY:C | 7 | 1.29 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 2 | 1.29 |
| (1,591) | 1:200:I:THR:C | 1:201:I:ILE:N | 1:201:I:ILE:CA | 1:201:I:ILE:C | 5 | 1.29 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 2 | 1.29 |
| (1,246) | 1:168:L:PHE:C | 1:169:L:TYR:N | 1:169:L:TYR:CA | 1:169:L:TYR:C | 10 | 1.29 |
| (1,1089) | 1:176:I:GLN:N | 1:176:I:GLN:CA | 1:176:I:GLN:C | 1:177:I:ALA:N | 9 | 1.28 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1 | 1.28 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 5 | 1.28 |
| (1,739) | 1:215:G:MET:N | 1:215:G:MET:CA | 1:215:G:MET:C | 1:216:G:THR:N | 10 | 1.28 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 10 | 1.28 |
| (1,399) | 1:183:I:ASN:C | 1:184:I:TRP:N | 1:184:I:TRP:CA | 1:184:I:TRP:C | 3 | 1.28 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 1 | 1.28 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,138) | 1:159:L:GLU:C | 1:160:L:PRO:N | 1:160:L:PRO:CA | 1:160:L:PRO:C | 2 | 1.28 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 6 | 1.28 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 10 | 1.28 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 8 | 1.27 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 10 | 1.26 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1 | 1.26 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 5 | 1.26 |
| (1,977) | 1:235:K:MET:C | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 7 | 1.25 |
| (1,852) | 1:225:L:GLY:N | 1:225:L:GLY:CA | 1:225:L:GLY:C | 1:226:L:HIS:N | 9 | 1.25 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 7 | 1.25 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 5 | 1.24 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 5 | 1.24 |
| (1,162) | 1:161:L:PHE:C | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1 | 1.24 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 9 | 1.23 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 4 | 1.23 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 9 | 1.22 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 10 | 1.22 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 7 | 1.22 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 7 | 1.21 |
| (1,744) | 1:215:L:MET:N | 1:215:L:MET:CA | 1:215:L:MET:C | 1:216:L:THR:N | 7 | 1.21 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 10 | 1.2 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 7 | 1.2 |
| (1,386) | 1:182:H:LYS:C | 1:183:H:ASN:N | 1:183:H:ASN:CA | 1:183:H:ASN:C | 2 | 1.2 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 4 | 1.2 |
| (1,656) | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 1:209:H:ALA:N | 4 | 1.18 |
| (1,407) | 1:184:K:TRP:N | 1:184:K:TRP:CA | 1:184:K:TRP:C | 1:185:K:MET:N | 9 | 1.18 |
| (1,473) | 1:189:K:LEU:C | 1:190:K:LEU:N | 1:190:K:LEU:CA | 1:190:K:LEU:C | 8 | 1.17 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 4 | 1.17 |
| (1,347) | 1:179:K:GLN:N | 1:179:K:GLN:CA | 1:179:K:GLN:C | 1:180:K:GLU:N | 5 | 1.17 |
| (1,190) | 1:164:J:TYR:N | 1:164:J:TYR:CA | 1:164:J:TYR:C | 1:165:J:VAL:N | 10 | 1.17 |
| (1,908) | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 1:231:H:LEU:N | 7 | 1.16 |
| (1,649) | 1:207:G:PRO:C | 1:208:G:GLY:N | 1:208:G:GLY:CA | 1:208:G:GLY:C | 10 | 1.16 |
| (1,562) | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 1:199:J:LYS:N | 4 | 1.16 |
| (1,346) | 1:179:J:GLN:N | 1:179:J:GLN:CA | 1:179:J:GLN:C | 1:180:J:GLU:N | 7 | 1.16 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 3 | 1.16 |
| (1,1000) | 1:237:J:GLN:C | 1:238:J:VAL:N | 1:238:J:VAL:CA | 1:238:J:VAL:C | 5 | 1.15 |
| (1,996) | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 1:238:L:VAL:N | 4 | 1.15 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 1 | 1.15 |
| (1,1105) | 1:241:G:THR:C | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1 | 1.14 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 6 | 1.14 |
| (1,731) | 1:214:K:MET:N | 1:214:K:MET:CA | 1:214:K:MET:C | 1:215:K:MET:N | 10 | 1.14 |
| (1,466) | 1:189:J:LEU:N | 1:189:J:LEU:CA | 1:189:J:LEU:C | 1:190:J:LEU:N | 5 | 1.14 |
| (1,458) | 1:188:H:THR:C | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 5 | 1.14 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 4 | 1.14 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 3 | 1.14 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 4 | 1.14 |
| (1,1081) | 1:175:G:GLU:C | 1:176:G:GLN:N | 1:176:G:GLN:CA | 1:176:G:GLN:C | 7 | 1.13 |
| (1,631) | 1:204:G:ALA:N | 1:204:G:ALA:CA | 1:204:G:ALA:C | 1:205:G:LEU:N | 9 | 1.13 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 9 | 1.13 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 3 | 1.13 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 3 | 1.13 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,130) | 1:159:J:GLU:N | 1:159:J:GLU:CA | 1:159:J:GLU:C | 1:160:J:PRO:N | 2 | 1.12 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 10 | 1.12 |
| (1,833) | 1:223:K:GLY:C | 1:224:K:PRO:N | 1:224:K:PRO:CA | 1:224:K:PRO:C | 9 | 1.11 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 9 | 1.11 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 3 | 1.11 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 9 | 1.1 |
| (1,457) | 1:188:G:THR:C | 1:189:G:LEU:N | 1:189:G:LEU:CA | 1:189:G:LEU:C | 3 | 1.1 |
| (1,770) | 1:217:H:ALA:C | 1:218:H:CYS:N | 1:218:H:CYS:CA | 1:218:H:CYS:C | 10 | 1.09 |
| (1,695) | 1:211:K:LEU:N | 1:211:K:LEU:CA | 1:211:K:LEU:C | 1:212:K:GLU:N | 1 | 1.09 |
| (1,240) | 1:168:L:PHE:N | 1:168:L:PHE:CA | 1:168:L:PHE:C | 1:169:L:TYR:N | 7 | 1.09 |
| (1,553) | 1:197:G:ASP:C | 1:198:G:CYS:N | 1:198:G:CYS:CA | 1:198:G:CYS:C | 2 | 1.08 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 6 | 1.08 |
| (1,276) | 1:171:L:THR:N | 1:171:L:THR:CA | 1:171:L:THR:C | 1:172:L:LEU:N | 10 | 1.08 |
| (1,1108) | 1:241:J:THR:C | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 9 | 1.07 |
| (1,1086) | 1:175:L:GLU:C | 1:176:L:GLN:N | 1:176:L:GLN:CA | 1:176:L:GLN:C | 6 | 1.07 |
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 1 | 1.07 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 2 | 1.07 |
| (1,425) | 1:185:K:MET:C | 1:186:K:THR:N | 1:186:K:THR:CA | 1:186:K:THR:C | 2 | 1.07 |
| (1,1071) | 1:174:I:ALA:C | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1 | 1.06 |
| (1,650) | 1:207:H:PRO:C | 1:208:H:GLY:N | 1:208:H:GLY:CA | 1:208:H:GLY:C | 3 | 1.06 |
| (1,995) | 1:237:K:GLN:N | 1:237:K:GLN:CA | 1:237:K:GLN:C | 1:238:K:VAL:N | 3 | 1.05 |
| (1,770) | 1:217:H:ALA:C | 1:218:H:CYS:N | 1:218:H:CYS:CA | 1:218:H:CYS:C | 5 | 1.05 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 7 | 1.05 |
| (1,167) | 1:162:K:ARG:N | 1:162:K:ARG:CA | 1:162:K:ARG:C | 1:163:K:ASP:N | 8 | 1.05 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 9 | 1.04 |
| (1,464) | 1:189:H:LEU:N | 1:189:H:LEU:CA | 1:189:H:LEU:C | 1:190:H:LEU:N | 4 | 1.04 |
| (1,356) | 1:180:H:GLU:N | 1:180:H:GLU:CA | 1:180:H:GLU:C | 1:181:H:VAL:N | 9 | 1.04 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 6 | 1.03 |
| (1,812) | 1:221:H:VAL:N | 1:221:H:VAL:CA | 1:221:H:VAL:C | 1:222:H:GLY:N | 8 | 1.03 |
| (1,938) | 1:232:H:ALA:C | 1:233:H:GLU:N | 1:233:H:GLU:CA | 1:233:H:GLU:C | 4 | 1.02 |
| (1,853) | 1:225:G:GLY:C | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 4 | 1.02 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 3 | 1.02 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 5 | 1.02 |
| (1,554) | 1:197:H:ASP:C | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 7 | 1.02 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 8 | 1.02 |
| (1,142) | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 1:161:J:PHE:N | 10 | 1.02 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 10 | 1.01 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 10 | 1.01 |
| (1,985) | 1:236:G:SER:C | 1:237:G:GLN:N | 1:237:G:GLN:CA | 1:237:G:GLN:C | 6 | 1.0 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 9 | 1.0 |