



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:10 pm GMT

PDB ID : 2MLR
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Alpha-face
Authors : Koppiseti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.
Deposited on : 2014-03-04

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | trunk28760 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

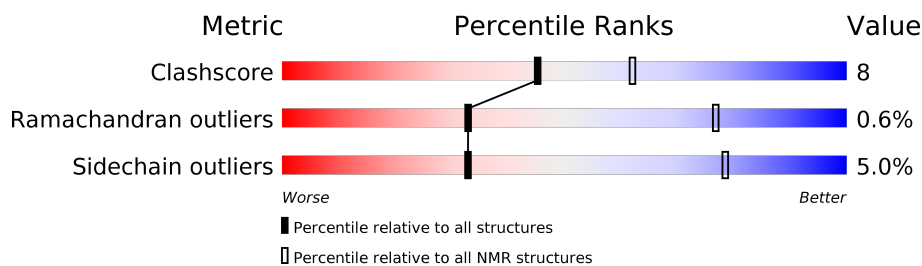
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 | 125131 | 11601 |
| Ramachandran outliers | 121729 | 10391 |
| Sidechain outliers | 121581 | 10367 |

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 | A | 164 | |

2 Ensemble composition and analysis

This entry contains 14 models. Model 3 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 | A:100-A:187, A:192-A:263 (160) | 0.38 | 3 |

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 4 clusters. No single-model clusters were found.

| Cluster number | Models |
|----------------|------------------|
| 1 | 8, 9, 10, 11, 13 |
| 2 | 1, 2, 3, 4, 5 |
| 3 | 6, 7 |
| 4 | 12, 14 |

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1 | A | 164 | Total | C | H | N | O | S | 0 |
| | | | 2508 | 824 | 1221 | 225 | 234 | 4 | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 219 | ALA | GLU | ENGINEERED MUTATION | UNP P39900 |

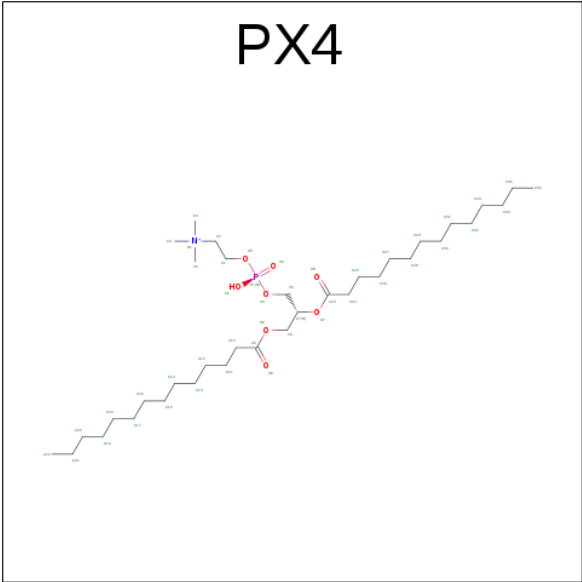
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 2 | A | 2 | Total | Zn |
| | | | 2 | 2 |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 3 | A | 3 | Total | Ca |
| | | | 3 | 3 |

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |

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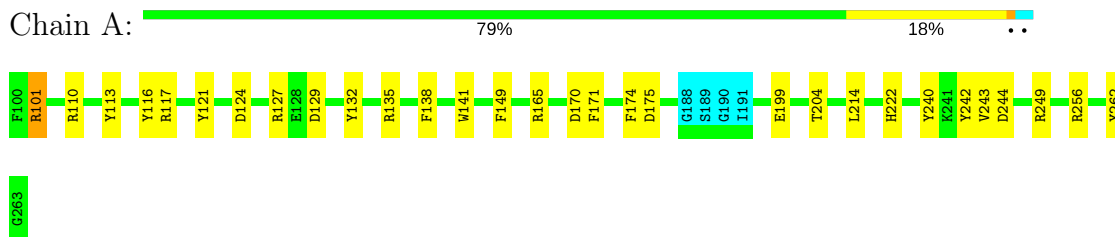
| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |
| 4 | A | 1 | Total | C | N | O | P |
| | | | 46 | 36 | 1 | 8 | 1 |

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Macrophage metalloelastase

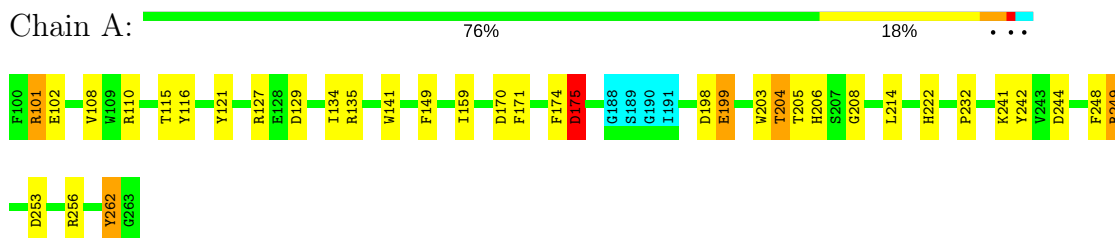


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

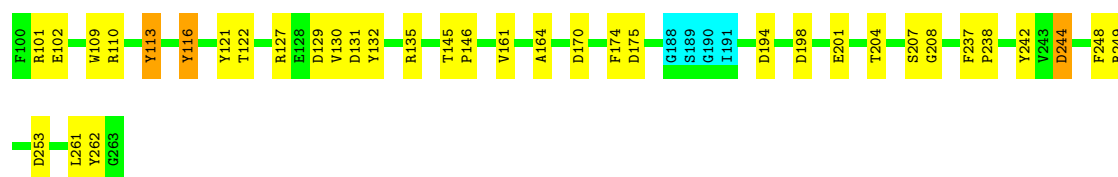
- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase





4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Macrophage metalloelastase

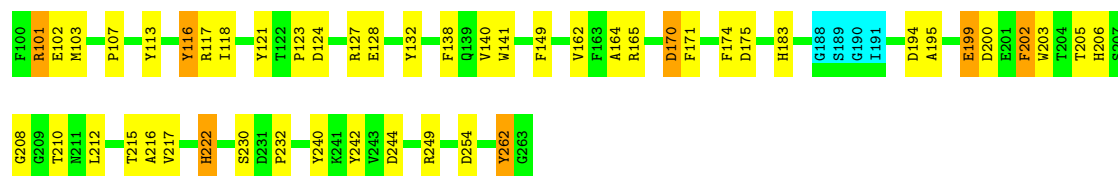
Chain A: 79% 16% ..



4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase

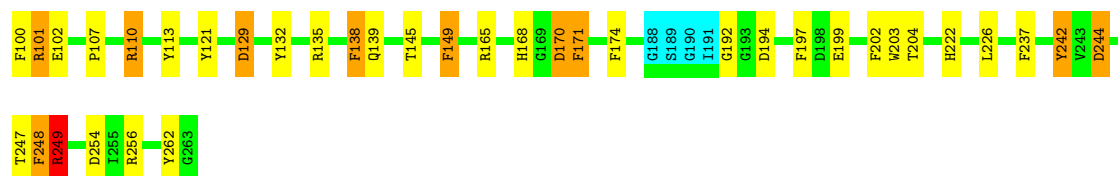
Chain A: 68% 26% ..



4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase

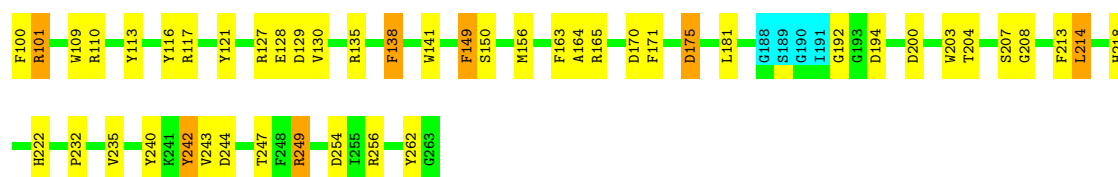
Chain A: 75% 16% 6% ..



4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase

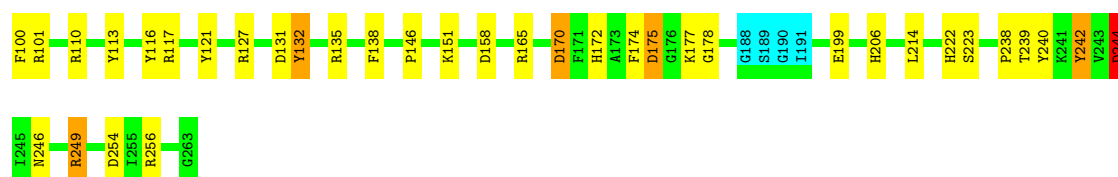
Chain A: 69% 24% ..



4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase

Chain A: 76% 18% ...



4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase

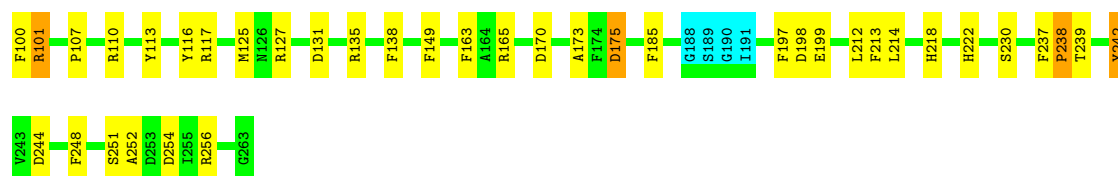
Chain A: 74% 21% ..



4.2.9 Score per residue for model 9

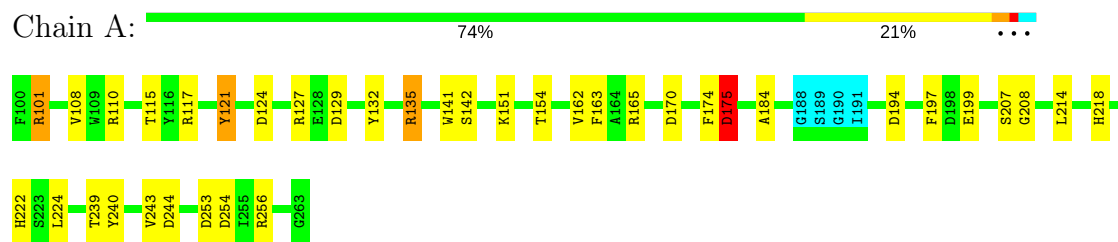
- Molecule 1: Macrophage metalloelastase

Chain A: 74% 21% ..



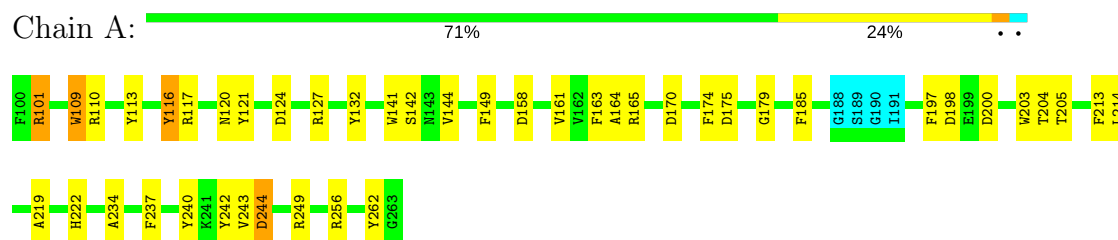
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



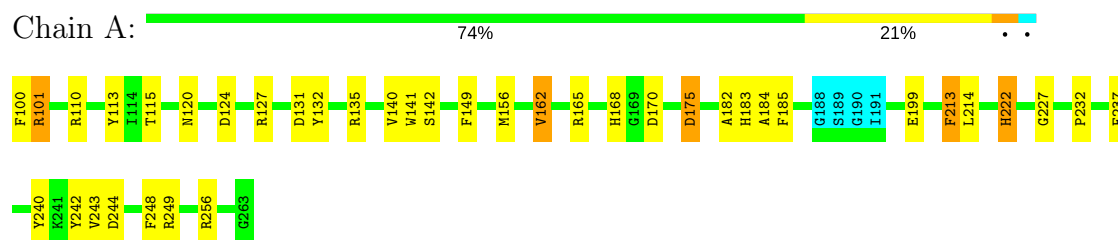
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



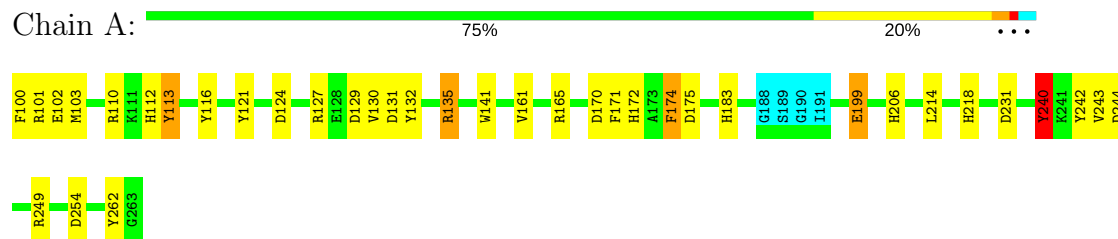
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



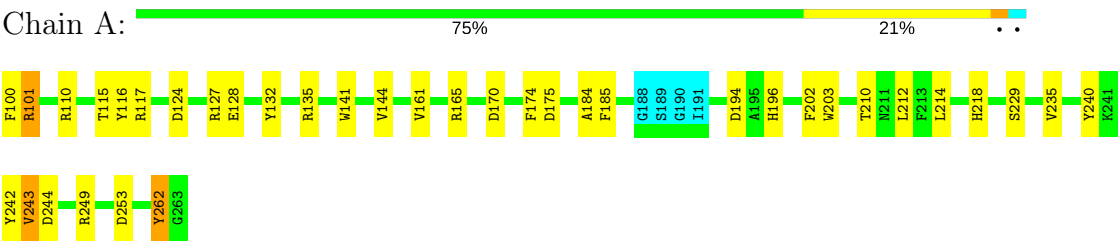
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



4.2.14 Score per residue for model 14

● Molecule 1: Macrophage metalloelastase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 14 calculated structures, 14 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 |
|---------------|----------------|---------|
| GROMACS | refinement | |

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) | 2mlr_cs.str |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1762 |
| Number of shifts mapped to atoms | 1762 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 83% |

No validations of the models with respect to experimental NMR restraints is performed at this time.

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: ZN, CA, PX4

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 | A | 0.58±0.01 | 0±0/1305 (0.0±0.0%) | 2.04±0.06 | 42±6/1768 (2.4±0.4%) |
| All | All | 0.58 | 0/18270 (0.0%) | 2.05 | 584/24752 (2.4%) |

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 | A | 0.0±0.0 | 5.1±1.9 |
| All | All | 0 | 71 |

There are no bond-length outliers.

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 | A | 249 | ARG | NE-CZ-NH1 | 19.17 | 129.88 | 120.30 | 11 | 6 |
| 1 | A | 127 | ARG | NE-CZ-NH2 | -18.79 | 110.91 | 120.30 | 11 | 8 |
| 1 | A | 165 | ARG | NE-CZ-NH2 | -18.12 | 111.24 | 120.30 | 5 | 4 |
| 1 | A | 262 | TYR | CB-CG-CD2 | -17.25 | 110.65 | 121.00 | 14 | 4 |
| 1 | A | 240 | TYR | CB-CG-CD1 | -14.90 | 112.06 | 121.00 | 6 | 5 |
| 1 | A | 110 | ARG | NE-CZ-NH2 | -14.86 | 112.87 | 120.30 | 13 | 6 |
| 1 | A | 174 | PHE | CB-CG-CD1 | -14.06 | 110.95 | 120.80 | 8 | 6 |
| 1 | A | 113 | TYR | CB-CG-CD2 | -14.02 | 112.59 | 121.00 | 2 | 3 |
| 1 | A | 165 | ARG | NE-CZ-NH1 | 14.01 | 127.31 | 120.30 | 3 | 8 |
| 1 | A | 101 | ARG | NE-CZ-NH2 | -13.97 | 113.31 | 120.30 | 12 | 7 |
| 1 | A | 117 | ARG | NE-CZ-NH2 | -12.67 | 113.97 | 120.30 | 3 | 5 |
| 1 | A | 135 | ARG | NE-CZ-NH2 | -12.59 | 114.00 | 120.30 | 7 | 9 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 256 | ARG | NE-CZ-NH2 | -12.30 | 114.15 | 120.30 | 11 | 5 |
| 1 | A | 101 | ARG | NE-CZ-NH1 | 12.20 | 126.40 | 120.30 | 4 | 6 |
| 1 | A | 127 | ARG | NE-CZ-NH1 | 12.07 | 126.33 | 120.30 | 9 | 6 |
| 1 | A | 110 | ARG | NE-CZ-NH1 | -11.95 | 114.33 | 120.30 | 12 | 7 |
| 1 | A | 135 | ARG | NE-CZ-NH1 | 11.80 | 126.20 | 120.30 | 13 | 6 |
| 1 | A | 248 | PHE | CB-CG-CD1 | -11.62 | 112.66 | 120.80 | 1 | 3 |
| 1 | A | 100 | PHE | CB-CG-CD2 | 11.57 | 128.90 | 120.80 | 9 | 5 |
| 1 | A | 254 | ASP | CB-CG-OD2 | -11.53 | 107.92 | 118.30 | 10 | 6 |
| 1 | A | 117 | ARG | NE-CZ-NH1 | 10.99 | 125.80 | 120.30 | 3 | 3 |
| 1 | A | 132 | TYR | CB-CG-CD2 | -10.80 | 114.52 | 121.00 | 10 | 4 |
| 1 | A | 256 | ARG | NE-CZ-NH1 | 10.79 | 125.69 | 120.30 | 11 | 4 |
| 1 | A | 113 | TYR | CG-CD1-CE1 | -10.52 | 112.89 | 121.30 | 9 | 2 |
| 1 | A | 113 | TYR | CD1-CE1-CZ | -10.37 | 110.46 | 119.80 | 5 | 2 |
| 1 | A | 213 | PHE | CB-CG-CD1 | -10.26 | 113.62 | 120.80 | 6 | 3 |
| 1 | A | 249 | ARG | NE-CZ-NH2 | -10.21 | 115.19 | 120.30 | 11 | 6 |
| 1 | A | 163 | PHE | CB-CG-CD2 | 10.18 | 127.93 | 120.80 | 11 | 2 |
| 1 | A | 175 | ASP | CB-CG-OD1 | 10.08 | 127.37 | 118.30 | 12 | 8 |
| 1 | A | 113 | TYR | CB-CG-CD1 | -10.07 | 114.96 | 121.00 | 9 | 7 |
| 1 | A | 199 | GLU | OE1-CD-OE2 | -10.05 | 111.24 | 123.30 | 4 | 2 |
| 1 | A | 175 | ASP | CB-CG-OD2 | 10.01 | 127.31 | 118.30 | 11 | 4 |
| 1 | A | 170 | ASP | CB-CG-OD1 | 9.97 | 127.27 | 118.30 | 14 | 11 |
| 1 | A | 124 | ASP | CB-CG-OD1 | 9.87 | 127.18 | 118.30 | 10 | 6 |
| 1 | A | 185 | PHE | CB-CG-CD2 | -9.86 | 113.90 | 120.80 | 14 | 3 |
| 1 | A | 194 | ASP | CB-CG-OD1 | 9.75 | 127.08 | 118.30 | 2 | 6 |
| 1 | A | 113 | TYR | CG-CD2-CE2 | -9.56 | 113.66 | 121.30 | 13 | 2 |
| 1 | A | 156 | MET | CG-SD-CE | 9.52 | 115.43 | 100.20 | 6 | 1 |
| 1 | A | 116 | TYR | CB-CG-CD1 | -9.48 | 115.31 | 121.00 | 11 | 4 |
| 1 | A | 262 | TYR | CB-CG-CD1 | 9.38 | 126.63 | 121.00 | 14 | 4 |
| 1 | A | 121 | TYR | CB-CG-CD2 | 9.29 | 126.57 | 121.00 | 10 | 5 |
| 1 | A | 100 | PHE | CB-CG-CD1 | -9.26 | 114.32 | 120.80 | 9 | 3 |
| 1 | A | 116 | TYR | CG-CD1-CE1 | -9.17 | 113.97 | 121.30 | 4 | 1 |
| 1 | A | 170 | ASP | OD1-CG-OD2 | -9.04 | 106.13 | 123.30 | 8 | 14 |
| 1 | A | 242 | TYR | CB-CG-CD1 | -9.02 | 115.59 | 121.00 | 2 | 5 |
| 1 | A | 132 | TYR | CB-CG-CD1 | 8.98 | 126.39 | 121.00 | 10 | 4 |
| 1 | A | 204 | THR | CA-CB-CG2 | 8.97 | 124.96 | 112.40 | 8 | 3 |
| 1 | A | 161 | VAL | CA-CB-CG1 | 8.94 | 124.31 | 110.90 | 14 | 2 |
| 1 | A | 170 | ASP | CB-CG-OD2 | 8.93 | 126.34 | 118.30 | 11 | 10 |
| 1 | A | 102 | GLU | OE1-CD-OE2 | -8.90 | 112.62 | 123.30 | 13 | 5 |
| 1 | A | 202 | PHE | CB-CG-CD2 | -8.86 | 114.60 | 120.80 | 5 | 2 |
| 1 | A | 121 | TYR | CB-CG-CD1 | -8.83 | 115.70 | 121.00 | 3 | 4 |
| 1 | A | 253 | ASP | CB-CG-OD2 | -8.44 | 110.70 | 118.30 | 14 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 163 | PHE | CB-CG-CD1 | -8.39 | 114.93 | 120.80 | 11 | 2 |
| 1 | A | 101 | ARG | CD-NE-CZ | 8.38 | 135.32 | 123.60 | 14 | 1 |
| 1 | A | 254 | ASP | CB-CG-OD1 | -8.36 | 110.78 | 118.30 | 5 | 3 |
| 1 | A | 194 | ASP | CB-CG-OD2 | 8.35 | 125.82 | 118.30 | 8 | 3 |
| 1 | A | 138 | PHE | CB-CG-CD1 | 8.31 | 126.62 | 120.80 | 5 | 4 |
| 1 | A | 262 | TYR | CZ-CE2-CD2 | -8.26 | 112.37 | 119.80 | 4 | 2 |
| 1 | A | 174 | PHE | CB-CG-CD2 | -8.15 | 115.09 | 120.80 | 2 | 4 |
| 1 | A | 248 | PHE | CB-CG-CD2 | -8.13 | 115.11 | 120.80 | 5 | 3 |
| 1 | A | 141 | TRP | CD1-NE1-CE2 | 8.13 | 116.32 | 109.00 | 14 | 4 |
| 1 | A | 115 | THR | CA-CB-CG2 | 8.11 | 123.76 | 112.40 | 1 | 3 |
| 1 | A | 231 | ASP | CB-CG-OD1 | -8.08 | 111.03 | 118.30 | 13 | 1 |
| 1 | A | 141 | TRP | NE1-CE2-CD2 | -7.98 | 99.32 | 107.30 | 14 | 3 |
| 1 | A | 203 | TRP | CG-CD2-CE3 | 7.91 | 141.02 | 133.90 | 11 | 2 |
| 1 | A | 116 | TYR | CB-CG-CD2 | -7.88 | 116.27 | 121.00 | 3 | 5 |
| 1 | A | 141 | TRP | NE1-CE2-CZ2 | 7.83 | 139.01 | 130.40 | 14 | 2 |
| 1 | A | 161 | VAL | CA-CB-CG2 | 7.82 | 122.62 | 110.90 | 13 | 2 |
| 1 | A | 213 | PHE | CB-CG-CD2 | -7.77 | 115.36 | 120.80 | 9 | 3 |
| 1 | A | 238 | PRO | N-CA-CB | 7.76 | 112.61 | 103.30 | 2 | 3 |
| 1 | A | 237 | PHE | CB-CG-CD2 | 7.72 | 126.20 | 120.80 | 11 | 1 |
| 1 | A | 131 | ASP | CB-CG-OD2 | -7.68 | 111.39 | 118.30 | 13 | 2 |
| 1 | A | 240 | TYR | CB-CG-CD2 | -7.67 | 116.40 | 121.00 | 8 | 3 |
| 1 | A | 140 | VAL | CA-CB-CG1 | 7.62 | 122.33 | 110.90 | 4 | 3 |
| 1 | A | 185 | PHE | CB-CG-CD1 | 7.59 | 126.11 | 120.80 | 14 | 2 |
| 1 | A | 116 | TYR | CD1-CE1-CZ | 7.50 | 126.55 | 119.80 | 4 | 2 |
| 1 | A | 129 | ASP | CB-CG-OD1 | 7.49 | 125.04 | 118.30 | 5 | 6 |
| 1 | A | 138 | PHE | CB-CG-CD2 | -7.48 | 115.57 | 120.80 | 7 | 3 |
| 1 | A | 109 | TRP | CD1-NE1-CE2 | 7.41 | 115.66 | 109.00 | 11 | 3 |
| 1 | A | 256 | ARG | CD-NE-CZ | 7.39 | 133.95 | 123.60 | 9 | 1 |
| 1 | A | 184 | ALA | N-CA-CB | -7.39 | 99.75 | 110.10 | 12 | 2 |
| 1 | A | 203 | TRP | CD1-NE1-CE2 | 7.39 | 115.65 | 109.00 | 1 | 3 |
| 1 | A | 232 | PRO | N-CA-CB | 7.29 | 112.05 | 103.30 | 1 | 3 |
| 1 | A | 135 | ARG | CD-NE-CZ | 7.25 | 133.75 | 123.60 | 14 | 2 |
| 1 | A | 197 | PHE | CB-CG-CD2 | -7.20 | 115.76 | 120.80 | 8 | 2 |
| 1 | A | 203 | TRP | CD1-CG-CD2 | 7.18 | 112.04 | 106.30 | 5 | 2 |
| 1 | A | 210 | THR | CA-CB-CG2 | 7.10 | 122.34 | 112.40 | 14 | 1 |
| 1 | A | 194 | ASP | OD1-CG-OD2 | -7.09 | 109.82 | 123.30 | 8 | 2 |
| 1 | A | 109 | TRP | NE1-CE2-CD2 | -7.07 | 100.23 | 107.30 | 11 | 3 |
| 1 | A | 262 | TYR | CG-CD1-CE1 | -7.07 | 115.64 | 121.30 | 6 | 1 |
| 1 | A | 253 | ASP | CB-CG-OD1 | 7.06 | 124.66 | 118.30 | 10 | 3 |
| 1 | A | 197 | PHE | CB-CG-CD1 | 7.04 | 125.73 | 120.80 | 8 | 3 |
| 1 | A | 149 | PHE | CZ-CE2-CD2 | -7.00 | 111.70 | 120.10 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 122 | THR | CA-CB-CG2 | 6.95 | 122.13 | 112.40 | 8 | 1 |
| 1 | A | 127 | ARG | NH1-CZ-NH2 | 6.94 | 127.04 | 119.40 | 11 | 2 |
| 1 | A | 132 | TYR | CG-CD2-CE2 | -6.93 | 115.75 | 121.30 | 11 | 2 |
| 1 | A | 244 | ASP | CB-CG-OD1 | -6.93 | 112.06 | 118.30 | 7 | 1 |
| 1 | A | 141 | TRP | CB-CG-CD2 | 6.91 | 135.58 | 126.60 | 11 | 1 |
| 1 | A | 201 | GLU | CB-CA-C | -6.90 | 96.60 | 110.40 | 2 | 1 |
| 1 | A | 222 | HIS | CA-CB-CG | 6.90 | 125.32 | 113.60 | 4 | 2 |
| 1 | A | 149 | PHE | CB-CG-CD1 | -6.89 | 115.98 | 120.80 | 9 | 4 |
| 1 | A | 171 | PHE | CB-CG-CD2 | -6.83 | 116.02 | 120.80 | 1 | 1 |
| 1 | A | 239 | THR | N-CA-CB | -6.81 | 97.36 | 110.30 | 7 | 1 |
| 1 | A | 172 | HIS | CA-CB-CG | 6.79 | 125.15 | 113.60 | 7 | 2 |
| 1 | A | 235 | VAL | CA-CB-CG1 | 6.78 | 121.06 | 110.90 | 14 | 2 |
| 1 | A | 242 | TYR | CB-CG-CD2 | -6.73 | 116.96 | 121.00 | 14 | 5 |
| 1 | A | 141 | TRP | CB-CG-CD1 | -6.61 | 118.40 | 127.00 | 11 | 1 |
| 1 | A | 101 | ARG | NH1-CZ-NH2 | 6.58 | 126.63 | 119.40 | 6 | 2 |
| 1 | A | 158 | ASP | CB-CG-OD2 | -6.54 | 112.42 | 118.30 | 7 | 3 |
| 1 | A | 218 | HIS | CA-CB-CG | 6.54 | 124.71 | 113.60 | 13 | 5 |
| 1 | A | 239 | THR | CA-CB-CG2 | 6.51 | 121.52 | 112.40 | 10 | 2 |
| 1 | A | 141 | TRP | CZ3-CH2-CZ2 | -6.48 | 113.83 | 121.60 | 6 | 2 |
| 1 | A | 175 | ASP | OD1-CG-OD2 | -6.47 | 111.01 | 123.30 | 12 | 6 |
| 1 | A | 131 | ASP | CB-CG-OD1 | 6.45 | 124.10 | 118.30 | 9 | 3 |
| 1 | A | 240 | TYR | CG-CD1-CE1 | -6.45 | 116.14 | 121.30 | 6 | 3 |
| 1 | A | 164 | ALA | CB-CA-C | 6.43 | 119.75 | 110.10 | 4 | 2 |
| 1 | A | 168 | HIS | C-N-CA | 6.41 | 135.76 | 122.30 | 5 | 2 |
| 1 | A | 110 | ARG | CD-NE-CZ | 6.41 | 132.57 | 123.60 | 12 | 2 |
| 1 | A | 262 | TYR | CG-CD2-CE2 | -6.40 | 116.18 | 121.30 | 3 | 3 |
| 1 | A | 210 | THR | O-C-N | -6.39 | 112.47 | 122.70 | 4 | 1 |
| 1 | A | 174 | PHE | CG-CD2-CE2 | -6.35 | 113.81 | 120.80 | 8 | 1 |
| 1 | A | 174 | PHE | CD1-CG-CD2 | 6.33 | 126.52 | 118.30 | 11 | 2 |
| 1 | A | 227 | GLY | N-CA-C | -6.28 | 97.41 | 113.10 | 12 | 1 |
| 1 | A | 248 | PHE | CG-CD1-CE1 | -6.25 | 113.92 | 120.80 | 9 | 1 |
| 1 | A | 117 | ARG | CD-NE-CZ | 6.25 | 132.34 | 123.60 | 6 | 2 |
| 1 | A | 130 | VAL | CA-CB-CG1 | 6.23 | 120.24 | 110.90 | 13 | 2 |
| 1 | A | 151 | LYS | C-N-CA | 6.23 | 137.27 | 121.70 | 7 | 1 |
| 1 | A | 174 | PHE | CB-CA-C | 6.22 | 122.84 | 110.40 | 14 | 4 |
| 1 | A | 237 | PHE | CB-CG-CD1 | 6.21 | 125.15 | 120.80 | 2 | 3 |
| 1 | A | 216 | ALA | CB-CA-C | -6.21 | 100.79 | 110.10 | 4 | 1 |
| 1 | A | 158 | ASP | CB-CG-OD1 | -6.20 | 112.72 | 118.30 | 3 | 1 |
| 1 | A | 254 | ASP | CA-CB-CG | 6.18 | 126.99 | 113.40 | 4 | 1 |
| 1 | A | 183 | HIS | CA-CB-CG | 6.17 | 124.10 | 113.60 | 13 | 1 |
| 1 | A | 113 | TYR | CZ-CE2-CD2 | 6.16 | 125.35 | 119.80 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 128 | GLU | OE1-CD-OE2 | -6.14 | 115.93 | 123.30 | 14 | 2 |
| 1 | A | 212 | LEU | CB-CG-CD1 | 6.14 | 121.44 | 111.00 | 14 | 2 |
| 1 | A | 243 | VAL | CA-CB-CG2 | 6.13 | 120.10 | 110.90 | 14 | 1 |
| 1 | A | 162 | VAL | CA-CB-CG1 | 6.13 | 120.10 | 110.90 | 3 | 3 |
| 1 | A | 247 | THR | O-C-N | -6.11 | 112.92 | 122.70 | 6 | 2 |
| 1 | A | 223 | SER | N-CA-CB | -6.10 | 101.34 | 110.50 | 7 | 1 |
| 1 | A | 202 | PHE | CB-CG-CD1 | -6.05 | 116.56 | 120.80 | 14 | 1 |
| 1 | A | 116 | TYR | CA-CB-CG | 6.04 | 124.88 | 113.40 | 3 | 1 |
| 1 | A | 200 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 | 6 | 1 |
| 1 | A | 200 | ASP | CB-CG-OD1 | 6.03 | 123.73 | 118.30 | 4 | 1 |
| 1 | A | 175 | ASP | CB-CA-C | 6.01 | 122.42 | 110.40 | 4 | 1 |
| 1 | A | 165 | ARG | CB-CA-C | 5.97 | 122.35 | 110.40 | 9 | 2 |
| 1 | A | 116 | TYR | CB-CA-C | 5.97 | 122.34 | 110.40 | 6 | 1 |
| 1 | A | 150 | SER | N-CA-CB | -5.96 | 101.56 | 110.50 | 6 | 1 |
| 1 | A | 231 | ASP | CB-CG-OD2 | 5.95 | 123.65 | 118.30 | 13 | 1 |
| 1 | A | 229 | SER | N-CA-CB | -5.91 | 101.63 | 110.50 | 14 | 1 |
| 1 | A | 135 | ARG | NH1-CZ-NH2 | 5.89 | 125.89 | 119.40 | 12 | 1 |
| 1 | A | 165 | ARG | NH1-CZ-NH2 | 5.88 | 125.86 | 119.40 | 5 | 1 |
| 1 | A | 205 | THR | CA-CB-OG1 | 5.84 | 121.26 | 109.00 | 11 | 1 |
| 1 | A | 141 | TRP | CE2-CD2-CG | 5.82 | 111.95 | 107.30 | 14 | 3 |
| 1 | A | 149 | PHE | CB-CG-CD2 | -5.81 | 116.73 | 120.80 | 6 | 2 |
| 1 | A | 198 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 | 1 | 2 |
| 1 | A | 132 | TYR | CG-CD1-CE1 | -5.79 | 116.67 | 121.30 | 2 | 1 |
| 1 | A | 219 | ALA | N-CA-CB | -5.77 | 102.02 | 110.10 | 11 | 1 |
| 1 | A | 262 | TYR | CA-CB-CG | 5.77 | 124.36 | 113.40 | 1 | 1 |
| 1 | A | 102 | GLU | N-CA-CB | -5.76 | 100.24 | 110.60 | 13 | 1 |
| 1 | A | 145 | THR | CA-CB-CG2 | 5.73 | 120.43 | 112.40 | 5 | 1 |
| 1 | A | 130 | VAL | CG1-CB-CG2 | -5.71 | 101.77 | 110.90 | 2 | 1 |
| 1 | A | 124 | ASP | CB-CG-OD2 | 5.68 | 123.41 | 118.30 | 4 | 2 |
| 1 | A | 109 | TRP | CE2-CD2-CG | 5.65 | 111.82 | 107.30 | 8 | 1 |
| 1 | A | 203 | TRP | CG-CD1-NE1 | -5.63 | 104.47 | 110.10 | 5 | 2 |
| 1 | A | 103 | MET | N-CA-CB | -5.63 | 100.46 | 110.60 | 4 | 1 |
| 1 | A | 192 | GLY | CA-C-N | 5.62 | 127.43 | 116.20 | 5 | 1 |
| 1 | A | 249 | ARG | NH1-CZ-NH2 | -5.61 | 113.23 | 119.40 | 3 | 1 |
| 1 | A | 129 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 | 2 | 3 |
| 1 | A | 108 | VAL | CA-CB-CG2 | 5.56 | 119.24 | 110.90 | 1 | 2 |
| 1 | A | 113 | TYR | CD1-CG-CD2 | 5.56 | 124.01 | 117.90 | 9 | 1 |
| 1 | A | 168 | HIS | CB-CA-C | 5.56 | 121.51 | 110.40 | 12 | 1 |
| 1 | A | 171 | PHE | CB-CG-CD1 | -5.55 | 116.92 | 120.80 | 5 | 1 |
| 1 | A | 124 | ASP | OD1-CG-OD2 | -5.55 | 112.76 | 123.30 | 8 | 1 |
| 1 | A | 257 | GLY | O-C-N | 5.54 | 131.57 | 122.70 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 107 | PRO | N-CD-CG | 5.53 | 111.50 | 103.20 | 3 | 1 |
| 1 | A | 112 | HIS | C-N-CA | 5.52 | 135.50 | 121.70 | 13 | 1 |
| 1 | A | 226 | LEU | CB-CG-CD2 | 5.51 | 120.37 | 111.00 | 5 | 1 |
| 1 | A | 163 | PHE | CZ-CE2-CD2 | -5.49 | 113.51 | 120.10 | 6 | 1 |
| 1 | A | 132 | TYR | CD1-CG-CD2 | 5.48 | 123.93 | 117.90 | 14 | 1 |
| 1 | A | 107 | PRO | C-N-CA | 5.48 | 135.39 | 121.70 | 9 | 1 |
| 1 | A | 240 | TYR | CD1-CG-CD2 | 5.47 | 123.92 | 117.90 | 6 | 1 |
| 1 | A | 125 | MET | N-CA-CB | 5.47 | 120.45 | 110.60 | 9 | 1 |
| 1 | A | 174 | PHE | CG-CD1-CE1 | 5.44 | 126.79 | 120.80 | 4 | 2 |
| 1 | A | 150 | SER | CB-CA-C | 5.42 | 120.39 | 110.10 | 3 | 1 |
| 1 | A | 230 | SER | N-CA-CB | -5.41 | 102.38 | 110.50 | 9 | 2 |
| 1 | A | 203 | TRP | NE1-CE2-CZ2 | 5.41 | 136.35 | 130.40 | 8 | 1 |
| 1 | A | 128 | GLU | O-C-N | -5.41 | 114.05 | 122.70 | 6 | 1 |
| 1 | A | 161 | VAL | CG1-CB-CG2 | -5.39 | 102.27 | 110.90 | 2 | 1 |
| 1 | A | 208 | GLY | CA-C-O | -5.37 | 110.94 | 120.60 | 4 | 1 |
| 1 | A | 203 | TRP | CA-CB-CG | 5.37 | 123.90 | 113.70 | 6 | 1 |
| 1 | A | 123 | PRO | C-N-CA | 5.35 | 135.07 | 121.70 | 4 | 1 |
| 1 | A | 162 | VAL | CB-CA-C | 5.34 | 121.55 | 111.40 | 4 | 1 |
| 1 | A | 241 | LYS | CB-CA-C | 5.33 | 121.06 | 110.40 | 1 | 1 |
| 1 | A | 249 | ARG | CD-NE-CZ | 5.33 | 131.06 | 123.60 | 12 | 1 |
| 1 | A | 208 | GLY | N-CA-C | -5.32 | 99.79 | 113.10 | 10 | 1 |
| 1 | A | 232 | PRO | N-CD-CG | 5.32 | 111.17 | 103.20 | 12 | 2 |
| 1 | A | 182 | ALA | CB-CA-C | 5.31 | 118.07 | 110.10 | 12 | 1 |
| 1 | A | 242 | TYR | C-N-CA | 5.30 | 134.95 | 121.70 | 13 | 2 |
| 1 | A | 132 | TYR | CZ-CE2-CD2 | 5.30 | 124.57 | 119.80 | 11 | 1 |
| 1 | A | 149 | PHE | CD1-CG-CD2 | 5.29 | 125.18 | 118.30 | 9 | 1 |
| 1 | A | 149 | PHE | CG-CD1-CE1 | -5.29 | 114.98 | 120.80 | 9 | 1 |
| 1 | A | 116 | TYR | CG-CD2-CE2 | -5.29 | 117.07 | 121.30 | 1 | 1 |
| 1 | A | 118 | ILE | N-CA-C | -5.28 | 96.73 | 111.00 | 4 | 1 |
| 1 | A | 235 | VAL | CG1-CB-CG2 | -5.28 | 102.46 | 110.90 | 6 | 1 |
| 1 | A | 202 | PHE | CG-CD2-CE2 | -5.27 | 115.00 | 120.80 | 14 | 1 |
| 1 | A | 125 | MET | CB-CA-C | 5.24 | 120.88 | 110.40 | 8 | 1 |
| 1 | A | 144 | VAL | CA-CB-CG2 | 5.24 | 118.76 | 110.90 | 14 | 2 |
| 1 | A | 129 | ASP | N-CA-CB | 5.24 | 120.03 | 110.60 | 3 | 1 |
| 1 | A | 240 | TYR | CZ-CE2-CD2 | -5.24 | 115.09 | 119.80 | 12 | 1 |
| 1 | A | 109 | TRP | CB-CG-CD1 | -5.23 | 120.20 | 127.00 | 2 | 1 |
| 1 | A | 240 | TYR | C-N-CA | 5.23 | 134.78 | 121.70 | 10 | 1 |
| 1 | A | 120 | ASN | CB-CA-C | 5.23 | 120.86 | 110.40 | 11 | 1 |
| 1 | A | 141 | TRP | CH2-CZ2-CE2 | 5.22 | 122.62 | 117.40 | 6 | 2 |
| 1 | A | 251 | SER | N-CA-CB | -5.21 | 102.68 | 110.50 | 9 | 1 |
| 1 | A | 165 | ARG | CD-NE-CZ | 5.20 | 130.88 | 123.60 | 11 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 163 | PHE | CG-CD2-CE2 | 5.19 | 126.51 | 120.80 | 6 | 1 |
| 1 | A | 130 | VAL | CA-CB-CG2 | 5.18 | 118.67 | 110.90 | 6 | 1 |
| 1 | A | 212 | LEU | O-C-N | -5.17 | 114.42 | 122.70 | 4 | 1 |
| 1 | A | 215 | THR | OG1-CB-CG2 | -5.17 | 98.11 | 110.00 | 4 | 1 |
| 1 | A | 246 | ASN | CB-CA-C | -5.15 | 100.10 | 110.40 | 7 | 1 |
| 1 | A | 256 | ARG | C-N-CA | 5.15 | 133.11 | 122.30 | 12 | 1 |
| 1 | A | 244 | ASP | CB-CG-OD2 | 5.14 | 122.93 | 118.30 | 11 | 1 |
| 1 | A | 240 | TYR | CG-CD2-CE2 | -5.14 | 117.19 | 121.30 | 10 | 1 |
| 1 | A | 184 | ALA | CB-CA-C | -5.14 | 102.39 | 110.10 | 14 | 1 |
| 1 | A | 101 | ARG | C-N-CA | 5.13 | 134.51 | 121.70 | 14 | 1 |
| 1 | A | 122 | THR | N-CA-CB | -5.12 | 100.58 | 110.30 | 8 | 1 |
| 1 | A | 181 | LEU | CB-CG-CD1 | 5.11 | 119.68 | 111.00 | 6 | 1 |
| 1 | A | 173 | ALA | N-CA-CB | 5.11 | 117.25 | 110.10 | 9 | 1 |
| 1 | A | 109 | TRP | NE1-CE2-CZ2 | 5.11 | 136.02 | 130.40 | 11 | 2 |
| 1 | A | 154 | THR | CA-CB-CG2 | 5.10 | 119.54 | 112.40 | 10 | 1 |
| 1 | A | 120 | ASN | N-CA-CB | 5.10 | 119.78 | 110.60 | 12 | 1 |
| 1 | A | 192 | GLY | C-N-CA | 5.09 | 132.99 | 122.30 | 6 | 1 |
| 1 | A | 242 | TYR | CG-CD1-CE1 | 5.09 | 125.37 | 121.30 | 12 | 1 |
| 1 | A | 110 | ARG | C-N-CA | 5.08 | 134.40 | 121.70 | 7 | 1 |
| 1 | A | 121 | TYR | CG-CD1-CE1 | -5.08 | 117.24 | 121.30 | 11 | 1 |
| 1 | A | 164 | ALA | O-C-N | -5.08 | 114.58 | 122.70 | 11 | 1 |
| 1 | A | 222 | HIS | CG-ND1-CE1 | -5.08 | 99.10 | 105.70 | 12 | 1 |
| 1 | A | 217 | VAL | O-C-N | -5.08 | 114.58 | 122.70 | 4 | 1 |
| 1 | A | 199 | GLU | CA-CB-CG | 5.08 | 124.57 | 113.40 | 13 | 1 |
| 1 | A | 261 | LEU | CB-CA-C | -5.06 | 100.59 | 110.20 | 2 | 1 |
| 1 | A | 206 | HIS | CA-CB-CG | 5.06 | 122.20 | 113.60 | 8 | 1 |
| 1 | A | 195 | ALA | N-CA-CB | -5.05 | 103.03 | 110.10 | 4 | 1 |
| 1 | A | 174 | PHE | C-N-CA | 5.03 | 134.28 | 121.70 | 1 | 1 |
| 1 | A | 262 | TYR | CB-CA-C | 5.01 | 120.42 | 110.40 | 2 | 1 |
| 1 | A | 173 | ALA | CB-CA-C | 5.00 | 117.61 | 110.10 | 3 | 1 |
| 1 | A | 185 | PHE | C-N-CA | 5.00 | 132.80 | 122.30 | 9 | 1 |
| 1 | A | 234 | ALA | C-N-CA | 5.00 | 134.20 | 121.70 | 11 | 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 | A | 242 | TYR | Sidechain,Peptide | 7 |
| 1 | A | 121 | TYR | Sidechain | 5 |
| 1 | A | 262 | TYR | Sidechain | 5 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|---------------------|----------------|
| 1 | A | 204 | THR | Peptide | 5 |
| 1 | A | 240 | TYR | Sidechain,Peptide | 4 |
| 1 | A | 132 | TYR | Sidechain | 3 |
| 1 | A | 116 | TYR | Sidechain,Mainchain | 3 |
| 1 | A | 113 | TYR | Sidechain | 3 |
| 1 | A | 197 | PHE | Sidechain | 2 |
| 1 | A | 185 | PHE | Sidechain | 2 |
| 1 | A | 110 | ARG | Sidechain | 2 |
| 1 | A | 248 | PHE | Sidechain,Peptide | 2 |
| 1 | A | 135 | ARG | Sidechain | 2 |
| 1 | A | 171 | PHE | Sidechain | 1 |
| 1 | A | 101 | ARG | Sidechain | 1 |
| 1 | A | 224 | LEU | Mainchain | 1 |
| 1 | A | 256 | ARG | Sidechain | 1 |
| 1 | A | 163 | PHE | Sidechain | 1 |
| 1 | A | 237 | PHE | Sidechain | 1 |
| 1 | A | 159 | ILE | Peptide | 1 |
| 1 | A | 222 | HIS | Sidechain | 1 |
| 1 | A | 199 | GLU | Sidechain | 1 |
| 1 | A | 100 | PHE | Sidechain | 1 |
| 1 | A | 151 | LYS | Peptide | 1 |
| 1 | A | 202 | PHE | Sidechain | 1 |
| 1 | A | 172 | HIS | Sidechain | 1 |
| 1 | A | 218 | HIS | Sidechain | 1 |
| 1 | A | 252 | ALA | Mainchain | 1 |
| 1 | A | 127 | ARG | Mainchain | 1 |
| 1 | A | 206 | HIS | Sidechain | 1 |
| 1 | A | 183 | HIS | Sidechain | 1 |
| 1 | A | 249 | ARG | Sidechain | 1 |
| 1 | A | 117 | ARG | Sidechain | 1 |
| 1 | A | 196 | HIS | Sidechain | 1 |
| 1 | A | 174 | PHE | Peptide | 1 |
| 1 | A | 164 | ALA | Peptide | 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 | A | 1265 | 1199 | 1196 | 2±1 |
| 4 | A | 5750 | 0 | 9000 | 131±13 |
| All | All | 98280 | 16786 | 142744 | 1846 |

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 8.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:388:PX4:H39 | 4:A:411:PX4:H17 | 0.99 | 1.35 | 4 | 1 |
| 4:A:337:PX4:H47 | 4:A:353:PX4:H15 | 0.93 | 1.41 | 8 | 2 |
| 4:A:413:PX4:H24 | 4:A:430:PX4:H63 | 0.92 | 1.40 | 10 | 1 |
| 4:A:320:PX4:H20 | 4:A:359:PX4:H57 | 0.92 | 1.42 | 5 | 1 |
| 4:A:368:PX4:H22 | 4:A:369:PX4:H51 | 0.90 | 1.40 | 6 | 1 |
| 4:A:342:PX4:H24 | 4:A:352:PX4:H47 | 0.88 | 1.43 | 11 | 1 |
| 4:A:378:PX4:H16 | 4:A:417:PX4:H47 | 0.85 | 1.46 | 7 | 9 |
| 4:A:309:PX4:H59 | 4:A:324:PX4:H57 | 0.84 | 1.50 | 12 | 1 |
| 4:A:355:PX4:H48 | 4:A:356:PX4:H14 | 0.83 | 1.49 | 4 | 2 |
| 4:A:332:PX4:H61 | 4:A:349:PX4:H51 | 0.83 | 1.51 | 6 | 1 |
| 4:A:329:PX4:H70 | 4:A:382:PX4:H26 | 0.82 | 1.50 | 7 | 1 |
| 4:A:316:PX4:H20 | 4:A:364:PX4:H47 | 0.82 | 1.49 | 9 | 1 |
| 4:A:386:PX4:H28 | 4:A:394:PX4:H50 | 0.82 | 1.50 | 11 | 1 |
| 4:A:313:PX4:H18 | 4:A:318:PX4:H46 | 0.81 | 1.50 | 9 | 2 |
| 4:A:416:PX4:H21 | 4:A:425:PX4:H46 | 0.81 | 1.51 | 11 | 1 |
| 4:A:335:PX4:H21 | 4:A:343:PX4:H22 | 0.81 | 1.52 | 5 | 1 |
| 4:A:317:PX4:H17 | 4:A:325:PX4:H52 | 0.81 | 1.53 | 9 | 1 |
| 4:A:384:PX4:H60 | 4:A:385:PX4:H35 | 0.80 | 1.54 | 2 | 1 |
| 4:A:387:PX4:H47 | 4:A:411:PX4:H17 | 0.79 | 1.54 | 12 | 1 |
| 4:A:340:PX4:H66 | 4:A:340:PX4:H31 | 0.79 | 1.55 | 5 | 1 |
| 4:A:387:PX4:H24 | 4:A:394:PX4:H53 | 0.78 | 1.55 | 1 | 2 |
| 4:A:404:PX4:H34 | 4:A:419:PX4:H22 | 0.78 | 1.55 | 8 | 1 |
| 4:A:376:PX4:H54 | 4:A:385:PX4:H17 | 0.77 | 1.57 | 13 | 1 |
| 4:A:317:PX4:H47 | 4:A:342:PX4:H69 | 0.77 | 1.57 | 12 | 1 |
| 4:A:421:PX4:H31 | 4:A:422:PX4:H39 | 0.77 | 1.55 | 2 | 1 |
| 4:A:310:PX4:H16 | 4:A:363:PX4:H20 | 0.76 | 1.56 | 9 | 2 |
| 4:A:368:PX4:H25 | 4:A:425:PX4:H42 | 0.76 | 1.58 | 4 | 1 |
| 4:A:413:PX4:H50 | 4:A:422:PX4:H33 | 0.75 | 1.58 | 2 | 1 |
| 4:A:321:PX4:H20 | 4:A:354:PX4:H48 | 0.75 | 1.56 | 10 | 1 |
| 4:A:393:PX4:H22 | 4:A:394:PX4:H19 | 0.75 | 1.58 | 7 | 1 |
| 4:A:326:PX4:H50 | 4:A:351:PX4:H18 | 0.75 | 1.58 | 4 | 1 |
| 4:A:400:PX4:H51 | 4:A:409:PX4:H20 | 0.75 | 1.57 | 12 | 1 |
| 4:A:321:PX4:H41 | 4:A:354:PX4:H59 | 0.75 | 1.58 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:417:PX4:H31 | 4:A:426:PX4:H61 | 0.74 | 1.58 | 6 | 1 |
| 4:A:398:PX4:H16 | 4:A:407:PX4:H49 | 0.74 | 1.58 | 14 | 1 |
| 4:A:330:PX4:H22 | 4:A:335:PX4:H19 | 0.74 | 1.60 | 2 | 1 |
| 4:A:345:PX4:H48 | 4:A:353:PX4:H46 | 0.74 | 1.59 | 4 | 1 |
| 4:A:330:PX4:H60 | 4:A:357:PX4:H24 | 0.73 | 1.60 | 10 | 2 |
| 4:A:306:PX4:H23 | 4:A:321:PX4:H39 | 0.73 | 1.60 | 5 | 1 |
| 4:A:332:PX4:H31 | 4:A:332:PX4:H51 | 0.73 | 1.58 | 7 | 1 |
| 4:A:395:PX4:H53 | 4:A:405:PX4:H22 | 0.72 | 1.60 | 4 | 1 |
| 4:A:392:PX4:H18 | 4:A:393:PX4:H50 | 0.72 | 1.61 | 1 | 1 |
| 4:A:317:PX4:H17 | 4:A:325:PX4:H49 | 0.72 | 1.60 | 1 | 1 |
| 4:A:403:PX4:H10 | 4:A:427:PX4:H49 | 0.72 | 1.61 | 3 | 2 |
| 4:A:325:PX4:H30 | 4:A:334:PX4:H18 | 0.72 | 1.60 | 4 | 1 |
| 4:A:376:PX4:H50 | 4:A:385:PX4:H17 | 0.72 | 1.60 | 11 | 2 |
| 4:A:383:PX4:H65 | 4:A:399:PX4:H31 | 0.72 | 1.60 | 8 | 1 |
| 4:A:317:PX4:H46 | 4:A:324:PX4:H17 | 0.72 | 1.60 | 8 | 1 |
| 4:A:371:PX4:H59 | 4:A:379:PX4:H33 | 0.72 | 1.61 | 4 | 1 |
| 4:A:367:PX4:H28 | 4:A:424:PX4:H52 | 0.72 | 1.62 | 4 | 1 |
| 4:A:323:PX4:H68 | 4:A:367:PX4:H40 | 0.72 | 1.62 | 3 | 1 |
| 4:A:378:PX4:H63 | 4:A:417:PX4:H62 | 0.72 | 1.62 | 11 | 1 |
| 4:A:321:PX4:H38 | 4:A:328:PX4:H57 | 0.72 | 1.61 | 13 | 1 |
| 4:A:385:PX4:H52 | 4:A:386:PX4:H26 | 0.71 | 1.61 | 14 | 1 |
| 4:A:383:PX4:H61 | 4:A:399:PX4:H29 | 0.71 | 1.60 | 6 | 1 |
| 4:A:402:PX4:H38 | 4:A:404:PX4:H62 | 0.71 | 1.59 | 14 | 1 |
| 4:A:376:PX4:H64 | 4:A:392:PX4:H29 | 0.71 | 1.60 | 5 | 1 |
| 4:A:387:PX4:H65 | 4:A:411:PX4:H54 | 0.71 | 1.63 | 8 | 1 |
| 4:A:409:PX4:H33 | 4:A:410:PX4:H46 | 0.71 | 1.60 | 2 | 1 |
| 4:A:332:PX4:H43 | 4:A:363:PX4:H72 | 0.71 | 1.63 | 12 | 1 |
| 4:A:402:PX4:H60 | 4:A:413:PX4:H41 | 0.71 | 1.63 | 7 | 1 |
| 4:A:363:PX4:H1 | 4:A:364:PX4:H20 | 0.71 | 1.61 | 11 | 1 |
| 4:A:391:PX4:H64 | 4:A:408:PX4:H55 | 0.71 | 1.63 | 7 | 1 |
| 4:A:321:PX4:H38 | 4:A:412:PX4:H43 | 0.70 | 1.62 | 14 | 1 |
| 4:A:370:PX4:H19 | 4:A:403:PX4:H17 | 0.70 | 1.63 | 11 | 2 |
| 4:A:419:PX4:H49 | 4:A:427:PX4:H49 | 0.70 | 1.63 | 13 | 1 |
| 4:A:308:PX4:H62 | 4:A:311:PX4:H41 | 0.70 | 1.64 | 13 | 1 |
| 4:A:325:PX4:H31 | 4:A:332:PX4:H25 | 0.70 | 1.63 | 11 | 1 |
| 4:A:306:PX4:H56 | 4:A:321:PX4:H55 | 0.69 | 1.64 | 13 | 1 |
| 4:A:384:PX4:H42 | 4:A:385:PX4:H43 | 0.69 | 1.62 | 8 | 1 |
| 4:A:317:PX4:H16 | 4:A:351:PX4:H24 | 0.69 | 1.64 | 14 | 1 |
| 4:A:408:PX4:H17 | 4:A:415:PX4:H20 | 0.69 | 1.64 | 8 | 1 |
| 4:A:322:PX4:H50 | 4:A:336:PX4:H27 | 0.69 | 1.63 | 1 | 1 |
| 4:A:332:PX4:H33 | 4:A:347:PX4:H62 | 0.69 | 1.64 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:358:PX4:H23 | 4:A:363:PX4:H53 | 0.69 | 1.64 | 9 | 1 |
| 4:A:374:PX4:H49 | 4:A:382:PX4:H46 | 0.69 | 1.62 | 8 | 2 |
| 4:A:315:PX4:H17 | 4:A:316:PX4:H49 | 0.69 | 1.64 | 13 | 1 |
| 4:A:360:PX4:H70 | 4:A:419:PX4:H41 | 0.69 | 1.62 | 4 | 1 |
| 4:A:368:PX4:H17 | 4:A:369:PX4:H53 | 0.69 | 1.63 | 9 | 1 |
| 4:A:399:PX4:H29 | 4:A:399:PX4:H63 | 0.69 | 1.64 | 2 | 1 |
| 4:A:331:PX4:H58 | 4:A:339:PX4:H22 | 0.69 | 1.63 | 4 | 1 |
| 4:A:396:PX4:H38 | 4:A:402:PX4:H41 | 0.69 | 1.64 | 12 | 1 |
| 4:A:422:PX4:H36 | 4:A:423:PX4:H23 | 0.68 | 1.65 | 5 | 1 |
| 4:A:388:PX4:H54 | 4:A:395:PX4:H30 | 0.68 | 1.65 | 12 | 1 |
| 4:A:368:PX4:H47 | 4:A:369:PX4:H56 | 0.68 | 1.63 | 1 | 1 |
| 4:A:429:PX4:H30 | 4:A:429:PX4:H55 | 0.68 | 1.63 | 11 | 1 |
| 4:A:337:PX4:H50 | 4:A:353:PX4:H21 | 0.68 | 1.64 | 4 | 1 |
| 4:A:328:PX4:H70 | 4:A:412:PX4:H70 | 0.68 | 1.65 | 13 | 1 |
| 4:A:395:PX4:H55 | 4:A:404:PX4:H46 | 0.68 | 1.66 | 1 | 1 |
| 4:A:416:PX4:H55 | 4:A:418:PX4:H30 | 0.68 | 1.66 | 12 | 1 |
| 4:A:388:PX4:H38 | 4:A:411:PX4:H46 | 0.68 | 1.65 | 5 | 1 |
| 4:A:306:PX4:H14 | 4:A:321:PX4:H28 | 0.68 | 1.66 | 12 | 1 |
| 4:A:316:PX4:H14 | 4:A:320:PX4:H22 | 0.68 | 1.64 | 10 | 1 |
| 4:A:378:PX4:H51 | 4:A:418:PX4:H50 | 0.68 | 1.65 | 13 | 1 |
| 4:A:376:PX4:H67 | 4:A:385:PX4:H30 | 0.68 | 1.64 | 2 | 1 |
| 4:A:391:PX4:H40 | 4:A:408:PX4:H42 | 0.67 | 1.66 | 2 | 1 |
| 4:A:370:PX4:H22 | 4:A:403:PX4:H17 | 0.67 | 1.65 | 9 | 2 |
| 4:A:306:PX4:H20 | 4:A:329:PX4:H52 | 0.67 | 1.66 | 9 | 1 |
| 4:A:346:PX4:H22 | 4:A:354:PX4:H21 | 0.67 | 1.65 | 9 | 1 |
| 4:A:331:PX4:H63 | 4:A:340:PX4:H71 | 0.67 | 1.67 | 14 | 1 |
| 4:A:312:PX4:H16 | 4:A:359:PX4:H5 | 0.67 | 1.64 | 14 | 1 |
| 4:A:330:PX4:H44 | 4:A:344:PX4:H45 | 0.67 | 1.66 | 12 | 1 |
| 4:A:384:PX4:H2 | 4:A:385:PX4:H18 | 0.67 | 1.66 | 1 | 4 |
| 4:A:331:PX4:H33 | 4:A:340:PX4:H69 | 0.67 | 1.66 | 3 | 1 |
| 4:A:315:PX4:H42 | 4:A:425:PX4:H31 | 0.67 | 1.67 | 4 | 1 |
| 4:A:332:PX4:H25 | 4:A:390:PX4:H41 | 0.67 | 1.67 | 6 | 1 |
| 4:A:308:PX4:H38 | 4:A:311:PX4:H69 | 0.67 | 1.65 | 12 | 1 |
| 4:A:417:PX4:H19 | 4:A:426:PX4:H24 | 0.67 | 1.66 | 12 | 1 |
| 4:A:424:PX4:H53 | 4:A:425:PX4:H22 | 0.66 | 1.67 | 2 | 1 |
| 4:A:331:PX4:H35 | 4:A:397:PX4:H44 | 0.66 | 1.66 | 7 | 1 |
| 4:A:395:PX4:H49 | 4:A:396:PX4:H24 | 0.66 | 1.67 | 14 | 1 |
| 4:A:350:PX4:H56 | 4:A:364:PX4:H37 | 0.66 | 1.66 | 3 | 1 |
| 4:A:371:PX4:H61 | 4:A:372:PX4:H27 | 0.66 | 1.68 | 4 | 1 |
| 4:A:306:PX4:H56 | 4:A:361:PX4:H59 | 0.66 | 1.66 | 5 | 1 |
| 4:A:378:PX4:H56 | 4:A:417:PX4:H58 | 0.66 | 1.68 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:311:PX4:H53 | 4:A:316:PX4:H20 | 0.66 | 1.68 | 6 | 1 |
| 4:A:326:PX4:H28 | 4:A:350:PX4:H24 | 0.65 | 1.68 | 5 | 1 |
| 4:A:391:PX4:H28 | 4:A:414:PX4:H46 | 0.65 | 1.69 | 5 | 1 |
| 4:A:313:PX4:H49 | 4:A:328:PX4:H17 | 0.65 | 1.65 | 4 | 1 |
| 4:A:311:PX4:H65 | 4:A:359:PX4:H71 | 0.65 | 1.66 | 7 | 1 |
| 4:A:383:PX4:H50 | 4:A:399:PX4:H17 | 0.65 | 1.67 | 8 | 1 |
| 4:A:380:PX4:H56 | 4:A:387:PX4:H50 | 0.65 | 1.68 | 11 | 1 |
| 4:A:373:PX4:H26 | 4:A:381:PX4:H53 | 0.65 | 1.68 | 9 | 1 |
| 4:A:311:PX4:H10 | 4:A:359:PX4:H51 | 0.65 | 1.68 | 2 | 1 |
| 4:A:345:PX4:H64 | 4:A:345:PX4:H40 | 0.65 | 1.69 | 4 | 1 |
| 4:A:321:PX4:H50 | 4:A:354:PX4:H27 | 0.65 | 1.66 | 6 | 1 |
| 4:A:316:PX4:H51 | 4:A:320:PX4:H27 | 0.65 | 1.69 | 12 | 1 |
| 4:A:417:PX4:H31 | 4:A:426:PX4:H37 | 0.65 | 1.67 | 13 | 1 |
| 4:A:387:PX4:H16 | 4:A:394:PX4:H9 | 0.65 | 1.69 | 2 | 1 |
| 4:A:356:PX4:H16 | 4:A:356:PX4:H10 | 0.65 | 1.68 | 8 | 1 |
| 4:A:333:PX4:H56 | 4:A:341:PX4:H54 | 0.65 | 1.68 | 12 | 1 |
| 4:A:382:PX4:H19 | 4:A:428:PX4:H23 | 0.64 | 1.69 | 1 | 1 |
| 4:A:421:PX4:H22 | 4:A:422:PX4:H26 | 0.64 | 1.68 | 6 | 1 |
| 4:A:317:PX4:H55 | 4:A:324:PX4:H31 | 0.64 | 1.69 | 14 | 1 |
| 4:A:388:PX4:H20 | 4:A:411:PX4:H14 | 0.64 | 1.70 | 3 | 1 |
| 4:A:306:PX4:H18 | 4:A:322:PX4:H51 | 0.64 | 1.69 | 13 | 1 |
| 4:A:354:PX4:H50 | 4:A:360:PX4:H55 | 0.64 | 1.69 | 4 | 1 |
| 4:A:371:PX4:H20 | 4:A:379:PX4:H21 | 0.64 | 1.68 | 14 | 1 |
| 4:A:403:PX4:H7 | 4:A:427:PX4:H52 | 0.64 | 1.68 | 9 | 1 |
| 4:A:385:PX4:H71 | 4:A:392:PX4:H30 | 0.64 | 1.69 | 5 | 1 |
| 4:A:314:PX4:H34 | 4:A:356:PX4:H33 | 0.64 | 1.67 | 7 | 1 |
| 4:A:326:PX4:O8 | 4:A:351:PX4:H17 | 0.64 | 1.91 | 6 | 1 |
| 4:A:307:PX4:H60 | 4:A:349:PX4:H45 | 0.64 | 1.69 | 14 | 1 |
| 4:A:418:PX4:H42 | 4:A:422:PX4:H59 | 0.64 | 1.68 | 1 | 1 |
| 4:A:360:PX4:H44 | 4:A:412:PX4:H60 | 0.64 | 1.69 | 4 | 1 |
| 4:A:406:PX4:H48 | 4:A:421:PX4:H53 | 0.64 | 1.69 | 12 | 1 |
| 4:A:335:PX4:H48 | 4:A:343:PX4:H21 | 0.64 | 1.67 | 11 | 1 |
| 4:A:311:PX4:H52 | 4:A:320:PX4:H24 | 0.64 | 1.68 | 5 | 1 |
| 4:A:317:PX4:H48 | 4:A:342:PX4:H54 | 0.64 | 1.69 | 5 | 1 |
| 4:A:391:PX4:H43 | 4:A:394:PX4:H34 | 0.64 | 1.70 | 5 | 1 |
| 4:A:371:PX4:H16 | 4:A:379:PX4:H20 | 0.64 | 1.70 | 14 | 2 |
| 4:A:391:PX4:H48 | 4:A:408:PX4:H16 | 0.64 | 1.69 | 2 | 3 |
| 4:A:306:PX4:H38 | 4:A:321:PX4:H43 | 0.64 | 1.68 | 12 | 1 |
| 4:A:403:PX4:H47 | 4:A:427:PX4:H48 | 0.64 | 1.68 | 12 | 1 |
| 4:A:395:PX4:H19 | 4:A:398:PX4:H54 | 0.64 | 1.68 | 4 | 1 |
| 4:A:387:PX4:H46 | 4:A:388:PX4:H37 | 0.64 | 1.68 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:308:PX4:H34 | 4:A:314:PX4:H58 | 0.64 | 1.70 | 8 | 1 |
| 4:A:345:PX4:H37 | 4:A:353:PX4:H64 | 0.64 | 1.68 | 1 | 1 |
| 4:A:404:PX4:H39 | 4:A:419:PX4:H30 | 0.63 | 1.68 | 9 | 1 |
| 4:A:409:PX4:H41 | 4:A:410:PX4:H24 | 0.63 | 1.70 | 4 | 1 |
| 4:A:404:PX4:H34 | 4:A:419:PX4:H48 | 0.63 | 1.70 | 3 | 1 |
| 4:A:350:PX4:H50 | 4:A:363:PX4:H51 | 0.63 | 1.68 | 11 | 2 |
| 4:A:385:PX4:H32 | 4:A:386:PX4:H32 | 0.63 | 1.70 | 7 | 1 |
| 4:A:421:PX4:H39 | 4:A:423:PX4:H33 | 0.63 | 1.68 | 11 | 1 |
| 4:A:424:PX4:H48 | 4:A:425:PX4:H21 | 0.63 | 1.70 | 9 | 1 |
| 4:A:404:PX4:H49 | 4:A:413:PX4:H21 | 0.63 | 1.68 | 5 | 1 |
| 4:A:313:PX4:H22 | 4:A:318:PX4:H51 | 0.63 | 1.70 | 11 | 1 |
| 4:A:324:PX4:H48 | 4:A:341:PX4:H3 | 0.63 | 1.69 | 8 | 1 |
| 4:A:322:PX4:H17 | 4:A:336:PX4:H23 | 0.63 | 1.70 | 11 | 1 |
| 4:A:428:PX4:H61 | 4:A:430:PX4:H29 | 0.63 | 1.71 | 7 | 1 |
| 4:A:355:PX4:H72 | 4:A:356:PX4:H53 | 0.63 | 1.70 | 3 | 1 |
| 4:A:408:PX4:H47 | 4:A:415:PX4:H21 | 0.63 | 1.70 | 9 | 1 |
| 4:A:382:PX4:H22 | 4:A:428:PX4:H32 | 0.63 | 1.68 | 5 | 1 |
| 4:A:410:PX4:H62 | 4:A:426:PX4:H37 | 0.63 | 1.69 | 4 | 1 |
| 4:A:320:PX4:H17 | 4:A:359:PX4:H56 | 0.63 | 1.71 | 7 | 1 |
| 4:A:395:PX4:H47 | 4:A:396:PX4:H20 | 0.63 | 1.71 | 12 | 1 |
| 4:A:311:PX4:H50 | 4:A:316:PX4:H19 | 0.63 | 1.71 | 14 | 1 |
| 4:A:363:PX4:H20 | 4:A:364:PX4:H33 | 0.63 | 1.69 | 1 | 1 |
| 4:A:372:PX4:H38 | 4:A:378:PX4:H42 | 0.63 | 1.70 | 13 | 1 |
| 4:A:325:PX4:H24 | 4:A:340:PX4:H53 | 0.63 | 1.70 | 5 | 1 |
| 4:A:370:PX4:H54 | 4:A:411:PX4:H50 | 0.62 | 1.71 | 12 | 1 |
| 4:A:362:PX4:H13 | 4:A:362:PX4:O2 | 0.62 | 1.93 | 11 | 1 |
| 4:A:308:PX4:H22 | 4:A:364:PX4:H14 | 0.62 | 1.71 | 3 | 1 |
| 4:A:375:PX4:H55 | 4:A:429:PX4:H41 | 0.62 | 1.70 | 5 | 1 |
| 4:A:377:PX4:H4 | 4:A:418:PX4:H49 | 0.62 | 1.71 | 6 | 1 |
| 4:A:320:PX4:H68 | 4:A:417:PX4:H72 | 0.62 | 1.71 | 1 | 1 |
| 4:A:353:PX4:H39 | 4:A:366:PX4:H26 | 0.62 | 1.70 | 1 | 1 |
| 4:A:309:PX4:H40 | 4:A:372:PX4:H45 | 0.62 | 1.69 | 11 | 1 |
| 4:A:317:PX4:H55 | 4:A:324:PX4:H20 | 0.62 | 1.70 | 2 | 1 |
| 4:A:331:PX4:H66 | 4:A:373:PX4:H45 | 0.62 | 1.71 | 13 | 1 |
| 4:A:330:PX4:H64 | 4:A:357:PX4:H28 | 0.62 | 1.71 | 10 | 1 |
| 4:A:337:PX4:H58 | 4:A:353:PX4:H27 | 0.62 | 1.69 | 5 | 1 |
| 4:A:378:PX4:H21 | 4:A:417:PX4:H48 | 0.62 | 1.72 | 3 | 1 |
| 4:A:395:PX4:H63 | 4:A:421:PX4:H20 | 0.62 | 1.70 | 9 | 1 |
| 4:A:317:PX4:H63 | 4:A:325:PX4:H59 | 0.62 | 1.71 | 5 | 1 |
| 4:A:326:PX4:H17 | 4:A:351:PX4:O8 | 0.62 | 1.95 | 14 | 2 |
| 4:A:389:PX4:H69 | 4:A:397:PX4:H45 | 0.62 | 1.71 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:345:PX4:H29 | 4:A:362:PX4:H65 | 0.62 | 1.71 | 12 | 1 |
| 4:A:354:PX4:H39 | 4:A:362:PX4:H33 | 0.62 | 1.70 | 8 | 1 |
| 4:A:378:PX4:H22 | 4:A:417:PX4:H48 | 0.62 | 1.69 | 8 | 1 |
| 4:A:405:PX4:H17 | 4:A:406:PX4:H54 | 0.62 | 1.70 | 1 | 2 |
| 4:A:331:PX4:H28 | 4:A:347:PX4:H49 | 0.62 | 1.71 | 4 | 1 |
| 4:A:307:PX4:H28 | 4:A:349:PX4:H23 | 0.62 | 1.71 | 14 | 1 |
| 4:A:314:PX4:H57 | 4:A:364:PX4:H53 | 0.61 | 1.71 | 9 | 1 |
| 4:A:317:PX4:H16 | 4:A:342:PX4:H52 | 0.61 | 1.70 | 5 | 1 |
| 4:A:329:PX4:H18 | 4:A:336:PX4:H53 | 0.61 | 1.69 | 8 | 1 |
| 4:A:426:PX4:H38 | 4:A:426:PX4:H64 | 0.61 | 1.72 | 1 | 1 |
| 4:A:306:PX4:H15 | 4:A:321:PX4:H42 | 0.61 | 1.70 | 10 | 1 |
| 4:A:417:PX4:O6 | 4:A:417:PX4:H4 | 0.61 | 1.95 | 5 | 1 |
| 4:A:369:PX4:H38 | 4:A:378:PX4:H68 | 0.61 | 1.72 | 14 | 1 |
| 4:A:376:PX4:H46 | 4:A:385:PX4:H17 | 0.61 | 1.71 | 10 | 1 |
| 4:A:380:PX4:H18 | 4:A:381:PX4:H15 | 0.61 | 1.71 | 4 | 3 |
| 4:A:391:PX4:H62 | 4:A:408:PX4:H52 | 0.61 | 1.72 | 4 | 1 |
| 4:A:320:PX4:H54 | 4:A:359:PX4:H26 | 0.61 | 1.70 | 6 | 1 |
| 4:A:316:PX4:H34 | 4:A:320:PX4:H37 | 0.61 | 1.71 | 3 | 1 |
| 4:A:307:PX4:H52 | 4:A:321:PX4:H59 | 0.61 | 1.72 | 13 | 1 |
| 4:A:403:PX4:H53 | 4:A:403:PX4:H32 | 0.61 | 1.73 | 12 | 1 |
| 4:A:376:PX4:H40 | 4:A:399:PX4:H64 | 0.61 | 1.73 | 1 | 1 |
| 4:A:398:PX4:H16 | 4:A:407:PX4:H48 | 0.61 | 1.72 | 9 | 1 |
| 4:A:386:PX4:O6 | 4:A:394:PX4:H18 | 0.61 | 1.94 | 7 | 1 |
| 4:A:368:PX4:H52 | 4:A:369:PX4:H64 | 0.61 | 1.73 | 3 | 1 |
| 4:A:423:PX4:H48 | 4:A:425:PX4:H18 | 0.61 | 1.73 | 12 | 1 |
| 4:A:369:PX4:H31 | 4:A:377:PX4:H62 | 0.61 | 1.73 | 13 | 1 |
| 4:A:360:PX4:H2 | 4:A:366:PX4:H16 | 0.61 | 1.71 | 6 | 2 |
| 4:A:380:PX4:H67 | 4:A:387:PX4:H65 | 0.61 | 1.73 | 12 | 1 |
| 4:A:306:PX4:H66 | 4:A:362:PX4:H45 | 0.61 | 1.71 | 10 | 1 |
| 1:A:214:LEU:HD12 | 1:A:240:TYR:CE1 | 0.61 | 2.30 | 13 | 1 |
| 4:A:347:PX4:H19 | 4:A:348:PX4:H14 | 0.61 | 1.72 | 13 | 1 |
| 4:A:317:PX4:H17 | 4:A:325:PX4:H46 | 0.60 | 1.73 | 7 | 2 |
| 4:A:371:PX4:H20 | 4:A:372:PX4:H17 | 0.60 | 1.71 | 7 | 1 |
| 4:A:406:PX4:O1 | 4:A:414:PX4:H9 | 0.60 | 1.95 | 8 | 1 |
| 4:A:391:PX4:H55 | 4:A:408:PX4:H55 | 0.60 | 1.72 | 3 | 1 |
| 4:A:367:PX4:H49 | 4:A:428:PX4:H51 | 0.60 | 1.73 | 1 | 1 |
| 4:A:329:PX4:H24 | 4:A:336:PX4:H60 | 0.60 | 1.73 | 3 | 1 |
| 4:A:363:PX4:H24 | 4:A:364:PX4:H37 | 0.60 | 1.71 | 1 | 1 |
| 4:A:393:PX4:O2 | 4:A:394:PX4:H17 | 0.60 | 1.96 | 10 | 2 |
| 4:A:347:PX4:H30 | 4:A:348:PX4:H19 | 0.60 | 1.72 | 14 | 1 |
| 4:A:306:PX4:H23 | 4:A:328:PX4:H54 | 0.60 | 1.73 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:404:PX4:H70 | 4:A:430:PX4:H65 | 0.60 | 1.73 | 11 | 1 |
| 4:A:325:PX4:H45 | 4:A:407:PX4:H29 | 0.60 | 1.72 | 7 | 1 |
| 4:A:401:PX4:H46 | 4:A:426:PX4:H56 | 0.60 | 1.72 | 13 | 1 |
| 4:A:371:PX4:H14 | 4:A:379:PX4:H20 | 0.60 | 1.71 | 11 | 1 |
| 4:A:398:PX4:H30 | 4:A:407:PX4:H18 | 0.60 | 1.72 | 10 | 1 |
| 4:A:378:PX4:H20 | 4:A:410:PX4:H52 | 0.60 | 1.73 | 12 | 2 |
| 4:A:350:PX4:H67 | 4:A:358:PX4:H33 | 0.60 | 1.71 | 3 | 1 |
| 4:A:311:PX4:H29 | 4:A:311:PX4:H60 | 0.60 | 1.74 | 9 | 1 |
| 4:A:348:PX4:H11 | 4:A:355:PX4:O2 | 0.60 | 1.95 | 5 | 2 |
| 1:A:244:ASP:OD2 | 4:A:349:PX4:H9 | 0.60 | 1.96 | 7 | 2 |
| 4:A:395:PX4:H64 | 4:A:406:PX4:H56 | 0.60 | 1.72 | 1 | 2 |
| 4:A:321:PX4:H26 | 4:A:360:PX4:H61 | 0.60 | 1.72 | 12 | 1 |
| 4:A:327:PX4:H20 | 4:A:328:PX4:H16 | 0.60 | 1.72 | 7 | 2 |
| 4:A:381:PX4:H51 | 4:A:396:PX4:H46 | 0.60 | 1.73 | 14 | 1 |
| 4:A:380:PX4:H52 | 4:A:387:PX4:H49 | 0.60 | 1.73 | 6 | 1 |
| 4:A:400:PX4:H71 | 4:A:426:PX4:H43 | 0.59 | 1.73 | 2 | 1 |
| 4:A:328:PX4:H72 | 4:A:374:PX4:H43 | 0.59 | 1.74 | 5 | 1 |
| 4:A:315:PX4:H55 | 4:A:323:PX4:H46 | 0.59 | 1.74 | 1 | 1 |
| 4:A:424:PX4:H47 | 4:A:429:PX4:H21 | 0.59 | 1.74 | 2 | 1 |
| 4:A:347:PX4:H64 | 4:A:356:PX4:H56 | 0.59 | 1.72 | 3 | 1 |
| 4:A:422:PX4:H35 | 4:A:423:PX4:H32 | 0.59 | 1.74 | 3 | 1 |
| 4:A:347:PX4:H35 | 4:A:348:PX4:H24 | 0.59 | 1.73 | 4 | 1 |
| 4:A:403:PX4:H2 | 4:A:427:PX4:H46 | 0.59 | 1.73 | 14 | 1 |
| 4:A:413:PX4:O2 | 4:A:430:PX4:H18 | 0.59 | 1.96 | 3 | 1 |
| 4:A:335:PX4:H28 | 4:A:343:PX4:H56 | 0.59 | 1.74 | 6 | 1 |
| 4:A:331:PX4:H31 | 4:A:340:PX4:H56 | 0.59 | 1.73 | 8 | 1 |
| 4:A:316:PX4:O6 | 4:A:364:PX4:H12 | 0.59 | 1.98 | 3 | 1 |
| 4:A:371:PX4:H54 | 4:A:379:PX4:H25 | 0.59 | 1.73 | 11 | 1 |
| 4:A:351:PX4:H50 | 4:A:358:PX4:H55 | 0.59 | 1.74 | 10 | 1 |
| 4:A:416:PX4:H58 | 4:A:423:PX4:H60 | 0.59 | 1.74 | 6 | 1 |
| 4:A:388:PX4:O6 | 4:A:395:PX4:H5 | 0.59 | 1.97 | 8 | 2 |
| 4:A:330:PX4:H25 | 4:A:343:PX4:H54 | 0.59 | 1.75 | 14 | 1 |
| 4:A:306:PX4:H29 | 4:A:329:PX4:H51 | 0.59 | 1.73 | 3 | 1 |
| 4:A:350:PX4:H60 | 4:A:364:PX4:H41 | 0.59 | 1.73 | 3 | 1 |
| 4:A:345:PX4:H33 | 4:A:362:PX4:H69 | 0.59 | 1.73 | 12 | 1 |
| 4:A:400:PX4:H46 | 4:A:408:PX4:H64 | 0.59 | 1.74 | 12 | 1 |
| 4:A:342:PX4:H24 | 4:A:352:PX4:C24 | 0.59 | 2.24 | 11 | 1 |
| 4:A:393:PX4:H45 | 4:A:394:PX4:H37 | 0.59 | 1.72 | 5 | 1 |
| 4:A:369:PX4:H20 | 4:A:377:PX4:H51 | 0.59 | 1.75 | 14 | 1 |
| 4:A:375:PX4:H65 | 4:A:412:PX4:H38 | 0.59 | 1.74 | 9 | 1 |
| 4:A:421:PX4:H44 | 4:A:428:PX4:H58 | 0.59 | 1.74 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:371:PX4:H34 | 4:A:377:PX4:H36 | 0.59 | 1.74 | 5 | 1 |
| 4:A:327:PX4:H26 | 4:A:327:PX4:H57 | 0.59 | 1.73 | 1 | 1 |
| 4:A:416:PX4:H49 | 4:A:425:PX4:H57 | 0.58 | 1.75 | 9 | 1 |
| 4:A:334:PX4:H42 | 4:A:391:PX4:H43 | 0.58 | 1.75 | 2 | 1 |
| 4:A:347:PX4:H34 | 4:A:348:PX4:H22 | 0.58 | 1.73 | 14 | 1 |
| 4:A:312:PX4:H61 | 4:A:359:PX4:H33 | 0.58 | 1.73 | 6 | 1 |
| 4:A:377:PX4:H72 | 4:A:425:PX4:H68 | 0.58 | 1.74 | 6 | 1 |
| 4:A:409:PX4:H51 | 4:A:415:PX4:H21 | 0.58 | 1.74 | 8 | 1 |
| 4:A:383:PX4:H63 | 4:A:399:PX4:H67 | 0.58 | 1.74 | 3 | 1 |
| 4:A:337:PX4:H71 | 4:A:353:PX4:H62 | 0.58 | 1.75 | 10 | 1 |
| 4:A:350:PX4:H9 | 4:A:358:PX4:O6 | 0.58 | 1.99 | 12 | 2 |
| 4:A:354:PX4:H51 | 4:A:360:PX4:H18 | 0.58 | 1.74 | 4 | 1 |
| 4:A:360:PX4:H62 | 4:A:360:PX4:H25 | 0.58 | 1.73 | 4 | 1 |
| 4:A:377:PX4:H34 | 4:A:379:PX4:H27 | 0.58 | 1.76 | 7 | 1 |
| 4:A:404:PX4:O2 | 4:A:413:PX4:H17 | 0.58 | 1.97 | 7 | 1 |
| 4:A:428:PX4:H52 | 4:A:430:PX4:H53 | 0.58 | 1.75 | 7 | 1 |
| 4:A:308:PX4:H24 | 4:A:364:PX4:H22 | 0.58 | 1.74 | 12 | 1 |
| 4:A:382:PX4:H69 | 4:A:412:PX4:H71 | 0.58 | 1.75 | 13 | 1 |
| 4:A:395:PX4:H67 | 4:A:406:PX4:H56 | 0.58 | 1.75 | 2 | 1 |
| 4:A:375:PX4:H42 | 4:A:424:PX4:H69 | 0.58 | 1.76 | 2 | 1 |
| 4:A:307:PX4:H56 | 4:A:362:PX4:H23 | 0.58 | 1.75 | 14 | 1 |
| 4:A:378:PX4:H20 | 4:A:410:PX4:H48 | 0.58 | 1.75 | 13 | 1 |
| 4:A:374:PX4:H31 | 4:A:427:PX4:H20 | 0.58 | 1.74 | 10 | 1 |
| 4:A:363:PX4:H24 | 4:A:365:PX4:H22 | 0.58 | 1.75 | 13 | 2 |
| 4:A:350:PX4:H54 | 4:A:415:PX4:H43 | 0.58 | 1.76 | 7 | 1 |
| 4:A:392:PX4:H66 | 4:A:415:PX4:H39 | 0.58 | 1.75 | 8 | 1 |
| 4:A:412:PX4:H55 | 4:A:427:PX4:H22 | 0.58 | 1.75 | 3 | 1 |
| 4:A:354:PX4:H60 | 4:A:360:PX4:H63 | 0.58 | 1.76 | 7 | 1 |
| 4:A:314:PX4:H34 | 4:A:362:PX4:H16 | 0.58 | 1.75 | 3 | 1 |
| 4:A:318:PX4:H53 | 4:A:359:PX4:H25 | 0.58 | 1.75 | 2 | 1 |
| 4:A:316:PX4:H61 | 4:A:323:PX4:H70 | 0.58 | 1.76 | 12 | 1 |
| 4:A:382:PX4:H21 | 4:A:428:PX4:H29 | 0.58 | 1.76 | 9 | 1 |
| 4:A:351:PX4:H28 | 4:A:352:PX4:H26 | 0.58 | 1.76 | 4 | 1 |
| 4:A:329:PX4:H69 | 4:A:382:PX4:H41 | 0.58 | 1.75 | 8 | 1 |
| 4:A:410:PX4:H51 | 4:A:426:PX4:H25 | 0.58 | 1.74 | 3 | 1 |
| 4:A:400:PX4:H17 | 4:A:408:PX4:H61 | 0.58 | 1.76 | 12 | 1 |
| 4:A:395:PX4:H49 | 4:A:396:PX4:H20 | 0.58 | 1.74 | 13 | 1 |
| 4:A:317:PX4:H60 | 4:A:325:PX4:H68 | 0.58 | 1.76 | 9 | 1 |
| 4:A:323:PX4:H34 | 4:A:323:PX4:H55 | 0.58 | 1.74 | 9 | 1 |
| 4:A:314:PX4:H49 | 4:A:364:PX4:H18 | 0.58 | 1.75 | 10 | 2 |
| 4:A:326:PX4:H16 | 4:A:351:PX4:H16 | 0.58 | 1.76 | 4 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:348:PX4:H5 | 4:A:355:PX4:O3 | 0.58 | 1.99 | 3 | 1 |
| 4:A:370:PX4:H35 | 4:A:403:PX4:H67 | 0.58 | 1.75 | 3 | 1 |
| 4:A:388:PX4:H20 | 4:A:411:PX4:H19 | 0.58 | 1.74 | 1 | 1 |
| 4:A:372:PX4:H62 | 4:A:379:PX4:H61 | 0.57 | 1.75 | 2 | 1 |
| 4:A:403:PX4:H50 | 4:A:404:PX4:H28 | 0.57 | 1.75 | 8 | 1 |
| 4:A:409:PX4:H29 | 4:A:425:PX4:H71 | 0.57 | 1.76 | 8 | 1 |
| 4:A:393:PX4:H11 | 4:A:401:PX4:H16 | 0.57 | 1.75 | 11 | 1 |
| 4:A:332:PX4:H67 | 4:A:349:PX4:H57 | 0.57 | 1.76 | 12 | 1 |
| 4:A:352:PX4:H20 | 4:A:358:PX4:H15 | 0.57 | 1.75 | 9 | 1 |
| 4:A:410:PX4:H58 | 4:A:426:PX4:H32 | 0.57 | 1.76 | 4 | 1 |
| 4:A:340:PX4:H66 | 4:A:397:PX4:H31 | 0.57 | 1.74 | 11 | 1 |
| 4:A:391:PX4:H62 | 4:A:400:PX4:H32 | 0.57 | 1.76 | 9 | 1 |
| 4:A:402:PX4:H15 | 4:A:404:PX4:H14 | 0.57 | 1.75 | 2 | 1 |
| 4:A:378:PX4:H30 | 4:A:417:PX4:H56 | 0.57 | 1.76 | 10 | 1 |
| 4:A:349:PX4:H17 | 4:A:356:PX4:H21 | 0.57 | 1.76 | 7 | 2 |
| 4:A:337:PX4:H63 | 4:A:353:PX4:H56 | 0.57 | 1.77 | 8 | 1 |
| 4:A:420:PX4:H72 | 4:A:426:PX4:H40 | 0.57 | 1.76 | 8 | 1 |
| 4:A:400:PX4:H28 | 4:A:408:PX4:H52 | 0.57 | 1.75 | 7 | 1 |
| 4:A:334:PX4:H69 | 4:A:352:PX4:H32 | 0.57 | 1.77 | 6 | 1 |
| 4:A:319:PX4:H39 | 4:A:324:PX4:H37 | 0.57 | 1.77 | 14 | 1 |
| 4:A:367:PX4:O2 | 4:A:424:PX4:H1 | 0.57 | 1.99 | 3 | 1 |
| 4:A:318:PX4:H27 | 4:A:327:PX4:H56 | 0.57 | 1.75 | 12 | 1 |
| 4:A:393:PX4:H46 | 4:A:401:PX4:H19 | 0.57 | 1.75 | 4 | 1 |
| 4:A:333:PX4:H39 | 4:A:375:PX4:H28 | 0.57 | 1.76 | 1 | 1 |
| 4:A:330:PX4:H21 | 4:A:335:PX4:H22 | 0.57 | 1.75 | 12 | 1 |
| 4:A:352:PX4:H33 | 4:A:358:PX4:H64 | 0.57 | 1.74 | 4 | 1 |
| 4:A:388:PX4:H17 | 4:A:396:PX4:H22 | 0.57 | 1.75 | 8 | 1 |
| 4:A:334:PX4:H37 | 4:A:407:PX4:H43 | 0.57 | 1.75 | 12 | 1 |
| 4:A:351:PX4:H62 | 4:A:358:PX4:H30 | 0.57 | 1.76 | 13 | 1 |
| 4:A:331:PX4:H11 | 4:A:340:PX4:O1 | 0.57 | 1.99 | 2 | 1 |
| 4:A:314:PX4:H69 | 4:A:350:PX4:H55 | 0.57 | 1.77 | 5 | 1 |
| 4:A:326:PX4:H47 | 4:A:334:PX4:H56 | 0.57 | 1.77 | 8 | 1 |
| 4:A:376:PX4:H52 | 4:A:385:PX4:H21 | 0.57 | 1.77 | 8 | 1 |
| 4:A:342:PX4:O2 | 4:A:352:PX4:H4 | 0.57 | 1.99 | 14 | 1 |
| 4:A:345:PX4:H15 | 4:A:353:PX4:H16 | 0.57 | 1.76 | 2 | 1 |
| 4:A:320:PX4:H20 | 4:A:359:PX4:C29 | 0.57 | 2.26 | 5 | 1 |
| 4:A:371:PX4:H56 | 4:A:378:PX4:H62 | 0.57 | 1.75 | 5 | 1 |
| 4:A:337:PX4:H17 | 4:A:345:PX4:H46 | 0.57 | 1.76 | 4 | 2 |
| 4:A:312:PX4:H65 | 4:A:359:PX4:H37 | 0.57 | 1.76 | 6 | 1 |
| 4:A:344:PX4:H28 | 4:A:348:PX4:H21 | 0.57 | 1.76 | 3 | 1 |
| 4:A:380:PX4:H67 | 4:A:388:PX4:H62 | 0.56 | 1.77 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:375:PX4:H14 | 4:A:375:PX4:H10 | 0.56 | 1.77 | 14 | 1 |
| 4:A:311:PX4:H70 | 4:A:312:PX4:H69 | 0.56 | 1.77 | 3 | 1 |
| 4:A:424:PX4:H17 | 4:A:429:PX4:O6 | 0.56 | 2.00 | 3 | 1 |
| 4:A:349:PX4:H56 | 4:A:350:PX4:H30 | 0.56 | 1.77 | 12 | 1 |
| 4:A:362:PX4:H38 | 4:A:430:PX4:H69 | 0.56 | 1.76 | 12 | 1 |
| 4:A:367:PX4:H47 | 4:A:428:PX4:H48 | 0.56 | 1.76 | 11 | 1 |
| 1:A:207:SER:O | 4:A:321:PX4:H4 | 0.56 | 2.00 | 2 | 1 |
| 4:A:317:PX4:H31 | 4:A:326:PX4:H62 | 0.56 | 1.76 | 5 | 1 |
| 4:A:371:PX4:H68 | 4:A:379:PX4:H41 | 0.56 | 1.76 | 9 | 1 |
| 4:A:393:PX4:H20 | 4:A:401:PX4:H16 | 0.56 | 1.77 | 5 | 2 |
| 4:A:360:PX4:H33 | 4:A:366:PX4:H64 | 0.56 | 1.76 | 5 | 1 |
| 4:A:391:PX4:H21 | 4:A:392:PX4:H47 | 0.56 | 1.78 | 5 | 1 |
| 4:A:400:PX4:H59 | 4:A:426:PX4:H40 | 0.56 | 1.76 | 6 | 1 |
| 4:A:336:PX4:H70 | 4:A:382:PX4:H42 | 0.56 | 1.76 | 8 | 1 |
| 4:A:309:PX4:H63 | 4:A:316:PX4:H65 | 0.56 | 1.77 | 14 | 1 |
| 4:A:329:PX4:H26 | 4:A:336:PX4:H60 | 0.56 | 1.75 | 11 | 1 |
| 4:A:373:PX4:H31 | 4:A:381:PX4:H30 | 0.56 | 1.77 | 11 | 1 |
| 4:A:318:PX4:H27 | 4:A:359:PX4:H23 | 0.56 | 1.76 | 2 | 1 |
| 4:A:320:PX4:C10 | 4:A:359:PX4:H57 | 0.56 | 2.25 | 5 | 1 |
| 4:A:388:PX4:H23 | 4:A:402:PX4:H16 | 0.56 | 1.75 | 3 | 1 |
| 4:A:429:PX4:H53 | 4:A:429:PX4:H33 | 0.56 | 1.77 | 9 | 1 |
| 4:A:315:PX4:H29 | 4:A:361:PX4:H24 | 0.56 | 1.77 | 4 | 1 |
| 4:A:310:PX4:H20 | 4:A:365:PX4:H21 | 0.56 | 1.76 | 14 | 1 |
| 4:A:318:PX4:H64 | 4:A:318:PX4:H43 | 0.56 | 1.78 | 11 | 1 |
| 4:A:379:PX4:H58 | 4:A:420:PX4:H31 | 0.56 | 1.78 | 11 | 1 |
| 4:A:313:PX4:H58 | 4:A:327:PX4:H23 | 0.56 | 1.78 | 2 | 1 |
| 4:A:320:PX4:H19 | 4:A:359:PX4:H59 | 0.56 | 1.77 | 14 | 1 |
| 4:A:316:PX4:H48 | 4:A:320:PX4:H26 | 0.56 | 1.77 | 3 | 1 |
| 4:A:352:PX4:O8 | 4:A:365:PX4:H11 | 0.56 | 2.00 | 1 | 1 |
| 4:A:332:PX4:H56 | 4:A:349:PX4:H48 | 0.56 | 1.76 | 3 | 1 |
| 4:A:402:PX4:H3 | 4:A:404:PX4:O1 | 0.56 | 2.01 | 3 | 1 |
| 4:A:307:PX4:H65 | 4:A:349:PX4:H28 | 0.56 | 1.76 | 11 | 1 |
| 4:A:369:PX4:H56 | 4:A:416:PX4:H69 | 0.56 | 1.78 | 9 | 1 |
| 4:A:400:PX4:H53 | 4:A:410:PX4:H50 | 0.56 | 1.78 | 12 | 1 |
| 4:A:408:PX4:H43 | 4:A:414:PX4:H64 | 0.56 | 1.76 | 12 | 1 |
| 4:A:338:PX4:H71 | 4:A:395:PX4:H40 | 0.56 | 1.78 | 13 | 1 |
| 4:A:389:PX4:H30 | 4:A:397:PX4:H54 | 0.55 | 1.79 | 4 | 1 |
| 1:A:177:LYS:O | 4:A:354:PX4:H13 | 0.55 | 2.01 | 7 | 1 |
| 4:A:337:PX4:H62 | 4:A:366:PX4:H53 | 0.55 | 1.77 | 8 | 1 |
| 4:A:377:PX4:H16 | 4:A:418:PX4:H7 | 0.55 | 1.78 | 8 | 1 |
| 4:A:358:PX4:H19 | 4:A:363:PX4:H49 | 0.55 | 1.77 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:309:PX4:H55 | 4:A:324:PX4:H53 | 0.55 | 1.77 | 12 | 1 |
| 4:A:381:PX4:H29 | 4:A:386:PX4:H58 | 0.55 | 1.77 | 12 | 1 |
| 4:A:380:PX4:H66 | 4:A:411:PX4:H22 | 0.55 | 1.77 | 2 | 1 |
| 4:A:375:PX4:H58 | 4:A:382:PX4:H71 | 0.55 | 1.78 | 6 | 1 |
| 4:A:395:PX4:H36 | 4:A:397:PX4:H61 | 0.55 | 1.76 | 6 | 1 |
| 4:A:330:PX4:H19 | 4:A:338:PX4:H19 | 0.55 | 1.77 | 1 | 1 |
| 4:A:347:PX4:H69 | 4:A:407:PX4:H68 | 0.55 | 1.77 | 11 | 1 |
| 4:A:349:PX4:H54 | 4:A:355:PX4:H34 | 0.55 | 1.76 | 11 | 1 |
| 4:A:412:PX4:H20 | 4:A:428:PX4:H46 | 0.55 | 1.77 | 11 | 1 |
| 4:A:337:PX4:H55 | 4:A:353:PX4:H47 | 0.55 | 1.77 | 10 | 1 |
| 4:A:341:PX4:H34 | 4:A:399:PX4:H69 | 0.55 | 1.78 | 14 | 1 |
| 4:A:326:PX4:H18 | 4:A:334:PX4:H72 | 0.55 | 1.79 | 11 | 1 |
| 4:A:360:PX4:H47 | 4:A:366:PX4:H46 | 0.55 | 1.77 | 11 | 1 |
| 4:A:399:PX4:H25 | 4:A:399:PX4:H59 | 0.55 | 1.77 | 2 | 1 |
| 4:A:392:PX4:H35 | 4:A:399:PX4:H56 | 0.55 | 1.77 | 10 | 1 |
| 4:A:338:PX4:H34 | 4:A:357:PX4:H27 | 0.55 | 1.78 | 9 | 1 |
| 4:A:412:PX4:H19 | 4:A:428:PX4:H54 | 0.55 | 1.79 | 5 | 1 |
| 4:A:354:PX4:H56 | 4:A:360:PX4:H59 | 0.55 | 1.77 | 7 | 1 |
| 4:A:357:PX4:H29 | 4:A:365:PX4:H62 | 0.55 | 1.78 | 14 | 1 |
| 4:A:313:PX4:H64 | 4:A:328:PX4:H68 | 0.55 | 1.77 | 1 | 1 |
| 4:A:416:PX4:H25 | 4:A:422:PX4:H56 | 0.55 | 1.77 | 6 | 1 |
| 4:A:375:PX4:H68 | 4:A:428:PX4:H54 | 0.55 | 1.78 | 14 | 1 |
| 4:A:367:PX4:H2 | 4:A:428:PX4:O8 | 0.55 | 2.02 | 14 | 1 |
| 4:A:329:PX4:H46 | 4:A:336:PX4:H18 | 0.55 | 1.78 | 2 | 1 |
| 4:A:346:PX4:H70 | 4:A:357:PX4:H31 | 0.55 | 1.77 | 6 | 1 |
| 4:A:369:PX4:H38 | 4:A:416:PX4:H63 | 0.55 | 1.78 | 11 | 1 |
| 4:A:360:PX4:H45 | 4:A:404:PX4:H41 | 0.55 | 1.78 | 9 | 1 |
| 4:A:385:PX4:H45 | 4:A:386:PX4:H45 | 0.55 | 1.78 | 10 | 1 |
| 4:A:348:PX4:H69 | 4:A:355:PX4:H27 | 0.55 | 1.79 | 14 | 1 |
| 4:A:316:PX4:H36 | 4:A:364:PX4:H55 | 0.55 | 1.78 | 3 | 1 |
| 4:A:306:PX4:H49 | 4:A:321:PX4:H22 | 0.55 | 1.77 | 1 | 1 |
| 4:A:373:PX4:H20 | 4:A:381:PX4:H18 | 0.55 | 1.78 | 1 | 1 |
| 4:A:395:PX4:H19 | 4:A:396:PX4:H14 | 0.55 | 1.79 | 12 | 1 |
| 4:A:317:PX4:H51 | 4:A:324:PX4:H17 | 0.55 | 1.79 | 11 | 1 |
| 4:A:314:PX4:H46 | 4:A:364:PX4:H18 | 0.55 | 1.79 | 11 | 1 |
| 4:A:392:PX4:H2 | 4:A:392:PX4:O6 | 0.55 | 2.02 | 9 | 1 |
| 4:A:416:PX4:H30 | 4:A:423:PX4:H30 | 0.55 | 1.79 | 2 | 1 |
| 4:A:392:PX4:H60 | 4:A:408:PX4:H31 | 0.55 | 1.78 | 7 | 1 |
| 4:A:339:PX4:H50 | 4:A:339:PX4:H32 | 0.54 | 1.78 | 9 | 1 |
| 4:A:332:PX4:H17 | 4:A:356:PX4:H7 | 0.54 | 1.78 | 2 | 1 |
| 4:A:408:PX4:H72 | 4:A:426:PX4:H69 | 0.54 | 1.79 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:382:PX4:H45 | 4:A:428:PX4:H43 | 0.54 | 1.78 | 8 | 1 |
| 4:A:389:PX4:H63 | 4:A:397:PX4:H35 | 0.54 | 1.78 | 14 | 1 |
| 4:A:307:PX4:H31 | 4:A:364:PX4:H57 | 0.54 | 1.79 | 1 | 1 |
| 4:A:383:PX4:H57 | 4:A:407:PX4:H24 | 0.54 | 1.80 | 9 | 1 |
| 4:A:318:PX4:O2 | 4:A:359:PX4:H14 | 0.54 | 2.03 | 5 | 1 |
| 4:A:321:PX4:H71 | 4:A:322:PX4:H33 | 0.54 | 1.79 | 8 | 1 |
| 4:A:355:PX4:H52 | 4:A:356:PX4:H14 | 0.54 | 1.77 | 1 | 1 |
| 4:A:416:PX4:H20 | 4:A:422:PX4:H48 | 0.54 | 1.80 | 4 | 1 |
| 4:A:330:PX4:H25 | 4:A:343:PX4:H51 | 0.54 | 1.77 | 6 | 1 |
| 4:A:380:PX4:H32 | 4:A:381:PX4:H59 | 0.54 | 1.77 | 3 | 1 |
| 4:A:323:PX4:H55 | 4:A:424:PX4:H70 | 0.54 | 1.77 | 6 | 1 |
| 4:A:307:PX4:H43 | 4:A:311:PX4:H43 | 0.54 | 1.78 | 12 | 1 |
| 4:A:383:PX4:H54 | 4:A:407:PX4:H20 | 0.54 | 1.78 | 9 | 1 |
| 4:A:404:PX4:H21 | 4:A:419:PX4:H10 | 0.54 | 1.79 | 9 | 1 |
| 4:A:317:PX4:H21 | 4:A:342:PX4:H68 | 0.54 | 1.78 | 10 | 1 |
| 4:A:308:PX4:H54 | 4:A:364:PX4:H31 | 0.54 | 1.79 | 4 | 1 |
| 4:A:403:PX4:H61 | 4:A:427:PX4:H62 | 0.54 | 1.78 | 6 | 1 |
| 4:A:372:PX4:H51 | 4:A:420:PX4:H19 | 0.54 | 1.78 | 3 | 1 |
| 4:A:325:PX4:H53 | 4:A:334:PX4:H36 | 0.54 | 1.78 | 12 | 1 |
| 4:A:332:PX4:O8 | 4:A:347:PX4:H52 | 0.54 | 2.03 | 13 | 1 |
| 4:A:331:PX4:H56 | 4:A:339:PX4:H22 | 0.54 | 1.80 | 2 | 1 |
| 4:A:351:PX4:H67 | 4:A:358:PX4:H36 | 0.54 | 1.79 | 2 | 1 |
| 4:A:354:PX4:H28 | 4:A:362:PX4:H17 | 0.54 | 1.79 | 5 | 1 |
| 4:A:372:PX4:H58 | 4:A:379:PX4:H57 | 0.54 | 1.80 | 5 | 1 |
| 4:A:428:PX4:H70 | 4:A:430:PX4:H32 | 0.54 | 1.79 | 1 | 1 |
| 4:A:386:PX4:H25 | 4:A:394:PX4:H20 | 0.54 | 1.79 | 9 | 1 |
| 4:A:338:PX4:H59 | 4:A:348:PX4:H57 | 0.54 | 1.78 | 12 | 1 |
| 4:A:406:PX4:H12 | 4:A:406:PX4:H15 | 0.54 | 1.80 | 9 | 1 |
| 4:A:419:PX4:H63 | 4:A:427:PX4:H60 | 0.54 | 1.80 | 2 | 1 |
| 4:A:423:PX4:H13 | 4:A:430:PX4:H46 | 0.54 | 1.80 | 10 | 1 |
| 4:A:327:PX4:H19 | 4:A:329:PX4:H23 | 0.54 | 1.78 | 5 | 1 |
| 4:A:373:PX4:H25 | 4:A:397:PX4:H15 | 0.54 | 1.79 | 7 | 1 |
| 4:A:416:PX4:H48 | 4:A:425:PX4:H49 | 0.54 | 1.79 | 14 | 1 |
| 4:A:369:PX4:H21 | 4:A:377:PX4:H56 | 0.54 | 1.78 | 1 | 1 |
| 4:A:377:PX4:H51 | 4:A:418:PX4:H52 | 0.54 | 1.79 | 13 | 1 |
| 4:A:370:PX4:H23 | 4:A:427:PX4:H59 | 0.54 | 1.80 | 9 | 1 |
| 4:A:372:PX4:H52 | 4:A:420:PX4:H21 | 0.54 | 1.80 | 4 | 1 |
| 4:A:384:PX4:O2 | 4:A:385:PX4:H18 | 0.54 | 2.03 | 8 | 2 |
| 4:A:307:PX4:H4 | 4:A:322:PX4:O8 | 0.54 | 2.03 | 3 | 1 |
| 4:A:308:PX4:H43 | 4:A:425:PX4:H68 | 0.54 | 1.79 | 13 | 1 |
| 1:A:208:GLY:HA3 | 4:A:307:PX4:H15 | 0.53 | 1.80 | 2 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:340:PX4:H63 | 4:A:397:PX4:H30 | 0.53 | 1.81 | 10 | 1 |
| 4:A:409:PX4:H16 | 4:A:410:PX4:H8 | 0.53 | 1.80 | 4 | 1 |
| 4:A:412:PX4:H48 | 4:A:419:PX4:H22 | 0.53 | 1.80 | 4 | 2 |
| 4:A:367:PX4:H22 | 4:A:424:PX4:H16 | 0.53 | 1.79 | 7 | 1 |
| 4:A:381:PX4:H57 | 4:A:397:PX4:H46 | 0.53 | 1.80 | 6 | 1 |
| 4:A:412:PX4:H54 | 4:A:427:PX4:H22 | 0.53 | 1.79 | 6 | 1 |
| 4:A:391:PX4:H23 | 4:A:414:PX4:H51 | 0.53 | 1.80 | 1 | 1 |
| 4:A:381:PX4:H35 | 4:A:381:PX4:H62 | 0.53 | 1.79 | 11 | 1 |
| 4:A:317:PX4:H26 | 4:A:334:PX4:H40 | 0.53 | 1.80 | 9 | 1 |
| 4:A:400:PX4:H51 | 4:A:409:PX4:H21 | 0.53 | 1.80 | 9 | 1 |
| 4:A:378:PX4:H49 | 4:A:410:PX4:H23 | 0.53 | 1.80 | 6 | 1 |
| 4:A:307:PX4:H29 | 4:A:361:PX4:H28 | 0.53 | 1.80 | 8 | 1 |
| 4:A:337:PX4:H64 | 4:A:345:PX4:H63 | 0.53 | 1.78 | 1 | 1 |
| 4:A:393:PX4:H66 | 4:A:399:PX4:H69 | 0.53 | 1.79 | 12 | 1 |
| 4:A:332:PX4:H44 | 4:A:389:PX4:H57 | 0.53 | 1.79 | 13 | 1 |
| 4:A:371:PX4:H21 | 4:A:379:PX4:H20 | 0.53 | 1.80 | 13 | 1 |
| 4:A:311:PX4:O2 | 4:A:359:PX4:H13 | 0.53 | 2.03 | 5 | 1 |
| 4:A:406:PX4:H27 | 4:A:415:PX4:H59 | 0.53 | 1.80 | 7 | 1 |
| 4:A:328:PX4:H55 | 4:A:329:PX4:H47 | 0.53 | 1.79 | 1 | 1 |
| 4:A:421:PX4:H4 | 4:A:422:PX4:O6 | 0.53 | 2.03 | 1 | 1 |
| 4:A:430:PX4:H28 | 4:A:430:PX4:H71 | 0.53 | 1.79 | 11 | 1 |
| 4:A:388:PX4:H58 | 4:A:397:PX4:H54 | 0.53 | 1.78 | 9 | 1 |
| 4:A:311:PX4:H43 | 4:A:425:PX4:H68 | 0.53 | 1.78 | 5 | 1 |
| 4:A:389:PX4:H48 | 4:A:390:PX4:H49 | 0.53 | 1.79 | 5 | 2 |
| 4:A:311:PX4:H17 | 4:A:359:PX4:H51 | 0.53 | 1.79 | 6 | 2 |
| 4:A:367:PX4:H59 | 4:A:424:PX4:H21 | 0.53 | 1.81 | 4 | 1 |
| 4:A:363:PX4:H70 | 4:A:392:PX4:H66 | 0.53 | 1.81 | 7 | 1 |
| 4:A:345:PX4:H37 | 4:A:403:PX4:H45 | 0.53 | 1.80 | 14 | 1 |
| 4:A:352:PX4:H48 | 4:A:358:PX4:H50 | 0.53 | 1.79 | 3 | 1 |
| 4:A:329:PX4:H66 | 4:A:375:PX4:H35 | 0.53 | 1.79 | 1 | 1 |
| 4:A:395:PX4:H44 | 4:A:398:PX4:H69 | 0.53 | 1.81 | 4 | 1 |
| 4:A:345:PX4:H44 | 4:A:402:PX4:H67 | 0.53 | 1.81 | 6 | 1 |
| 4:A:388:PX4:H18 | 4:A:411:PX4:O2 | 0.53 | 2.04 | 6 | 1 |
| 4:A:386:PX4:H35 | 4:A:394:PX4:H36 | 0.53 | 1.81 | 3 | 1 |
| 4:A:429:PX4:H15 | 4:A:429:PX4:H10 | 0.53 | 1.80 | 3 | 1 |
| 4:A:384:PX4:H19 | 4:A:385:PX4:H23 | 0.53 | 1.79 | 1 | 1 |
| 4:A:350:PX4:H68 | 4:A:351:PX4:H58 | 0.53 | 1.81 | 2 | 1 |
| 4:A:308:PX4:H16 | 4:A:311:PX4:H20 | 0.53 | 1.78 | 5 | 1 |
| 4:A:391:PX4:H49 | 4:A:408:PX4:H16 | 0.53 | 1.80 | 7 | 1 |
| 4:A:338:PX4:H32 | 4:A:348:PX4:H33 | 0.53 | 1.81 | 6 | 1 |
| 4:A:395:PX4:H58 | 4:A:404:PX4:H48 | 0.53 | 1.79 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:398:PX4:H38 | 4:A:414:PX4:H47 | 0.53 | 1.80 | 6 | 1 |
| 4:A:317:PX4:H20 | 4:A:351:PX4:O6 | 0.53 | 2.04 | 11 | 1 |
| 4:A:358:PX4:H29 | 4:A:363:PX4:H26 | 0.53 | 1.79 | 10 | 1 |
| 4:A:325:PX4:H15 | 4:A:341:PX4:H17 | 0.53 | 1.79 | 5 | 1 |
| 4:A:311:PX4:H48 | 4:A:320:PX4:H21 | 0.53 | 1.79 | 4 | 1 |
| 4:A:351:PX4:H66 | 4:A:358:PX4:H32 | 0.53 | 1.79 | 3 | 1 |
| 4:A:345:PX4:H42 | 4:A:388:PX4:H40 | 0.53 | 1.79 | 12 | 1 |
| 4:A:310:PX4:H65 | 4:A:312:PX4:H52 | 0.53 | 1.80 | 9 | 1 |
| 4:A:370:PX4:H69 | 4:A:411:PX4:H65 | 0.53 | 1.80 | 2 | 1 |
| 4:A:416:PX4:H51 | 4:A:418:PX4:H26 | 0.53 | 1.79 | 4 | 1 |
| 4:A:307:PX4:H37 | 4:A:423:PX4:H39 | 0.53 | 1.78 | 4 | 1 |
| 4:A:329:PX4:H30 | 4:A:336:PX4:H68 | 0.53 | 1.79 | 8 | 1 |
| 4:A:400:PX4:H28 | 4:A:426:PX4:H59 | 0.53 | 1.81 | 12 | 1 |
| 4:A:410:PX4:H16 | 4:A:418:PX4:H28 | 0.53 | 1.80 | 12 | 1 |
| 4:A:361:PX4:H34 | 4:A:423:PX4:H35 | 0.53 | 1.80 | 12 | 1 |
| 4:A:309:PX4:H51 | 4:A:316:PX4:H48 | 0.53 | 1.80 | 5 | 1 |
| 4:A:376:PX4:H26 | 4:A:399:PX4:H48 | 0.53 | 1.81 | 4 | 1 |
| 4:A:405:PX4:H22 | 4:A:406:PX4:H61 | 0.53 | 1.79 | 13 | 1 |
| 4:A:335:PX4:H31 | 4:A:343:PX4:H55 | 0.53 | 1.79 | 11 | 1 |
| 4:A:337:PX4:H40 | 4:A:338:PX4:H47 | 0.53 | 1.79 | 10 | 1 |
| 4:A:311:PX4:H24 | 4:A:311:PX4:H60 | 0.53 | 1.81 | 6 | 1 |
| 4:A:392:PX4:H68 | 4:A:400:PX4:H45 | 0.53 | 1.80 | 1 | 1 |
| 4:A:413:PX4:H61 | 4:A:430:PX4:H42 | 0.52 | 1.81 | 9 | 1 |
| 4:A:349:PX4:H58 | 4:A:356:PX4:H42 | 0.52 | 1.80 | 10 | 1 |
| 4:A:398:PX4:H39 | 4:A:414:PX4:H31 | 0.52 | 1.81 | 10 | 1 |
| 4:A:367:PX4:H64 | 4:A:375:PX4:H57 | 0.52 | 1.80 | 7 | 1 |
| 4:A:347:PX4:H20 | 4:A:348:PX4:H14 | 0.52 | 1.81 | 6 | 1 |
| 4:A:412:PX4:H12 | 4:A:419:PX4:O1 | 0.52 | 2.04 | 12 | 1 |
| 4:A:398:PX4:H21 | 4:A:407:PX4:H49 | 0.52 | 1.80 | 10 | 1 |
| 4:A:337:PX4:H56 | 4:A:345:PX4:H59 | 0.52 | 1.81 | 5 | 1 |
| 4:A:306:PX4:H47 | 4:A:322:PX4:H50 | 0.52 | 1.81 | 7 | 1 |
| 4:A:389:PX4:H32 | 4:A:397:PX4:H22 | 0.52 | 1.82 | 6 | 1 |
| 4:A:314:PX4:H53 | 4:A:364:PX4:H18 | 0.52 | 1.81 | 1 | 1 |
| 4:A:326:PX4:H48 | 4:A:334:PX4:H35 | 0.52 | 1.79 | 5 | 1 |
| 4:A:315:PX4:H10 | 4:A:315:PX4:O6 | 0.52 | 2.04 | 4 | 1 |
| 4:A:361:PX4:H26 | 4:A:364:PX4:H54 | 0.52 | 1.81 | 3 | 1 |
| 4:A:346:PX4:H19 | 4:A:354:PX4:H28 | 0.52 | 1.80 | 1 | 1 |
| 4:A:311:PX4:H44 | 4:A:314:PX4:H65 | 0.52 | 1.82 | 13 | 1 |
| 4:A:407:PX4:H30 | 4:A:414:PX4:H61 | 0.52 | 1.81 | 11 | 1 |
| 4:A:410:PX4:H67 | 4:A:417:PX4:H37 | 0.52 | 1.81 | 14 | 1 |
| 4:A:388:PX4:H49 | 4:A:396:PX4:H21 | 0.52 | 1.81 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:313:PX4:H56 | 4:A:327:PX4:H27 | 0.52 | 1.82 | 13 | 1 |
| 4:A:415:PX4:H56 | 4:A:422:PX4:H53 | 0.52 | 1.81 | 13 | 1 |
| 4:A:314:PX4:H33 | 4:A:362:PX4:O8 | 0.52 | 2.04 | 9 | 1 |
| 4:A:329:PX4:H56 | 4:A:336:PX4:H35 | 0.52 | 1.82 | 6 | 2 |
| 4:A:310:PX4:H34 | 4:A:365:PX4:H34 | 0.52 | 1.81 | 3 | 1 |
| 4:A:325:PX4:H55 | 4:A:334:PX4:H40 | 0.52 | 1.81 | 11 | 1 |
| 4:A:313:PX4:H28 | 4:A:366:PX4:H21 | 0.52 | 1.81 | 9 | 1 |
| 4:A:340:PX4:H22 | 4:A:341:PX4:H63 | 0.52 | 1.81 | 2 | 1 |
| 4:A:404:PX4:H21 | 4:A:413:PX4:H30 | 0.52 | 1.81 | 10 | 1 |
| 4:A:308:PX4:H21 | 4:A:311:PX4:H55 | 0.52 | 1.82 | 7 | 1 |
| 4:A:329:PX4:H60 | 4:A:336:PX4:H40 | 0.52 | 1.82 | 8 | 1 |
| 4:A:405:PX4:H51 | 4:A:406:PX4:H51 | 0.52 | 1.81 | 3 | 1 |
| 4:A:400:PX4:H46 | 4:A:409:PX4:H23 | 0.52 | 1.81 | 1 | 1 |
| 4:A:340:PX4:H36 | 4:A:340:PX4:H59 | 0.52 | 1.79 | 12 | 1 |
| 4:A:307:PX4:H45 | 4:A:422:PX4:H39 | 0.52 | 1.80 | 13 | 1 |
| 4:A:317:PX4:H21 | 4:A:326:PX4:H53 | 0.52 | 1.81 | 13 | 1 |
| 4:A:390:PX4:H1 | 4:A:399:PX4:O6 | 0.52 | 2.05 | 13 | 1 |
| 4:A:393:PX4:H71 | 4:A:414:PX4:H53 | 0.52 | 1.81 | 11 | 1 |
| 4:A:342:PX4:H29 | 4:A:352:PX4:H60 | 0.52 | 1.82 | 9 | 1 |
| 4:A:306:PX4:H61 | 4:A:362:PX4:H37 | 0.52 | 1.82 | 9 | 1 |
| 4:A:354:PX4:H69 | 4:A:360:PX4:H27 | 0.52 | 1.81 | 2 | 1 |
| 4:A:405:PX4:H55 | 4:A:406:PX4:H51 | 0.52 | 1.82 | 2 | 1 |
| 4:A:331:PX4:H38 | 4:A:340:PX4:H40 | 0.52 | 1.82 | 10 | 1 |
| 4:A:348:PX4:H52 | 4:A:355:PX4:H67 | 0.52 | 1.81 | 5 | 1 |
| 4:A:312:PX4:H29 | 4:A:365:PX4:H24 | 0.52 | 1.82 | 3 | 1 |
| 4:A:380:PX4:H6 | 4:A:381:PX4:O1 | 0.52 | 2.04 | 11 | 1 |
| 4:A:370:PX4:H19 | 4:A:427:PX4:H55 | 0.52 | 1.82 | 9 | 1 |
| 4:A:410:PX4:H16 | 4:A:418:PX4:H31 | 0.52 | 1.81 | 10 | 1 |
| 4:A:383:PX4:H71 | 4:A:399:PX4:H67 | 0.52 | 1.80 | 5 | 1 |
| 4:A:419:PX4:H67 | 4:A:427:PX4:H69 | 0.52 | 1.81 | 5 | 1 |
| 4:A:310:PX4:H60 | 4:A:312:PX4:H53 | 0.52 | 1.82 | 4 | 2 |
| 4:A:341:PX4:H39 | 4:A:399:PX4:H72 | 0.52 | 1.81 | 5 | 1 |
| 4:A:371:PX4:H56 | 4:A:372:PX4:H23 | 0.52 | 1.82 | 4 | 1 |
| 4:A:306:PX4:H43 | 4:A:328:PX4:H67 | 0.52 | 1.82 | 8 | 1 |
| 4:A:361:PX4:H39 | 4:A:364:PX4:H65 | 0.52 | 1.81 | 9 | 1 |
| 4:A:327:PX4:H14 | 4:A:328:PX4:O2 | 0.52 | 2.05 | 7 | 1 |
| 4:A:308:PX4:H27 | 4:A:316:PX4:H27 | 0.52 | 1.81 | 8 | 1 |
| 4:A:314:PX4:H26 | 4:A:356:PX4:H25 | 0.52 | 1.82 | 12 | 1 |
| 4:A:313:PX4:H61 | 4:A:329:PX4:H25 | 0.52 | 1.81 | 13 | 1 |
| 4:A:324:PX4:H66 | 4:A:341:PX4:H32 | 0.51 | 1.82 | 9 | 1 |
| 4:A:377:PX4:H71 | 4:A:425:PX4:H19 | 0.51 | 1.81 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:409:PX4:H67 | 4:A:415:PX4:H33 | 0.51 | 1.81 | 3 | 1 |
| 4:A:354:PX4:H65 | 4:A:360:PX4:H20 | 0.51 | 1.81 | 1 | 1 |
| 4:A:338:PX4:H67 | 4:A:348:PX4:H58 | 0.51 | 1.82 | 10 | 1 |
| 4:A:321:PX4:H28 | 4:A:412:PX4:H41 | 0.51 | 1.80 | 5 | 1 |
| 4:A:387:PX4:H47 | 4:A:411:PX4:H54 | 0.51 | 1.80 | 5 | 1 |
| 4:A:393:PX4:H23 | 4:A:401:PX4:H16 | 0.51 | 1.81 | 4 | 1 |
| 4:A:421:PX4:H71 | 4:A:422:PX4:H32 | 0.51 | 1.81 | 4 | 1 |
| 4:A:360:PX4:H31 | 4:A:419:PX4:H42 | 0.51 | 1.80 | 7 | 1 |
| 4:A:416:PX4:H45 | 4:A:422:PX4:H67 | 0.51 | 1.81 | 12 | 1 |
| 4:A:323:PX4:H38 | 4:A:361:PX4:H54 | 0.51 | 1.82 | 6 | 1 |
| 4:A:350:PX4:H51 | 4:A:363:PX4:H62 | 0.51 | 1.82 | 8 | 1 |
| 4:A:398:PX4:H44 | 4:A:415:PX4:H27 | 0.51 | 1.82 | 14 | 1 |
| 4:A:360:PX4:H43 | 4:A:403:PX4:H65 | 0.51 | 1.82 | 3 | 1 |
| 4:A:368:PX4:H10 | 4:A:369:PX4:O2 | 0.51 | 2.05 | 1 | 1 |
| 4:A:380:PX4:H32 | 4:A:380:PX4:H60 | 0.51 | 1.80 | 12 | 1 |
| 4:A:400:PX4:H59 | 4:A:410:PX4:H62 | 0.51 | 1.82 | 5 | 1 |
| 4:A:308:PX4:H27 | 4:A:311:PX4:H31 | 0.51 | 1.81 | 4 | 1 |
| 4:A:347:PX4:H56 | 4:A:356:PX4:H58 | 0.51 | 1.83 | 4 | 1 |
| 4:A:417:PX4:H31 | 4:A:426:PX4:H66 | 0.51 | 1.83 | 7 | 1 |
| 4:A:322:PX4:H49 | 4:A:336:PX4:H25 | 0.51 | 1.83 | 9 | 1 |
| 4:A:378:PX4:H29 | 4:A:420:PX4:H57 | 0.51 | 1.82 | 4 | 1 |
| 4:A:402:PX4:H21 | 4:A:404:PX4:H67 | 0.51 | 1.83 | 14 | 1 |
| 4:A:404:PX4:H15 | 4:A:413:PX4:H20 | 0.51 | 1.81 | 1 | 1 |
| 4:A:393:PX4:H18 | 4:A:401:PX4:H20 | 0.51 | 1.83 | 12 | 1 |
| 4:A:345:PX4:H15 | 4:A:353:PX4:H14 | 0.51 | 1.81 | 4 | 2 |
| 4:A:358:PX4:H23 | 4:A:363:PX4:H55 | 0.51 | 1.83 | 12 | 1 |
| 4:A:312:PX4:H31 | 4:A:365:PX4:H46 | 0.51 | 1.82 | 14 | 1 |
| 4:A:346:PX4:H68 | 4:A:362:PX4:H72 | 0.51 | 1.82 | 14 | 1 |
| 4:A:314:PX4:H47 | 4:A:350:PX4:H43 | 0.51 | 1.82 | 14 | 1 |
| 4:A:372:PX4:H34 | 4:A:420:PX4:H29 | 0.51 | 1.82 | 14 | 1 |
| 4:A:363:PX4:H71 | 4:A:392:PX4:H66 | 0.51 | 1.82 | 3 | 1 |
| 4:A:392:PX4:H57 | 4:A:401:PX4:H29 | 0.51 | 1.81 | 13 | 1 |
| 4:A:349:PX4:H26 | 4:A:356:PX4:H38 | 0.51 | 1.83 | 11 | 1 |
| 4:A:306:PX4:H22 | 4:A:321:PX4:H35 | 0.51 | 1.82 | 9 | 1 |
| 4:A:306:PX4:H60 | 4:A:362:PX4:H38 | 0.51 | 1.83 | 10 | 1 |
| 4:A:321:PX4:H56 | 4:A:361:PX4:H54 | 0.51 | 1.82 | 10 | 1 |
| 4:A:311:PX4:O1 | 4:A:359:PX4:H3 | 0.51 | 2.06 | 5 | 2 |
| 4:A:355:PX4:H36 | 4:A:356:PX4:H41 | 0.51 | 1.81 | 4 | 1 |
| 4:A:372:PX4:H23 | 4:A:417:PX4:H46 | 0.51 | 1.83 | 8 | 1 |
| 4:A:410:PX4:H42 | 4:A:418:PX4:H42 | 0.51 | 1.82 | 14 | 1 |
| 4:A:346:PX4:H19 | 4:A:354:PX4:H31 | 0.51 | 1.82 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:343:PX4:H33 | 4:A:344:PX4:H30 | 0.51 | 1.83 | 12 | 1 |
| 4:A:316:PX4:H20 | 4:A:364:PX4:H14 | 0.51 | 1.81 | 12 | 1 |
| 4:A:378:PX4:H59 | 4:A:410:PX4:H26 | 0.51 | 1.82 | 12 | 1 |
| 4:A:309:PX4:H3 | 4:A:320:PX4:O1 | 0.51 | 2.05 | 13 | 1 |
| 4:A:409:PX4:O6 | 4:A:410:PX4:H5 | 0.51 | 2.06 | 13 | 1 |
| 4:A:318:PX4:H53 | 4:A:328:PX4:H22 | 0.51 | 1.81 | 11 | 1 |
| 4:A:333:PX4:H14 | 4:A:340:PX4:H1 | 0.51 | 1.82 | 11 | 1 |
| 4:A:354:PX4:H49 | 4:A:360:PX4:H49 | 0.51 | 1.83 | 4 | 1 |
| 4:A:410:PX4:H16 | 4:A:418:PX4:H29 | 0.51 | 1.81 | 6 | 1 |
| 4:A:333:PX4:H54 | 4:A:341:PX4:H54 | 0.51 | 1.83 | 11 | 1 |
| 4:A:388:PX4:H51 | 4:A:396:PX4:H48 | 0.51 | 1.81 | 10 | 1 |
| 4:A:395:PX4:H24 | 4:A:396:PX4:H64 | 0.51 | 1.83 | 4 | 1 |
| 4:A:320:PX4:H51 | 4:A:359:PX4:H25 | 0.51 | 1.81 | 8 | 1 |
| 4:A:319:PX4:H51 | 4:A:324:PX4:H16 | 0.51 | 1.83 | 1 | 1 |
| 4:A:400:PX4:H20 | 4:A:426:PX4:H50 | 0.51 | 1.82 | 12 | 1 |
| 4:A:390:PX4:H57 | 4:A:429:PX4:H60 | 0.51 | 1.82 | 11 | 1 |
| 4:A:327:PX4:H16 | 4:A:328:PX4:O6 | 0.50 | 2.05 | 5 | 1 |
| 4:A:313:PX4:H20 | 4:A:360:PX4:H15 | 0.50 | 1.82 | 7 | 1 |
| 4:A:344:PX4:H60 | 4:A:344:PX4:H25 | 0.50 | 1.83 | 14 | 1 |
| 4:A:363:PX4:H47 | 4:A:364:PX4:H37 | 0.50 | 1.81 | 14 | 1 |
| 4:A:337:PX4:H39 | 4:A:338:PX4:H51 | 0.50 | 1.83 | 9 | 1 |
| 4:A:307:PX4:H42 | 4:A:350:PX4:H45 | 0.50 | 1.82 | 2 | 1 |
| 4:A:345:PX4:H70 | 4:A:370:PX4:H39 | 0.50 | 1.83 | 10 | 1 |
| 4:A:369:PX4:H19 | 4:A:418:PX4:H15 | 0.50 | 1.83 | 10 | 1 |
| 4:A:388:PX4:H29 | 4:A:411:PX4:H24 | 0.50 | 1.83 | 5 | 1 |
| 1:A:206:HIS:ND1 | 4:A:314:PX4:H1 | 0.50 | 2.21 | 13 | 3 |
| 4:A:310:PX4:H48 | 4:A:365:PX4:H20 | 0.50 | 1.81 | 7 | 1 |
| 4:A:413:PX4:H63 | 4:A:430:PX4:H36 | 0.50 | 1.82 | 7 | 1 |
| 4:A:308:PX4:H18 | 4:A:311:PX4:O8 | 0.50 | 2.06 | 14 | 2 |
| 4:A:402:PX4:H21 | 4:A:403:PX4:H21 | 0.50 | 1.82 | 3 | 1 |
| 4:A:412:PX4:H47 | 4:A:419:PX4:H14 | 0.50 | 1.84 | 12 | 1 |
| 4:A:346:PX4:H12 | 4:A:360:PX4:H46 | 0.50 | 1.82 | 13 | 1 |
| 4:A:403:PX4:H3 | 4:A:427:PX4:H48 | 0.50 | 1.83 | 11 | 1 |
| 4:A:352:PX4:H61 | 4:A:358:PX4:H57 | 0.50 | 1.82 | 9 | 1 |
| 4:A:370:PX4:H17 | 4:A:403:PX4:O1 | 0.50 | 2.06 | 4 | 1 |
| 4:A:311:PX4:O4 | 4:A:359:PX4:H6 | 0.50 | 2.05 | 13 | 1 |
| 4:A:363:PX4:H25 | 4:A:365:PX4:H26 | 0.50 | 1.83 | 13 | 1 |
| 4:A:378:PX4:H35 | 4:A:410:PX4:H60 | 0.50 | 1.83 | 13 | 1 |
| 4:A:416:PX4:H53 | 4:A:418:PX4:H30 | 0.50 | 1.84 | 13 | 1 |
| 4:A:394:PX4:H9 | 4:A:394:PX4:O8 | 0.50 | 2.07 | 14 | 1 |
| 4:A:407:PX4:H9 | 4:A:414:PX4:H48 | 0.50 | 1.83 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:368:PX4:H32 | 4:A:425:PX4:H42 | 0.50 | 1.81 | 3 | 1 |
| 4:A:347:PX4:H35 | 4:A:348:PX4:H28 | 0.50 | 1.83 | 13 | 1 |
| 4:A:378:PX4:H50 | 4:A:418:PX4:H51 | 0.50 | 1.81 | 9 | 1 |
| 4:A:316:PX4:H65 | 4:A:320:PX4:H40 | 0.50 | 1.83 | 5 | 1 |
| 4:A:374:PX4:H22 | 4:A:428:PX4:H20 | 0.50 | 1.82 | 14 | 1 |
| 4:A:383:PX4:H46 | 4:A:399:PX4:H50 | 0.50 | 1.83 | 3 | 1 |
| 4:A:421:PX4:H13 | 4:A:423:PX4:O6 | 0.50 | 2.07 | 1 | 1 |
| 4:A:388:PX4:H24 | 4:A:402:PX4:O8 | 0.50 | 2.05 | 11 | 1 |
| 1:A:237:PHE:CD1 | 1:A:238:PRO:HD2 | 0.50 | 2.42 | 9 | 1 |
| 4:A:392:PX4:H27 | 4:A:393:PX4:H61 | 0.50 | 1.84 | 9 | 1 |
| 4:A:402:PX4:H4 | 4:A:404:PX4:O2 | 0.50 | 2.06 | 11 | 2 |
| 4:A:307:PX4:H67 | 4:A:307:PX4:H34 | 0.50 | 1.84 | 2 | 1 |
| 4:A:408:PX4:H2 | 4:A:408:PX4:H18 | 0.50 | 1.84 | 6 | 1 |
| 4:A:422:PX4:H38 | 4:A:423:PX4:H40 | 0.50 | 1.83 | 6 | 1 |
| 4:A:384:PX4:H56 | 4:A:385:PX4:H32 | 0.50 | 1.82 | 3 | 1 |
| 4:A:409:PX4:H54 | 4:A:422:PX4:H62 | 0.50 | 1.82 | 3 | 1 |
| 4:A:395:PX4:H42 | 4:A:405:PX4:H36 | 0.50 | 1.81 | 13 | 1 |
| 4:A:416:PX4:H24 | 4:A:422:PX4:H17 | 0.50 | 1.83 | 10 | 1 |
| 4:A:369:PX4:H18 | 4:A:425:PX4:H9 | 0.50 | 1.82 | 4 | 1 |
| 4:A:400:PX4:H30 | 4:A:401:PX4:H57 | 0.50 | 1.83 | 1 | 1 |
| 4:A:408:PX4:H17 | 4:A:415:PX4:O6 | 0.50 | 2.07 | 1 | 1 |
| 4:A:345:PX4:H46 | 4:A:346:PX4:H56 | 0.50 | 1.84 | 12 | 1 |
| 4:A:371:PX4:H68 | 4:A:371:PX4:H35 | 0.50 | 1.83 | 12 | 1 |
| 4:A:322:PX4:O2 | 4:A:333:PX4:H9 | 0.50 | 2.07 | 13 | 1 |
| 4:A:321:PX4:H24 | 4:A:354:PX4:H53 | 0.50 | 1.81 | 2 | 2 |
| 4:A:306:PX4:H19 | 4:A:321:PX4:H42 | 0.50 | 1.84 | 6 | 1 |
| 4:A:380:PX4:H49 | 4:A:381:PX4:H13 | 0.50 | 1.83 | 12 | 1 |
| 4:A:400:PX4:H68 | 4:A:410:PX4:H67 | 0.49 | 1.84 | 10 | 1 |
| 4:A:308:PX4:H40 | 4:A:316:PX4:H41 | 0.49 | 1.84 | 4 | 1 |
| 4:A:428:PX4:H63 | 4:A:430:PX4:H32 | 0.49 | 1.84 | 8 | 1 |
| 4:A:338:PX4:H17 | 4:A:348:PX4:H17 | 0.49 | 1.84 | 1 | 1 |
| 4:A:356:PX4:H32 | 4:A:362:PX4:H27 | 0.49 | 1.82 | 1 | 1 |
| 4:A:395:PX4:H58 | 4:A:404:PX4:H50 | 0.49 | 1.83 | 1 | 1 |
| 4:A:409:PX4:H51 | 4:A:415:PX4:C11 | 0.49 | 2.36 | 8 | 1 |
| 4:A:390:PX4:H62 | 4:A:397:PX4:H42 | 0.49 | 1.84 | 9 | 1 |
| 4:A:347:PX4:H22 | 4:A:348:PX4:H56 | 0.49 | 1.83 | 5 | 1 |
| 4:A:393:PX4:H3 | 4:A:401:PX4:O2 | 0.49 | 2.08 | 5 | 1 |
| 4:A:374:PX4:H18 | 4:A:382:PX4:O7 | 0.49 | 2.06 | 8 | 1 |
| 4:A:306:PX4:H22 | 4:A:322:PX4:H57 | 0.49 | 1.84 | 1 | 1 |
| 4:A:312:PX4:H29 | 4:A:365:PX4:H22 | 0.49 | 1.84 | 12 | 1 |
| 4:A:393:PX4:H37 | 4:A:401:PX4:H70 | 0.49 | 1.84 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:421:PX4:H67 | 4:A:423:PX4:H45 | 0.49 | 1.83 | 3 | 1 |
| 4:A:308:PX4:O6 | 4:A:364:PX4:H3 | 0.49 | 2.07 | 12 | 1 |
| 4:A:372:PX4:H20 | 4:A:420:PX4:H16 | 0.49 | 1.84 | 13 | 2 |
| 4:A:317:PX4:H14 | 4:A:351:PX4:H20 | 0.49 | 1.85 | 5 | 1 |
| 4:A:316:PX4:H51 | 4:A:320:PX4:C14 | 0.49 | 2.37 | 12 | 1 |
| 4:A:312:PX4:H35 | 4:A:365:PX4:H46 | 0.49 | 1.83 | 13 | 1 |
| 4:A:377:PX4:H42 | 4:A:379:PX4:H56 | 0.49 | 1.84 | 13 | 1 |
| 4:A:337:PX4:H9 | 4:A:357:PX4:H2 | 0.49 | 1.84 | 11 | 1 |
| 4:A:316:PX4:H29 | 4:A:361:PX4:H25 | 0.49 | 1.85 | 2 | 1 |
| 4:A:369:PX4:H20 | 4:A:377:PX4:H46 | 0.49 | 1.85 | 4 | 1 |
| 4:A:326:PX4:O6 | 4:A:363:PX4:H61 | 0.49 | 2.07 | 8 | 1 |
| 4:A:347:PX4:H21 | 4:A:348:PX4:H55 | 0.49 | 1.83 | 3 | 1 |
| 4:A:313:PX4:H65 | 4:A:360:PX4:H70 | 0.49 | 1.85 | 1 | 1 |
| 4:A:345:PX4:O1 | 4:A:346:PX4:H9 | 0.49 | 2.08 | 9 | 1 |
| 4:A:340:PX4:H42 | 4:A:389:PX4:H27 | 0.49 | 1.84 | 9 | 1 |
| 4:A:335:PX4:O6 | 4:A:343:PX4:H14 | 0.49 | 2.08 | 5 | 1 |
| 4:A:419:PX4:H42 | 4:A:427:PX4:H41 | 0.49 | 1.83 | 5 | 1 |
| 4:A:326:PX4:H19 | 4:A:334:PX4:H55 | 0.49 | 1.83 | 4 | 1 |
| 4:A:348:PX4:H35 | 4:A:380:PX4:H42 | 0.49 | 1.83 | 7 | 1 |
| 4:A:390:PX4:O1 | 4:A:399:PX4:H12 | 0.49 | 2.08 | 6 | 1 |
| 4:A:306:PX4:H59 | 4:A:361:PX4:H57 | 0.49 | 1.84 | 8 | 1 |
| 4:A:344:PX4:H56 | 4:A:347:PX4:H33 | 0.49 | 1.84 | 10 | 1 |
| 4:A:408:PX4:H4 | 4:A:414:PX4:O2 | 0.49 | 2.07 | 10 | 2 |
| 4:A:332:PX4:H53 | 4:A:356:PX4:H47 | 0.49 | 1.84 | 5 | 1 |
| 4:A:392:PX4:H70 | 4:A:415:PX4:H33 | 0.49 | 1.84 | 7 | 1 |
| 4:A:406:PX4:H23 | 4:A:415:PX4:H22 | 0.49 | 1.85 | 13 | 1 |
| 4:A:337:PX4:H31 | 4:A:338:PX4:H28 | 0.49 | 1.84 | 10 | 1 |
| 4:A:313:PX4:H51 | 4:A:354:PX4:H66 | 0.49 | 1.85 | 5 | 1 |
| 4:A:337:PX4:H42 | 4:A:347:PX4:H30 | 0.49 | 1.84 | 7 | 1 |
| 4:A:395:PX4:H19 | 4:A:396:PX4:H15 | 0.49 | 1.85 | 8 | 1 |
| 4:A:313:PX4:H15 | 4:A:360:PX4:C9 | 0.49 | 2.38 | 14 | 1 |
| 4:A:312:PX4:H25 | 4:A:365:PX4:H20 | 0.49 | 1.84 | 3 | 1 |
| 4:A:332:PX4:H52 | 4:A:347:PX4:H65 | 0.49 | 1.85 | 3 | 1 |
| 4:A:337:PX4:H48 | 4:A:345:PX4:H51 | 0.49 | 1.82 | 12 | 1 |
| 4:A:393:PX4:H32 | 4:A:401:PX4:H53 | 0.49 | 1.83 | 12 | 1 |
| 4:A:326:PX4:H69 | 4:A:393:PX4:H62 | 0.49 | 1.83 | 9 | 1 |
| 4:A:344:PX4:H52 | 4:A:347:PX4:H27 | 0.49 | 1.84 | 9 | 1 |
| 4:A:361:PX4:H37 | 4:A:423:PX4:H36 | 0.49 | 1.84 | 9 | 1 |
| 4:A:385:PX4:H49 | 4:A:393:PX4:H52 | 0.49 | 1.84 | 5 | 1 |
| 4:A:400:PX4:H39 | 4:A:401:PX4:H35 | 0.49 | 1.84 | 5 | 1 |
| 4:A:421:PX4:H26 | 4:A:423:PX4:H22 | 0.49 | 1.85 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:319:PX4:H17 | 4:A:324:PX4:O4 | 0.49 | 2.08 | 8 | 1 |
| 4:A:400:PX4:H57 | 4:A:408:PX4:H72 | 0.49 | 1.85 | 8 | 1 |
| 4:A:405:PX4:H64 | 4:A:406:PX4:H67 | 0.49 | 1.85 | 3 | 1 |
| 4:A:415:PX4:H56 | 4:A:421:PX4:H68 | 0.49 | 1.83 | 3 | 1 |
| 4:A:387:PX4:H47 | 4:A:411:PX4:C8 | 0.49 | 2.34 | 12 | 1 |
| 4:A:321:PX4:H34 | 4:A:322:PX4:H58 | 0.49 | 1.83 | 13 | 1 |
| 4:A:376:PX4:H59 | 4:A:385:PX4:H57 | 0.48 | 1.84 | 5 | 1 |
| 4:A:385:PX4:H23 | 4:A:386:PX4:H28 | 0.48 | 1.85 | 5 | 1 |
| 4:A:335:PX4:H1 | 4:A:344:PX4:O6 | 0.48 | 2.08 | 4 | 1 |
| 4:A:355:PX4:H54 | 4:A:356:PX4:H47 | 0.48 | 1.85 | 8 | 1 |
| 4:A:367:PX4:H18 | 4:A:424:PX4:O3 | 0.48 | 2.08 | 8 | 1 |
| 4:A:316:PX4:H64 | 4:A:323:PX4:H69 | 0.48 | 1.84 | 14 | 1 |
| 4:A:376:PX4:H61 | 4:A:392:PX4:H32 | 0.48 | 1.85 | 14 | 1 |
| 4:A:373:PX4:O2 | 4:A:382:PX4:H9 | 0.48 | 2.08 | 12 | 1 |
| 4:A:308:PX4:H19 | 4:A:311:PX4:H52 | 0.48 | 1.85 | 2 | 1 |
| 4:A:406:PX4:H28 | 4:A:421:PX4:H63 | 0.48 | 1.86 | 5 | 1 |
| 4:A:404:PX4:H48 | 4:A:413:PX4:O6 | 0.48 | 2.08 | 4 | 1 |
| 4:A:385:PX4:H28 | 4:A:386:PX4:H28 | 0.48 | 1.85 | 7 | 1 |
| 4:A:322:PX4:H56 | 4:A:336:PX4:H31 | 0.48 | 1.85 | 3 | 1 |
| 4:A:369:PX4:H32 | 4:A:410:PX4:H21 | 0.48 | 1.83 | 2 | 1 |
| 4:A:372:PX4:H25 | 4:A:420:PX4:H50 | 0.48 | 1.84 | 4 | 1 |
| 4:A:421:PX4:H40 | 4:A:423:PX4:H53 | 0.48 | 1.85 | 7 | 1 |
| 4:A:332:PX4:H43 | 4:A:407:PX4:H61 | 0.48 | 1.85 | 3 | 1 |
| 4:A:311:PX4:H31 | 4:A:364:PX4:H27 | 0.48 | 1.86 | 11 | 1 |
| 4:A:357:PX4:H29 | 4:A:357:PX4:H71 | 0.48 | 1.84 | 10 | 1 |
| 4:A:376:PX4:H60 | 4:A:392:PX4:H25 | 0.48 | 1.84 | 5 | 1 |
| 4:A:316:PX4:H24 | 4:A:364:PX4:H47 | 0.48 | 1.86 | 8 | 1 |
| 4:A:320:PX4:H71 | 4:A:378:PX4:H40 | 0.48 | 1.85 | 8 | 1 |
| 4:A:307:PX4:H71 | 4:A:349:PX4:H45 | 0.48 | 1.84 | 1 | 1 |
| 4:A:307:PX4:H22 | 4:A:321:PX4:H64 | 0.48 | 1.83 | 13 | 1 |
| 4:A:389:PX4:H51 | 4:A:390:PX4:H24 | 0.48 | 1.85 | 13 | 1 |
| 4:A:378:PX4:H2 | 4:A:410:PX4:O6 | 0.48 | 2.09 | 13 | 1 |
| 4:A:345:PX4:H20 | 4:A:346:PX4:H15 | 0.48 | 1.85 | 11 | 1 |
| 4:A:326:PX4:H21 | 4:A:350:PX4:H17 | 0.48 | 1.85 | 9 | 1 |
| 4:A:309:PX4:H65 | 4:A:320:PX4:H36 | 0.48 | 1.85 | 2 | 1 |
| 4:A:349:PX4:H38 | 4:A:421:PX4:H42 | 0.48 | 1.85 | 10 | 1 |
| 4:A:400:PX4:H46 | 4:A:409:PX4:H20 | 0.48 | 1.85 | 10 | 1 |
| 4:A:400:PX4:H40 | 4:A:401:PX4:H45 | 0.48 | 1.85 | 1 | 1 |
| 4:A:310:PX4:O6 | 4:A:365:PX4:H11 | 0.48 | 2.08 | 12 | 1 |
| 4:A:400:PX4:H60 | 4:A:410:PX4:H54 | 0.48 | 1.85 | 13 | 1 |
| 4:A:346:PX4:H50 | 4:A:362:PX4:H56 | 0.48 | 1.86 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:354:PX4:H24 | 4:A:362:PX4:H17 | 0.48 | 1.84 | 11 | 1 |
| 4:A:330:PX4:C11 | 4:A:335:PX4:H19 | 0.48 | 2.36 | 2 | 1 |
| 4:A:393:PX4:H42 | 4:A:401:PX4:H40 | 0.48 | 1.84 | 2 | 1 |
| 4:A:353:PX4:H70 | 4:A:412:PX4:H37 | 0.48 | 1.86 | 5 | 1 |
| 4:A:377:PX4:H60 | 4:A:416:PX4:H62 | 0.48 | 1.85 | 5 | 1 |
| 4:A:331:PX4:O6 | 4:A:340:PX4:H4 | 0.48 | 2.08 | 1 | 1 |
| 4:A:392:PX4:H67 | 4:A:408:PX4:H36 | 0.48 | 1.84 | 12 | 1 |
| 4:A:388:PX4:H23 | 4:A:396:PX4:H30 | 0.48 | 1.84 | 11 | 1 |
| 4:A:390:PX4:H62 | 4:A:397:PX4:C21 | 0.48 | 2.38 | 9 | 1 |
| 4:A:358:PX4:H27 | 4:A:363:PX4:H26 | 0.48 | 1.86 | 2 | 1 |
| 4:A:337:PX4:H50 | 4:A:353:PX4:H25 | 0.48 | 1.84 | 10 | 1 |
| 4:A:337:PX4:H30 | 4:A:338:PX4:H48 | 0.48 | 1.86 | 5 | 1 |
| 1:A:242:TYR:CD1 | 4:A:314:PX4:H19 | 0.48 | 2.43 | 4 | 1 |
| 4:A:374:PX4:H29 | 4:A:427:PX4:H31 | 0.48 | 1.86 | 7 | 1 |
| 4:A:319:PX4:H21 | 4:A:324:PX4:H19 | 0.48 | 1.84 | 6 | 1 |
| 4:A:369:PX4:H18 | 4:A:425:PX4:H1 | 0.48 | 1.86 | 1 | 1 |
| 4:A:395:PX4:H48 | 4:A:405:PX4:H19 | 0.48 | 1.86 | 12 | 2 |
| 1:A:145:THR:HB | 1:A:146:PRO:HD2 | 0.48 | 1.85 | 2 | 1 |
| 4:A:331:PX4:H18 | 4:A:340:PX4:H21 | 0.48 | 1.84 | 5 | 1 |
| 4:A:318:PX4:O2 | 4:A:359:PX4:H18 | 0.48 | 2.07 | 4 | 1 |
| 4:A:323:PX4:H26 | 4:A:333:PX4:H17 | 0.48 | 1.85 | 4 | 1 |
| 4:A:346:PX4:H51 | 4:A:355:PX4:H14 | 0.48 | 1.85 | 6 | 1 |
| 4:A:406:PX4:H18 | 4:A:415:PX4:O1 | 0.48 | 2.09 | 11 | 1 |
| 4:A:307:PX4:H49 | 4:A:321:PX4:H56 | 0.48 | 1.86 | 5 | 1 |
| 4:A:315:PX4:H45 | 4:A:425:PX4:H27 | 0.48 | 1.85 | 7 | 1 |
| 4:A:348:PX4:H55 | 4:A:388:PX4:H71 | 0.48 | 1.84 | 6 | 1 |
| 4:A:326:PX4:H20 | 4:A:350:PX4:H48 | 0.48 | 1.86 | 8 | 1 |
| 4:A:404:PX4:H53 | 4:A:413:PX4:H24 | 0.48 | 1.86 | 14 | 1 |
| 4:A:326:PX4:H49 | 4:A:351:PX4:H18 | 0.48 | 1.84 | 1 | 1 |
| 4:A:351:PX4:C5 | 4:A:352:PX4:H24 | 0.48 | 2.39 | 9 | 1 |
| 4:A:404:PX4:H59 | 4:A:430:PX4:H40 | 0.48 | 1.86 | 4 | 1 |
| 4:A:347:PX4:H13 | 4:A:348:PX4:O1 | 0.48 | 2.08 | 6 | 3 |
| 4:A:416:PX4:O3 | 4:A:416:PX4:H10 | 0.48 | 2.09 | 1 | 1 |
| 4:A:321:PX4:H15 | 4:A:354:PX4:H15 | 0.48 | 1.85 | 12 | 1 |
| 4:A:337:PX4:H22 | 4:A:337:PX4:H8 | 0.48 | 1.85 | 12 | 1 |
| 4:A:421:PX4:H30 | 4:A:423:PX4:H19 | 0.48 | 1.86 | 12 | 1 |
| 4:A:325:PX4:H62 | 4:A:334:PX4:H45 | 0.48 | 1.86 | 11 | 1 |
| 4:A:357:PX4:H39 | 4:A:402:PX4:H41 | 0.47 | 1.84 | 4 | 1 |
| 4:A:308:PX4:O1 | 4:A:311:PX4:H14 | 0.47 | 2.10 | 7 | 1 |
| 4:A:349:PX4:H30 | 4:A:356:PX4:H38 | 0.47 | 1.86 | 7 | 1 |
| 4:A:424:PX4:H69 | 4:A:429:PX4:H67 | 0.47 | 1.86 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:325:PX4:H17 | 4:A:341:PX4:H47 | 0.47 | 1.85 | 14 | 1 |
| 4:A:373:PX4:H60 | 4:A:381:PX4:H25 | 0.47 | 1.85 | 3 | 1 |
| 4:A:331:PX4:H14 | 4:A:347:PX4:H14 | 0.47 | 1.86 | 5 | 1 |
| 4:A:421:PX4:H30 | 4:A:430:PX4:H19 | 0.47 | 1.84 | 5 | 1 |
| 4:A:402:PX4:O2 | 4:A:402:PX4:H10 | 0.47 | 2.09 | 7 | 1 |
| 4:A:413:PX4:H50 | 4:A:430:PX4:H23 | 0.47 | 1.86 | 7 | 1 |
| 4:A:388:PX4:H17 | 4:A:396:PX4:O6 | 0.47 | 2.09 | 1 | 2 |
| 4:A:338:PX4:H68 | 4:A:396:PX4:H38 | 0.47 | 1.85 | 2 | 1 |
| 4:A:326:PX4:H35 | 4:A:350:PX4:H52 | 0.47 | 1.86 | 10 | 1 |
| 4:A:322:PX4:H25 | 4:A:361:PX4:H48 | 0.47 | 1.86 | 10 | 2 |
| 4:A:314:PX4:H61 | 4:A:364:PX4:H71 | 0.47 | 1.86 | 7 | 1 |
| 4:A:351:PX4:H55 | 4:A:358:PX4:H52 | 0.47 | 1.86 | 7 | 1 |
| 4:A:332:PX4:H3 | 4:A:356:PX4:O3 | 0.47 | 2.08 | 14 | 1 |
| 4:A:376:PX4:H68 | 4:A:385:PX4:H63 | 0.47 | 1.87 | 14 | 1 |
| 4:A:367:PX4:H28 | 4:A:423:PX4:H50 | 0.47 | 1.85 | 14 | 1 |
| 4:A:335:PX4:H24 | 4:A:344:PX4:H24 | 0.47 | 1.86 | 11 | 1 |
| 4:A:372:PX4:H55 | 4:A:379:PX4:H53 | 0.47 | 1.86 | 2 | 1 |
| 4:A:311:PX4:H69 | 4:A:320:PX4:H44 | 0.47 | 1.86 | 10 | 1 |
| 4:A:310:PX4:H48 | 4:A:312:PX4:H21 | 0.47 | 1.86 | 10 | 1 |
| 4:A:342:PX4:H54 | 4:A:351:PX4:H29 | 0.47 | 1.86 | 11 | 2 |
| 4:A:398:PX4:H40 | 4:A:414:PX4:H32 | 0.47 | 1.86 | 6 | 1 |
| 4:A:355:PX4:H20 | 4:A:362:PX4:H51 | 0.47 | 1.86 | 14 | 1 |
| 4:A:421:PX4:H5 | 4:A:423:PX4:O1 | 0.47 | 2.09 | 3 | 2 |
| 4:A:368:PX4:H1 | 4:A:369:PX4:O2 | 0.47 | 2.09 | 1 | 1 |
| 4:A:378:PX4:H52 | 4:A:410:PX4:H26 | 0.47 | 1.87 | 13 | 1 |
| 4:A:345:PX4:H19 | 4:A:346:PX4:H19 | 0.47 | 1.86 | 11 | 1 |
| 4:A:405:PX4:H54 | 4:A:414:PX4:H30 | 0.47 | 1.86 | 11 | 1 |
| 4:A:399:PX4:O1 | 4:A:407:PX4:H7 | 0.47 | 2.10 | 9 | 1 |
| 4:A:325:PX4:H12 | 4:A:325:PX4:H14 | 0.47 | 1.87 | 5 | 1 |
| 1:A:205:THR:O | 4:A:314:PX4:H9 | 0.47 | 2.09 | 4 | 1 |
| 4:A:338:PX4:H70 | 4:A:362:PX4:H44 | 0.47 | 1.86 | 4 | 1 |
| 4:A:317:PX4:O1 | 4:A:351:PX4:H20 | 0.47 | 2.09 | 4 | 1 |
| 4:A:412:PX4:H5 | 4:A:427:PX4:O1 | 0.47 | 2.10 | 7 | 1 |
| 4:A:326:PX4:H51 | 4:A:334:PX4:H40 | 0.47 | 1.87 | 3 | 1 |
| 4:A:351:PX4:H56 | 4:A:358:PX4:H56 | 0.47 | 1.86 | 3 | 1 |
| 4:A:325:PX4:H17 | 4:A:341:PX4:H17 | 0.47 | 1.87 | 1 | 1 |
| 4:A:400:PX4:H47 | 4:A:426:PX4:H26 | 0.47 | 1.85 | 12 | 1 |
| 4:A:417:PX4:H64 | 4:A:420:PX4:H60 | 0.47 | 1.86 | 4 | 1 |
| 4:A:340:PX4:H47 | 4:A:341:PX4:H61 | 0.47 | 1.87 | 7 | 1 |
| 4:A:405:PX4:O2 | 4:A:406:PX4:H12 | 0.47 | 2.09 | 7 | 1 |
| 4:A:424:PX4:H48 | 4:A:425:PX4:H22 | 0.47 | 1.86 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:358:PX4:H20 | 4:A:363:PX4:H18 | 0.47 | 1.86 | 14 | 2 |
| 4:A:361:PX4:H31 | 4:A:367:PX4:H42 | 0.47 | 1.84 | 1 | 1 |
| 4:A:316:PX4:H61 | 4:A:323:PX4:C36 | 0.47 | 2.38 | 12 | 1 |
| 4:A:309:PX4:O6 | 4:A:320:PX4:H4 | 0.47 | 2.09 | 9 | 1 |
| 4:A:358:PX4:H38 | 4:A:365:PX4:H34 | 0.47 | 1.86 | 9 | 1 |
| 4:A:396:PX4:H63 | 4:A:398:PX4:H50 | 0.47 | 1.86 | 9 | 1 |
| 4:A:400:PX4:O2 | 4:A:426:PX4:H14 | 0.47 | 2.09 | 9 | 1 |
| 4:A:359:PX4:H44 | 4:A:372:PX4:H40 | 0.47 | 1.87 | 2 | 1 |
| 4:A:346:PX4:H46 | 4:A:355:PX4:O1 | 0.47 | 2.10 | 10 | 1 |
| 4:A:306:PX4:H70 | 4:A:349:PX4:H35 | 0.47 | 1.86 | 5 | 1 |
| 4:A:346:PX4:H29 | 4:A:354:PX4:H19 | 0.47 | 1.86 | 5 | 1 |
| 4:A:322:PX4:H40 | 4:A:361:PX4:H54 | 0.47 | 1.84 | 5 | 1 |
| 4:A:395:PX4:H59 | 4:A:405:PX4:H42 | 0.47 | 1.84 | 5 | 1 |
| 4:A:310:PX4:H54 | 4:A:312:PX4:H22 | 0.47 | 1.87 | 5 | 1 |
| 4:A:308:PX4:H54 | 4:A:364:PX4:H30 | 0.47 | 1.85 | 5 | 1 |
| 4:A:349:PX4:H12 | 4:A:349:PX4:O6 | 0.47 | 2.09 | 4 | 1 |
| 4:A:336:PX4:H36 | 4:A:361:PX4:H67 | 0.47 | 1.86 | 4 | 1 |
| 1:A:214:LEU:HD23 | 1:A:214:LEU:H | 0.47 | 1.69 | 7 | 1 |
| 4:A:390:PX4:H60 | 4:A:390:PX4:H29 | 0.47 | 1.86 | 7 | 1 |
| 4:A:345:PX4:O1 | 4:A:346:PX4:H13 | 0.47 | 2.08 | 6 | 1 |
| 4:A:360:PX4:H3 | 4:A:366:PX4:O4 | 0.47 | 2.10 | 6 | 1 |
| 4:A:403:PX4:H52 | 4:A:419:PX4:H55 | 0.47 | 1.86 | 6 | 1 |
| 4:A:331:PX4:H69 | 4:A:347:PX4:H42 | 0.47 | 1.85 | 14 | 1 |
| 4:A:381:PX4:H52 | 4:A:388:PX4:H46 | 0.47 | 1.86 | 14 | 1 |
| 4:A:392:PX4:H51 | 4:A:408:PX4:H24 | 0.47 | 1.85 | 14 | 1 |
| 4:A:306:PX4:H29 | 4:A:336:PX4:H31 | 0.47 | 1.87 | 1 | 1 |
| 4:A:319:PX4:H12 | 4:A:342:PX4:O2 | 0.47 | 2.09 | 1 | 1 |
| 4:A:335:PX4:H48 | 4:A:343:PX4:H22 | 0.47 | 1.86 | 12 | 1 |
| 4:A:402:PX4:H37 | 4:A:413:PX4:H36 | 0.47 | 1.86 | 13 | 1 |
| 4:A:391:PX4:H64 | 4:A:409:PX4:H62 | 0.47 | 1.87 | 13 | 1 |
| 4:A:405:PX4:H9 | 4:A:405:PX4:O6 | 0.47 | 2.10 | 11 | 1 |
| 4:A:388:PX4:H52 | 4:A:411:PX4:H28 | 0.47 | 1.87 | 11 | 1 |
| 4:A:315:PX4:H28 | 4:A:322:PX4:H40 | 0.47 | 1.87 | 9 | 1 |
| 4:A:400:PX4:H48 | 4:A:410:PX4:H46 | 0.47 | 1.87 | 10 | 1 |
| 4:A:412:PX4:H27 | 4:A:413:PX4:H38 | 0.47 | 1.84 | 10 | 1 |
| 4:A:389:PX4:H21 | 4:A:396:PX4:H71 | 0.47 | 1.87 | 5 | 1 |
| 4:A:371:PX4:H71 | 4:A:378:PX4:H62 | 0.47 | 1.87 | 14 | 1 |
| 4:A:323:PX4:H43 | 4:A:424:PX4:H27 | 0.47 | 1.86 | 1 | 1 |
| 4:A:413:PX4:H66 | 4:A:422:PX4:H41 | 0.47 | 1.87 | 1 | 1 |
| 4:A:376:PX4:H23 | 4:A:399:PX4:H49 | 0.47 | 1.86 | 11 | 1 |
| 4:A:355:PX4:H61 | 4:A:355:PX4:H17 | 0.47 | 1.85 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:408:PX4:H72 | 4:A:426:PX4:H57 | 0.47 | 1.87 | 9 | 1 |
| 4:A:391:PX4:H41 | 4:A:408:PX4:H39 | 0.47 | 1.85 | 10 | 1 |
| 4:A:334:PX4:H41 | 4:A:408:PX4:H41 | 0.47 | 1.87 | 5 | 1 |
| 4:A:350:PX4:H49 | 4:A:363:PX4:H50 | 0.47 | 1.87 | 5 | 1 |
| 4:A:307:PX4:H64 | 4:A:321:PX4:H67 | 0.47 | 1.87 | 4 | 1 |
| 4:A:375:PX4:H68 | 4:A:419:PX4:H32 | 0.47 | 1.86 | 4 | 1 |
| 4:A:369:PX4:H32 | 4:A:377:PX4:H61 | 0.47 | 1.86 | 4 | 1 |
| 4:A:400:PX4:H17 | 4:A:408:PX4:H53 | 0.47 | 1.85 | 7 | 1 |
| 4:A:398:PX4:H16 | 4:A:407:PX4:H46 | 0.47 | 1.85 | 7 | 1 |
| 4:A:312:PX4:H28 | 4:A:365:PX4:H46 | 0.47 | 1.85 | 8 | 1 |
| 4:A:332:PX4:H37 | 4:A:390:PX4:H39 | 0.47 | 1.86 | 14 | 1 |
| 4:A:326:PX4:H36 | 4:A:349:PX4:H71 | 0.47 | 1.87 | 1 | 1 |
| 4:A:371:PX4:H39 | 4:A:420:PX4:H36 | 0.47 | 1.86 | 11 | 1 |
| 4:A:416:PX4:H57 | 4:A:423:PX4:H64 | 0.47 | 1.86 | 9 | 1 |
| 4:A:388:PX4:H34 | 4:A:402:PX4:H24 | 0.47 | 1.87 | 4 | 1 |
| 4:A:402:PX4:H51 | 4:A:404:PX4:H47 | 0.47 | 1.87 | 3 | 1 |
| 4:A:322:PX4:H25 | 4:A:361:PX4:H46 | 0.47 | 1.85 | 13 | 1 |
| 4:A:419:PX4:O8 | 4:A:427:PX4:H17 | 0.47 | 2.09 | 13 | 1 |
| 4:A:372:PX4:H26 | 4:A:378:PX4:H34 | 0.46 | 1.87 | 9 | 1 |
| 4:A:368:PX4:O2 | 4:A:369:PX4:H4 | 0.46 | 2.09 | 2 | 1 |
| 4:A:342:PX4:H19 | 4:A:352:PX4:H23 | 0.46 | 1.87 | 10 | 1 |
| 4:A:404:PX4:H41 | 4:A:412:PX4:H64 | 0.46 | 1.88 | 10 | 1 |
| 4:A:345:PX4:H20 | 4:A:346:PX4:H47 | 0.46 | 1.86 | 5 | 1 |
| 4:A:349:PX4:H41 | 4:A:422:PX4:H45 | 0.46 | 1.87 | 7 | 1 |
| 4:A:358:PX4:H31 | 4:A:364:PX4:H43 | 0.46 | 1.85 | 14 | 1 |
| 4:A:308:PX4:H62 | 4:A:363:PX4:H21 | 0.46 | 1.87 | 1 | 1 |
| 4:A:370:PX4:H68 | 4:A:403:PX4:H23 | 0.46 | 1.88 | 13 | 1 |
| 4:A:392:PX4:H18 | 4:A:393:PX4:H47 | 0.46 | 1.87 | 11 | 2 |
| 4:A:325:PX4:H47 | 4:A:341:PX4:H22 | 0.46 | 1.87 | 2 | 1 |
| 4:A:393:PX4:H38 | 4:A:401:PX4:H36 | 0.46 | 1.86 | 2 | 1 |
| 4:A:353:PX4:H27 | 4:A:366:PX4:H14 | 0.46 | 1.86 | 10 | 1 |
| 4:A:310:PX4:H71 | 4:A:311:PX4:H20 | 0.46 | 1.85 | 7 | 1 |
| 4:A:400:PX4:H31 | 4:A:426:PX4:H58 | 0.46 | 1.87 | 8 | 1 |
| 4:A:382:PX4:H59 | 4:A:428:PX4:H21 | 0.46 | 1.88 | 3 | 1 |
| 4:A:386:PX4:H29 | 4:A:387:PX4:H26 | 0.46 | 1.86 | 12 | 1 |
| 4:A:400:PX4:H29 | 4:A:401:PX4:H31 | 0.46 | 1.87 | 13 | 1 |
| 4:A:380:PX4:H52 | 4:A:387:PX4:H46 | 0.46 | 1.87 | 11 | 1 |
| 4:A:404:PX4:H15 | 4:A:413:PX4:O6 | 0.46 | 2.11 | 9 | 1 |
| 4:A:322:PX4:H38 | 4:A:413:PX4:H68 | 0.46 | 1.88 | 2 | 1 |
| 4:A:310:PX4:H63 | 4:A:311:PX4:H21 | 0.46 | 1.87 | 10 | 1 |
| 4:A:310:PX4:H72 | 4:A:311:PX4:H67 | 0.46 | 1.87 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:424:PX4:H40 | 4:A:429:PX4:H68 | 0.46 | 1.88 | 6 | 1 |
| 4:A:315:PX4:H5 | 4:A:361:PX4:O6 | 0.46 | 2.11 | 14 | 1 |
| 4:A:392:PX4:H49 | 4:A:393:PX4:H50 | 0.46 | 1.88 | 14 | 1 |
| 4:A:355:PX4:H40 | 4:A:356:PX4:H35 | 0.46 | 1.87 | 3 | 1 |
| 4:A:395:PX4:H35 | 4:A:397:PX4:H64 | 0.46 | 1.86 | 3 | 1 |
| 4:A:378:PX4:H19 | 4:A:410:PX4:H27 | 0.46 | 1.87 | 12 | 1 |
| 4:A:383:PX4:H59 | 4:A:399:PX4:H17 | 0.46 | 1.87 | 9 | 1 |
| 4:A:398:PX4:H19 | 4:A:407:PX4:H19 | 0.46 | 1.86 | 9 | 1 |
| 4:A:330:PX4:H30 | 4:A:338:PX4:H29 | 0.46 | 1.87 | 10 | 1 |
| 4:A:390:PX4:H61 | 4:A:397:PX4:H36 | 0.46 | 1.87 | 10 | 1 |
| 4:A:371:PX4:H60 | 4:A:378:PX4:H66 | 0.46 | 1.87 | 5 | 1 |
| 4:A:315:PX4:H17 | 4:A:316:PX4:H54 | 0.46 | 1.87 | 7 | 1 |
| 4:A:331:PX4:H42 | 4:A:397:PX4:H30 | 0.46 | 1.88 | 6 | 1 |
| 4:A:353:PX4:O6 | 4:A:366:PX4:H3 | 0.46 | 2.10 | 8 | 1 |
| 4:A:410:PX4:H60 | 4:A:417:PX4:H62 | 0.46 | 1.87 | 14 | 1 |
| 4:A:404:PX4:H69 | 4:A:412:PX4:H45 | 0.46 | 1.87 | 1 | 1 |
| 4:A:315:PX4:H21 | 4:A:316:PX4:H32 | 0.46 | 1.88 | 12 | 1 |
| 4:A:407:PX4:H18 | 4:A:414:PX4:H49 | 0.46 | 1.85 | 12 | 1 |
| 4:A:322:PX4:H24 | 4:A:361:PX4:H48 | 0.46 | 1.85 | 2 | 1 |
| 4:A:349:PX4:H56 | 4:A:350:PX4:H28 | 0.46 | 1.86 | 10 | 1 |
| 4:A:378:PX4:H42 | 4:A:410:PX4:H71 | 0.46 | 1.85 | 5 | 1 |
| 4:A:321:PX4:H68 | 4:A:361:PX4:H49 | 0.46 | 1.88 | 7 | 1 |
| 4:A:417:PX4:H20 | 4:A:426:PX4:H23 | 0.46 | 1.87 | 7 | 1 |
| 4:A:347:PX4:H43 | 4:A:348:PX4:H31 | 0.46 | 1.86 | 3 | 1 |
| 4:A:378:PX4:H17 | 4:A:410:PX4:H22 | 0.46 | 1.86 | 3 | 1 |
| 4:A:321:PX4:H70 | 4:A:423:PX4:H41 | 0.46 | 1.88 | 12 | 1 |
| 4:A:307:PX4:H39 | 4:A:349:PX4:H69 | 0.46 | 1.86 | 13 | 1 |
| 4:A:391:PX4:H29 | 4:A:414:PX4:H46 | 0.46 | 1.87 | 13 | 1 |
| 4:A:347:PX4:H72 | 4:A:356:PX4:H65 | 0.46 | 1.87 | 9 | 1 |
| 4:A:331:PX4:H28 | 4:A:347:PX4:C25 | 0.46 | 2.40 | 4 | 1 |
| 4:A:387:PX4:H14 | 4:A:387:PX4:H6 | 0.46 | 1.86 | 6 | 1 |
| 4:A:402:PX4:H18 | 4:A:404:PX4:H20 | 0.46 | 1.85 | 6 | 1 |
| 4:A:350:PX4:H69 | 4:A:351:PX4:H69 | 0.46 | 1.87 | 3 | 1 |
| 4:A:367:PX4:H25 | 4:A:424:PX4:H26 | 0.46 | 1.87 | 1 | 1 |
| 4:A:346:PX4:H30 | 4:A:353:PX4:H65 | 0.46 | 1.86 | 13 | 1 |
| 4:A:307:PX4:H55 | 4:A:362:PX4:H27 | 0.46 | 1.86 | 11 | 1 |
| 4:A:369:PX4:H25 | 4:A:418:PX4:H25 | 0.46 | 1.87 | 11 | 1 |
| 4:A:349:PX4:H64 | 4:A:405:PX4:H70 | 0.46 | 1.87 | 11 | 1 |
| 4:A:340:PX4:H36 | 4:A:397:PX4:H65 | 0.46 | 1.85 | 9 | 1 |
| 4:A:313:PX4:C19 | 4:A:337:PX4:H64 | 0.46 | 2.41 | 10 | 1 |
| 4:A:423:PX4:H55 | 4:A:425:PX4:H28 | 0.46 | 1.88 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:421:PX4:H43 | 4:A:423:PX4:H41 | 0.46 | 1.87 | 7 | 1 |
| 4:A:337:PX4:H47 | 4:A:353:PX4:C6 | 0.46 | 2.29 | 8 | 1 |
| 4:A:331:PX4:H29 | 4:A:347:PX4:H52 | 0.46 | 1.87 | 8 | 1 |
| 4:A:321:PX4:H61 | 4:A:361:PX4:H46 | 0.46 | 1.88 | 12 | 1 |
| 4:A:308:PX4:H52 | 4:A:363:PX4:H24 | 0.46 | 1.86 | 12 | 1 |
| 4:A:340:PX4:H65 | 4:A:340:PX4:H28 | 0.46 | 1.86 | 13 | 1 |
| 4:A:407:PX4:H7 | 4:A:407:PX4:O6 | 0.46 | 2.11 | 1 | 1 |
| 4:A:337:PX4:H65 | 4:A:353:PX4:H40 | 0.46 | 1.86 | 12 | 1 |
| 4:A:383:PX4:H20 | 4:A:392:PX4:H27 | 0.46 | 1.85 | 12 | 1 |
| 4:A:313:PX4:H60 | 4:A:327:PX4:H31 | 0.46 | 1.87 | 13 | 1 |
| 4:A:390:PX4:H57 | 4:A:397:PX4:H35 | 0.46 | 1.86 | 13 | 1 |
| 4:A:396:PX4:H63 | 4:A:398:PX4:H51 | 0.46 | 1.88 | 11 | 1 |
| 4:A:367:PX4:H48 | 4:A:428:PX4:H50 | 0.46 | 1.86 | 9 | 1 |
| 4:A:330:PX4:H13 | 4:A:338:PX4:O6 | 0.46 | 2.11 | 5 | 1 |
| 4:A:391:PX4:H17 | 4:A:408:PX4:H2 | 0.46 | 1.88 | 7 | 1 |
| 4:A:317:PX4:H42 | 4:A:342:PX4:H72 | 0.46 | 1.88 | 6 | 1 |
| 4:A:344:PX4:H31 | 4:A:348:PX4:H25 | 0.46 | 1.88 | 8 | 1 |
| 4:A:392:PX4:H68 | 4:A:408:PX4:H35 | 0.46 | 1.88 | 8 | 1 |
| 4:A:325:PX4:H42 | 4:A:334:PX4:H59 | 0.46 | 1.87 | 14 | 1 |
| 4:A:357:PX4:H43 | 4:A:358:PX4:H44 | 0.46 | 1.86 | 13 | 1 |
| 4:A:392:PX4:H29 | 4:A:393:PX4:H61 | 0.46 | 1.88 | 11 | 1 |
| 4:A:311:PX4:H20 | 4:A:311:PX4:H55 | 0.46 | 1.88 | 10 | 1 |
| 4:A:332:PX4:H29 | 4:A:347:PX4:H66 | 0.46 | 1.87 | 5 | 1 |
| 4:A:311:PX4:H51 | 4:A:359:PX4:H59 | 0.46 | 1.86 | 7 | 1 |
| 4:A:388:PX4:H14 | 4:A:396:PX4:H18 | 0.46 | 1.88 | 7 | 1 |
| 4:A:362:PX4:H26 | 4:A:413:PX4:H72 | 0.46 | 1.88 | 7 | 1 |
| 4:A:338:PX4:H47 | 4:A:348:PX4:C23 | 0.46 | 2.41 | 8 | 1 |
| 4:A:382:PX4:H60 | 4:A:412:PX4:H64 | 0.46 | 1.88 | 8 | 1 |
| 4:A:398:PX4:H32 | 4:A:414:PX4:H55 | 0.46 | 1.86 | 8 | 1 |
| 4:A:370:PX4:H42 | 4:A:403:PX4:H38 | 0.46 | 1.86 | 1 | 1 |
| 4:A:340:PX4:H37 | 4:A:397:PX4:H29 | 0.46 | 1.88 | 1 | 1 |
| 4:A:402:PX4:H20 | 4:A:411:PX4:O8 | 0.46 | 2.11 | 1 | 1 |
| 4:A:398:PX4:H48 | 4:A:407:PX4:H57 | 0.46 | 1.86 | 12 | 1 |
| 4:A:334:PX4:H33 | 4:A:407:PX4:H38 | 0.45 | 1.88 | 9 | 1 |
| 4:A:330:PX4:H19 | 4:A:330:PX4:C4 | 0.45 | 2.41 | 10 | 1 |
| 4:A:410:PX4:O2 | 4:A:416:PX4:H3 | 0.45 | 2.10 | 14 | 2 |
| 4:A:409:PX4:H64 | 4:A:415:PX4:H60 | 0.45 | 1.88 | 4 | 1 |
| 4:A:312:PX4:H32 | 4:A:357:PX4:H55 | 0.45 | 1.88 | 14 | 1 |
| 4:A:361:PX4:H19 | 4:A:364:PX4:H46 | 0.45 | 1.87 | 14 | 1 |
| 4:A:404:PX4:H26 | 4:A:419:PX4:H9 | 0.45 | 1.87 | 3 | 1 |
| 4:A:391:PX4:H16 | 4:A:392:PX4:H46 | 0.45 | 1.88 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:326:PX4:H55 | 4:A:408:PX4:H44 | 0.45 | 1.87 | 11 | 1 |
| 4:A:380:PX4:H62 | 4:A:388:PX4:H42 | 0.45 | 1.88 | 9 | 1 |
| 4:A:421:PX4:H7 | 4:A:422:PX4:O6 | 0.45 | 2.11 | 9 | 1 |
| 4:A:413:PX4:H35 | 4:A:419:PX4:H27 | 0.45 | 1.87 | 10 | 1 |
| 4:A:308:PX4:H16 | 4:A:311:PX4:C9 | 0.45 | 2.41 | 7 | 1 |
| 4:A:308:PX4:H21 | 4:A:311:PX4:H49 | 0.45 | 1.88 | 7 | 1 |
| 4:A:316:PX4:H48 | 4:A:320:PX4:H21 | 0.45 | 1.87 | 7 | 1 |
| 4:A:317:PX4:H51 | 4:A:341:PX4:H19 | 0.45 | 1.87 | 8 | 1 |
| 4:A:360:PX4:H43 | 4:A:382:PX4:H64 | 0.45 | 1.88 | 8 | 1 |
| 4:A:367:PX4:H16 | 4:A:424:PX4:H14 | 0.45 | 1.87 | 14 | 1 |
| 4:A:323:PX4:H4 | 4:A:333:PX4:O2 | 0.45 | 2.11 | 3 | 1 |
| 4:A:333:PX4:H33 | 4:A:389:PX4:H45 | 0.45 | 1.88 | 11 | 1 |
| 4:A:351:PX4:H12 | 4:A:352:PX4:H24 | 0.45 | 1.88 | 9 | 1 |
| 4:A:345:PX4:C36 | 4:A:370:PX4:H39 | 0.45 | 2.41 | 10 | 1 |
| 4:A:354:PX4:H63 | 4:A:360:PX4:H63 | 0.45 | 1.88 | 4 | 1 |
| 4:A:422:PX4:H3 | 4:A:423:PX4:O2 | 0.45 | 2.10 | 4 | 1 |
| 4:A:331:PX4:C21 | 4:A:397:PX4:H30 | 0.45 | 2.41 | 6 | 1 |
| 4:A:391:PX4:H48 | 4:A:392:PX4:H46 | 0.45 | 1.87 | 8 | 1 |
| 4:A:317:PX4:H59 | 4:A:319:PX4:H56 | 0.45 | 1.88 | 14 | 1 |
| 4:A:383:PX4:O4 | 4:A:392:PX4:H1 | 0.45 | 2.10 | 3 | 1 |
| 4:A:393:PX4:H31 | 4:A:394:PX4:C11 | 0.45 | 2.41 | 3 | 1 |
| 4:A:403:PX4:H46 | 4:A:419:PX4:H51 | 0.45 | 1.88 | 1 | 1 |
| 4:A:390:PX4:H1 | 4:A:399:PX4:H18 | 0.45 | 1.88 | 12 | 1 |
| 4:A:328:PX4:H47 | 4:A:329:PX4:H28 | 0.45 | 1.89 | 9 | 1 |
| 4:A:380:PX4:H20 | 4:A:381:PX4:H48 | 0.45 | 1.89 | 9 | 1 |
| 4:A:310:PX4:H70 | 4:A:359:PX4:H59 | 0.45 | 1.88 | 5 | 1 |
| 4:A:331:PX4:H40 | 4:A:340:PX4:H63 | 0.45 | 1.88 | 5 | 1 |
| 4:A:313:PX4:H21 | 4:A:366:PX4:H18 | 0.45 | 1.88 | 5 | 1 |
| 4:A:307:PX4:H37 | 4:A:416:PX4:H42 | 0.45 | 1.88 | 5 | 1 |
| 4:A:405:PX4:H47 | 4:A:406:PX4:H48 | 0.45 | 1.88 | 4 | 1 |
| 4:A:337:PX4:H48 | 4:A:345:PX4:H49 | 0.45 | 1.88 | 6 | 1 |
| 4:A:348:PX4:H55 | 4:A:388:PX4:H70 | 0.45 | 1.88 | 1 | 1 |
| 4:A:348:PX4:H59 | 4:A:362:PX4:H54 | 0.45 | 1.89 | 13 | 1 |
| 4:A:369:PX4:H21 | 4:A:377:PX4:H71 | 0.45 | 1.87 | 10 | 1 |
| 4:A:338:PX4:H66 | 4:A:395:PX4:H38 | 0.45 | 1.89 | 4 | 1 |
| 4:A:381:PX4:H59 | 4:A:397:PX4:H47 | 0.45 | 1.87 | 7 | 1 |
| 4:A:349:PX4:O1 | 4:A:350:PX4:H14 | 0.45 | 2.11 | 10 | 1 |
| 4:A:313:PX4:H42 | 4:A:403:PX4:H62 | 0.45 | 1.87 | 5 | 1 |
| 4:A:421:PX4:H24 | 4:A:423:PX4:H19 | 0.45 | 1.87 | 5 | 1 |
| 4:A:323:PX4:H36 | 4:A:424:PX4:H67 | 0.45 | 1.87 | 4 | 1 |
| 4:A:307:PX4:H5 | 4:A:321:PX4:H48 | 0.45 | 1.87 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:412:PX4:O8 | 4:A:428:PX4:H17 | 0.45 | 2.11 | 8 | 1 |
| 4:A:378:PX4:H19 | 4:A:410:PX4:C14 | 0.45 | 2.42 | 12 | 1 |
| 4:A:375:PX4:H50 | 4:A:428:PX4:H14 | 0.45 | 1.88 | 13 | 1 |
| 4:A:371:PX4:H58 | 4:A:379:PX4:H32 | 0.45 | 1.89 | 13 | 1 |
| 4:A:391:PX4:H46 | 4:A:401:PX4:O6 | 0.45 | 2.12 | 11 | 1 |
| 4:A:313:PX4:H42 | 4:A:403:PX4:H66 | 0.45 | 1.89 | 2 | 1 |
| 4:A:368:PX4:H37 | 4:A:418:PX4:H72 | 0.45 | 1.89 | 4 | 1 |
| 4:A:416:PX4:H27 | 4:A:423:PX4:H24 | 0.45 | 1.87 | 7 | 1 |
| 1:A:214:LEU:HD11 | 1:A:243:VAL:H | 0.45 | 1.71 | 14 | 1 |
| 4:A:322:PX4:H22 | 4:A:323:PX4:H19 | 0.45 | 1.89 | 1 | 1 |
| 4:A:393:PX4:H56 | 4:A:401:PX4:H35 | 0.45 | 1.89 | 1 | 1 |
| 4:A:391:PX4:H40 | 4:A:392:PX4:H56 | 0.45 | 1.88 | 13 | 1 |
| 4:A:312:PX4:H62 | 4:A:320:PX4:H67 | 0.45 | 1.87 | 11 | 1 |
| 4:A:373:PX4:O6 | 4:A:397:PX4:H12 | 0.45 | 2.12 | 11 | 1 |
| 4:A:419:PX4:H12 | 4:A:419:PX4:H18 | 0.45 | 1.87 | 11 | 1 |
| 4:A:367:PX4:H17 | 4:A:428:PX4:H54 | 0.45 | 1.88 | 9 | 1 |
| 4:A:373:PX4:H36 | 4:A:381:PX4:H45 | 0.45 | 1.88 | 2 | 1 |
| 4:A:330:PX4:H21 | 4:A:338:PX4:H22 | 0.45 | 1.87 | 10 | 1 |
| 4:A:342:PX4:H27 | 4:A:358:PX4:H58 | 0.45 | 1.89 | 5 | 1 |
| 4:A:331:PX4:H53 | 4:A:340:PX4:H34 | 0.45 | 1.87 | 4 | 1 |
| 4:A:402:PX4:H57 | 4:A:404:PX4:H60 | 0.45 | 1.88 | 4 | 1 |
| 1:A:243:VAL:HG12 | 4:A:356:PX4:H23 | 0.45 | 1.88 | 6 | 1 |
| 4:A:331:PX4:H43 | 4:A:389:PX4:H29 | 0.45 | 1.88 | 6 | 1 |
| 4:A:316:PX4:H25 | 4:A:320:PX4:H33 | 0.45 | 1.88 | 3 | 1 |
| 4:A:394:PX4:H34 | 4:A:401:PX4:H39 | 0.45 | 1.89 | 3 | 1 |
| 4:A:337:PX4:H53 | 4:A:353:PX4:H25 | 0.45 | 1.89 | 4 | 1 |
| 4:A:378:PX4:H16 | 4:A:417:PX4:C24 | 0.45 | 2.33 | 7 | 1 |
| 4:A:398:PX4:H67 | 4:A:405:PX4:H57 | 0.45 | 1.88 | 6 | 1 |
| 4:A:306:PX4:H14 | 4:A:321:PX4:O6 | 0.45 | 2.12 | 3 | 1 |
| 4:A:370:PX4:H28 | 4:A:403:PX4:H57 | 0.45 | 1.89 | 1 | 1 |
| 4:A:310:PX4:H17 | 4:A:365:PX4:O5 | 0.45 | 2.11 | 13 | 1 |
| 4:A:392:PX4:H25 | 4:A:393:PX4:H66 | 0.45 | 1.87 | 13 | 1 |
| 4:A:330:PX4:H19 | 4:A:330:PX4:H7 | 0.45 | 1.87 | 11 | 1 |
| 4:A:383:PX4:H24 | 4:A:383:PX4:H31 | 0.45 | 1.89 | 5 | 1 |
| 4:A:384:PX4:H34 | 4:A:384:PX4:H61 | 0.45 | 1.89 | 5 | 1 |
| 4:A:417:PX4:H24 | 4:A:426:PX4:H26 | 0.45 | 1.89 | 4 | 1 |
| 4:A:389:PX4:O2 | 4:A:398:PX4:H4 | 0.45 | 2.12 | 14 | 1 |
| 4:A:350:PX4:H1 | 4:A:358:PX4:O2 | 0.45 | 2.12 | 12 | 1 |
| 4:A:369:PX4:H52 | 4:A:425:PX4:H21 | 0.45 | 1.89 | 11 | 1 |
| 4:A:412:PX4:H23 | 4:A:413:PX4:H31 | 0.44 | 1.89 | 9 | 1 |
| 4:A:347:PX4:H10 | 4:A:348:PX4:O1 | 0.44 | 2.13 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:352:PX4:H52 | 4:A:358:PX4:H50 | 0.44 | 1.89 | 10 | 1 |
| 4:A:380:PX4:H26 | 4:A:381:PX4:H36 | 0.44 | 1.87 | 8 | 1 |
| 4:A:406:PX4:H25 | 4:A:415:PX4:H22 | 0.44 | 1.88 | 14 | 1 |
| 4:A:383:PX4:H66 | 4:A:399:PX4:H69 | 0.44 | 1.89 | 1 | 1 |
| 4:A:306:PX4:H59 | 4:A:361:PX4:H54 | 0.44 | 1.89 | 13 | 1 |
| 4:A:369:PX4:H44 | 4:A:418:PX4:H68 | 0.44 | 1.87 | 11 | 1 |
| 4:A:398:PX4:H13 | 4:A:398:PX4:H15 | 0.44 | 1.90 | 11 | 1 |
| 4:A:322:PX4:H62 | 4:A:412:PX4:H42 | 0.44 | 1.88 | 11 | 1 |
| 4:A:398:PX4:H45 | 4:A:414:PX4:H21 | 0.44 | 1.89 | 9 | 1 |
| 4:A:353:PX4:H20 | 4:A:366:PX4:H2 | 0.44 | 1.88 | 10 | 1 |
| 4:A:319:PX4:H26 | 4:A:324:PX4:H24 | 0.44 | 1.88 | 5 | 1 |
| 4:A:311:PX4:H53 | 4:A:359:PX4:H56 | 0.44 | 1.89 | 5 | 1 |
| 4:A:317:PX4:O2 | 4:A:325:PX4:H10 | 0.44 | 2.12 | 7 | 1 |
| 4:A:334:PX4:O6 | 4:A:334:PX4:H3 | 0.44 | 2.12 | 7 | 1 |
| 4:A:347:PX4:H19 | 4:A:347:PX4:H9 | 0.44 | 1.89 | 6 | 1 |
| 4:A:367:PX4:H48 | 4:A:424:PX4:H19 | 0.44 | 1.88 | 6 | 1 |
| 4:A:389:PX4:H30 | 4:A:396:PX4:H60 | 0.44 | 1.89 | 8 | 1 |
| 4:A:410:PX4:H66 | 4:A:426:PX4:H41 | 0.44 | 1.89 | 12 | 1 |
| 4:A:313:PX4:H47 | 4:A:328:PX4:H17 | 0.44 | 1.90 | 11 | 1 |
| 4:A:307:PX4:H51 | 4:A:362:PX4:H22 | 0.44 | 1.90 | 6 | 1 |
| 4:A:396:PX4:H31 | 4:A:411:PX4:H34 | 0.44 | 1.90 | 8 | 1 |
| 4:A:375:PX4:H21 | 4:A:429:PX4:H45 | 0.44 | 1.88 | 1 | 1 |
| 4:A:423:PX4:H16 | 4:A:425:PX4:O8 | 0.44 | 2.12 | 13 | 1 |
| 4:A:318:PX4:H18 | 4:A:328:PX4:H19 | 0.44 | 1.88 | 11 | 1 |
| 4:A:419:PX4:H60 | 4:A:427:PX4:H58 | 0.44 | 1.89 | 11 | 1 |
| 4:A:321:PX4:H68 | 4:A:322:PX4:H30 | 0.44 | 1.90 | 9 | 1 |
| 4:A:311:PX4:O3 | 4:A:311:PX4:H6 | 0.44 | 2.10 | 2 | 1 |
| 4:A:377:PX4:H10 | 4:A:418:PX4:O8 | 0.44 | 2.13 | 2 | 1 |
| 4:A:387:PX4:H54 | 4:A:388:PX4:H38 | 0.44 | 1.89 | 10 | 1 |
| 4:A:422:PX4:H34 | 4:A:423:PX4:H45 | 0.44 | 1.88 | 6 | 1 |
| 4:A:337:PX4:H15 | 4:A:353:PX4:O1 | 0.44 | 2.13 | 1 | 2 |
| 4:A:329:PX4:H67 | 4:A:424:PX4:H40 | 0.44 | 1.90 | 14 | 1 |
| 4:A:400:PX4:H47 | 4:A:409:PX4:H23 | 0.44 | 1.89 | 3 | 1 |
| 4:A:402:PX4:H54 | 4:A:404:PX4:H59 | 0.44 | 1.89 | 11 | 1 |
| 4:A:370:PX4:H26 | 4:A:427:PX4:H57 | 0.44 | 1.89 | 11 | 1 |
| 4:A:319:PX4:H66 | 4:A:324:PX4:H58 | 0.44 | 1.88 | 9 | 1 |
| 4:A:405:PX4:H53 | 4:A:414:PX4:H33 | 0.44 | 1.89 | 9 | 1 |
| 4:A:337:PX4:H52 | 4:A:345:PX4:H55 | 0.44 | 1.88 | 7 | 2 |
| 4:A:338:PX4:H55 | 4:A:348:PX4:H53 | 0.44 | 1.90 | 14 | 1 |
| 4:A:412:PX4:H27 | 4:A:430:PX4:H60 | 0.44 | 1.89 | 14 | 1 |
| 4:A:342:PX4:H29 | 4:A:351:PX4:H30 | 0.44 | 1.89 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:369:PX4:O1 | 4:A:425:PX4:H4 | 0.44 | 2.13 | 12 | 3 |
| 4:A:345:PX4:H35 | 4:A:346:PX4:H37 | 0.44 | 1.89 | 12 | 1 |
| 4:A:389:PX4:H48 | 4:A:398:PX4:H17 | 0.44 | 1.89 | 12 | 1 |
| 4:A:320:PX4:H54 | 4:A:359:PX4:H30 | 0.44 | 1.90 | 13 | 1 |
| 4:A:326:PX4:H66 | 4:A:399:PX4:H65 | 0.44 | 1.88 | 11 | 1 |
| 4:A:380:PX4:H46 | 4:A:387:PX4:H20 | 0.44 | 1.89 | 11 | 1 |
| 4:A:321:PX4:H37 | 4:A:354:PX4:H59 | 0.44 | 1.90 | 9 | 1 |
| 4:A:400:PX4:C24 | 4:A:409:PX4:H23 | 0.44 | 2.42 | 2 | 1 |
| 1:A:207:SER:O | 4:A:321:PX4:H6 | 0.44 | 2.13 | 10 | 1 |
| 4:A:355:PX4:H38 | 4:A:356:PX4:H44 | 0.44 | 1.88 | 7 | 1 |
| 4:A:315:PX4:H5 | 4:A:364:PX4:O8 | 0.44 | 2.11 | 7 | 1 |
| 4:A:389:PX4:H30 | 4:A:396:PX4:C31 | 0.44 | 2.42 | 8 | 1 |
| 4:A:390:PX4:H30 | 4:A:398:PX4:H19 | 0.44 | 1.89 | 8 | 1 |
| 4:A:310:PX4:O6 | 4:A:365:PX4:H4 | 0.44 | 2.12 | 1 | 1 |
| 4:A:391:PX4:H25 | 4:A:393:PX4:H64 | 0.44 | 1.89 | 1 | 1 |
| 4:A:346:PX4:H39 | 4:A:354:PX4:H31 | 0.44 | 1.89 | 5 | 1 |
| 4:A:315:PX4:H20 | 4:A:320:PX4:H28 | 0.44 | 1.89 | 4 | 1 |
| 4:A:338:PX4:H64 | 4:A:411:PX4:H36 | 0.44 | 1.89 | 4 | 1 |
| 4:A:333:PX4:H61 | 4:A:368:PX4:H72 | 0.44 | 1.90 | 4 | 1 |
| 4:A:393:PX4:H14 | 4:A:394:PX4:C9 | 0.44 | 2.43 | 8 | 1 |
| 4:A:331:PX4:H44 | 4:A:340:PX4:H71 | 0.44 | 1.89 | 3 | 1 |
| 4:A:391:PX4:H58 | 4:A:401:PX4:H36 | 0.44 | 1.89 | 13 | 1 |
| 4:A:312:PX4:H25 | 4:A:363:PX4:H32 | 0.44 | 1.90 | 9 | 1 |
| 4:A:318:PX4:H24 | 4:A:320:PX4:H46 | 0.44 | 1.90 | 2 | 1 |
| 4:A:393:PX4:O6 | 4:A:394:PX4:H15 | 0.44 | 2.13 | 2 | 1 |
| 4:A:393:PX4:H41 | 4:A:394:PX4:H40 | 0.44 | 1.89 | 10 | 1 |
| 4:A:392:PX4:H35 | 4:A:399:PX4:H61 | 0.44 | 1.89 | 4 | 1 |
| 4:A:400:PX4:H38 | 4:A:401:PX4:H38 | 0.44 | 1.87 | 7 | 1 |
| 4:A:322:PX4:H34 | 4:A:361:PX4:H22 | 0.44 | 1.88 | 6 | 1 |
| 4:A:344:PX4:H37 | 4:A:347:PX4:H45 | 0.44 | 1.90 | 8 | 1 |
| 4:A:377:PX4:H16 | 4:A:418:PX4:C3 | 0.44 | 2.42 | 8 | 1 |
| 4:A:403:PX4:H9 | 4:A:427:PX4:O8 | 0.44 | 2.13 | 8 | 1 |
| 4:A:313:PX4:H57 | 4:A:327:PX4:H21 | 0.44 | 1.87 | 14 | 1 |
| 4:A:310:PX4:H23 | 4:A:358:PX4:H49 | 0.44 | 1.89 | 14 | 1 |
| 4:A:406:PX4:H35 | 4:A:414:PX4:H32 | 0.44 | 1.90 | 3 | 1 |
| 4:A:402:PX4:H36 | 4:A:403:PX4:H35 | 0.44 | 1.89 | 1 | 1 |
| 4:A:338:PX4:H17 | 4:A:348:PX4:O6 | 0.44 | 2.13 | 13 | 1 |
| 4:A:358:PX4:H22 | 4:A:363:PX4:H53 | 0.44 | 1.89 | 13 | 1 |
| 4:A:314:PX4:H69 | 4:A:364:PX4:H45 | 0.44 | 1.89 | 10 | 1 |
| 4:A:413:PX4:H69 | 4:A:428:PX4:H70 | 0.44 | 1.88 | 4 | 1 |
| 4:A:367:PX4:H46 | 4:A:428:PX4:H47 | 0.44 | 1.90 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:352:PX4:H32 | 4:A:358:PX4:H62 | 0.44 | 1.90 | 14 | 1 |
| 4:A:370:PX4:H34 | 4:A:403:PX4:H67 | 0.44 | 1.90 | 14 | 1 |
| 4:A:382:PX4:H52 | 4:A:428:PX4:H28 | 0.44 | 1.88 | 3 | 1 |
| 4:A:323:PX4:H16 | 4:A:333:PX4:H51 | 0.44 | 1.90 | 1 | 1 |
| 4:A:326:PX4:H57 | 4:A:334:PX4:H34 | 0.44 | 1.90 | 11 | 1 |
| 4:A:351:PX4:O7 | 4:A:352:PX4:H23 | 0.43 | 2.13 | 2 | 1 |
| 4:A:416:PX4:O1 | 4:A:422:PX4:H10 | 0.43 | 2.13 | 2 | 1 |
| 4:A:351:PX4:H8 | 4:A:352:PX4:O1 | 0.43 | 2.13 | 4 | 1 |
| 4:A:374:PX4:H32 | 4:A:427:PX4:H23 | 0.43 | 1.90 | 14 | 1 |
| 4:A:340:PX4:H62 | 4:A:341:PX4:H66 | 0.43 | 1.90 | 1 | 1 |
| 4:A:308:PX4:H44 | 4:A:311:PX4:H70 | 0.43 | 1.90 | 12 | 1 |
| 4:A:318:PX4:H35 | 4:A:327:PX4:H65 | 0.43 | 1.89 | 12 | 1 |
| 4:A:330:PX4:H52 | 4:A:338:PX4:H24 | 0.43 | 1.90 | 12 | 1 |
| 4:A:417:PX4:H28 | 4:A:426:PX4:H32 | 0.43 | 1.90 | 12 | 1 |
| 4:A:312:PX4:H69 | 4:A:359:PX4:H37 | 0.43 | 1.89 | 13 | 1 |
| 4:A:321:PX4:H67 | 4:A:361:PX4:H24 | 0.43 | 1.90 | 13 | 1 |
| 4:A:376:PX4:H66 | 4:A:385:PX4:H30 | 0.43 | 1.90 | 13 | 1 |
| 4:A:330:PX4:H63 | 4:A:338:PX4:H42 | 0.43 | 1.88 | 2 | 1 |
| 4:A:312:PX4:H44 | 4:A:365:PX4:H68 | 0.43 | 1.89 | 5 | 1 |
| 4:A:310:PX4:H43 | 4:A:365:PX4:H37 | 0.43 | 1.90 | 7 | 1 |
| 4:A:393:PX4:H45 | 4:A:401:PX4:H45 | 0.43 | 1.90 | 6 | 1 |
| 4:A:328:PX4:H25 | 4:A:328:PX4:H20 | 0.43 | 1.38 | 8 | 1 |
| 4:A:416:PX4:O8 | 4:A:418:PX4:H40 | 0.43 | 2.13 | 8 | 1 |
| 4:A:361:PX4:H40 | 4:A:423:PX4:H66 | 0.43 | 1.90 | 3 | 1 |
| 4:A:346:PX4:H46 | 4:A:362:PX4:H46 | 0.43 | 1.90 | 12 | 1 |
| 4:A:311:PX4:H5 | 4:A:320:PX4:O4 | 0.43 | 2.13 | 13 | 1 |
| 1:A:244:ASP:OD2 | 4:A:349:PX4:H3 | 0.43 | 2.14 | 2 | 1 |
| 4:A:378:PX4:H29 | 4:A:378:PX4:H23 | 0.43 | 1.63 | 2 | 1 |
| 4:A:386:PX4:H38 | 4:A:394:PX4:H67 | 0.43 | 1.89 | 10 | 1 |
| 4:A:347:PX4:O4 | 4:A:348:PX4:H6 | 0.43 | 2.13 | 5 | 1 |
| 4:A:418:PX4:O1 | 4:A:425:PX4:H5 | 0.43 | 2.13 | 3 | 1 |
| 4:A:326:PX4:H37 | 4:A:350:PX4:H32 | 0.43 | 1.89 | 1 | 1 |
| 4:A:395:PX4:H43 | 4:A:405:PX4:H40 | 0.43 | 1.89 | 13 | 1 |
| 4:A:430:PX4:H38 | 4:A:430:PX4:H44 | 0.43 | 1.51 | 11 | 1 |
| 4:A:315:PX4:H10 | 4:A:316:PX4:O6 | 0.43 | 2.13 | 2 | 1 |
| 4:A:334:PX4:H69 | 4:A:352:PX4:H37 | 0.43 | 1.89 | 2 | 1 |
| 4:A:389:PX4:H33 | 4:A:397:PX4:H21 | 0.43 | 1.90 | 2 | 1 |
| 4:A:307:PX4:H61 | 4:A:362:PX4:H27 | 0.43 | 1.91 | 10 | 1 |
| 4:A:378:PX4:O1 | 4:A:417:PX4:H17 | 0.43 | 2.12 | 10 | 1 |
| 4:A:418:PX4:H41 | 4:A:418:PX4:H36 | 0.43 | 1.56 | 5 | 1 |
| 4:A:341:PX4:H58 | 4:A:390:PX4:H72 | 0.43 | 1.89 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:320:PX4:H32 | 4:A:359:PX4:H63 | 0.43 | 1.90 | 8 | 1 |
| 4:A:314:PX4:H31 | 4:A:356:PX4:H28 | 0.43 | 1.90 | 11 | 1 |
| 4:A:410:PX4:O2 | 4:A:416:PX4:H10 | 0.43 | 2.14 | 9 | 1 |
| 4:A:306:PX4:H51 | 4:A:306:PX4:H56 | 0.43 | 1.58 | 7 | 1 |
| 4:A:363:PX4:H30 | 4:A:363:PX4:H35 | 0.43 | 1.61 | 6 | 1 |
| 4:A:331:PX4:H51 | 4:A:347:PX4:H22 | 0.43 | 1.91 | 8 | 1 |
| 4:A:387:PX4:H5 | 4:A:411:PX4:O3 | 0.43 | 2.13 | 12 | 1 |
| 4:A:314:PX4:H71 | 4:A:409:PX4:H31 | 0.43 | 1.90 | 13 | 1 |
| 4:A:338:PX4:H70 | 4:A:395:PX4:H38 | 0.43 | 1.90 | 10 | 1 |
| 4:A:352:PX4:O8 | 4:A:365:PX4:H3 | 0.43 | 2.13 | 10 | 1 |
| 4:A:407:PX4:O6 | 4:A:414:PX4:H49 | 0.43 | 2.13 | 10 | 1 |
| 4:A:333:PX4:H53 | 4:A:341:PX4:H57 | 0.43 | 1.89 | 5 | 1 |
| 4:A:314:PX4:H37 | 4:A:362:PX4:H16 | 0.43 | 1.90 | 4 | 1 |
| 1:A:178:GLY:HA3 | 4:A:354:PX4:H1 | 0.43 | 1.89 | 7 | 1 |
| 4:A:376:PX4:H19 | 4:A:383:PX4:H19 | 0.43 | 1.90 | 7 | 1 |
| 4:A:374:PX4:H8 | 4:A:427:PX4:H20 | 0.43 | 1.91 | 8 | 1 |
| 4:A:369:PX4:H29 | 4:A:378:PX4:H51 | 0.43 | 1.89 | 1 | 1 |
| 4:A:341:PX4:H72 | 4:A:397:PX4:H35 | 0.43 | 1.89 | 1 | 1 |
| 4:A:316:PX4:H47 | 4:A:320:PX4:H23 | 0.43 | 1.90 | 12 | 1 |
| 4:A:393:PX4:H30 | 4:A:400:PX4:H31 | 0.43 | 1.91 | 13 | 1 |
| 4:A:342:PX4:C12 | 4:A:352:PX4:H47 | 0.43 | 2.31 | 11 | 1 |
| 4:A:374:PX4:H58 | 4:A:382:PX4:H50 | 0.43 | 1.91 | 11 | 1 |
| 4:A:423:PX4:H55 | 4:A:425:PX4:H27 | 0.43 | 1.90 | 11 | 1 |
| 4:A:410:PX4:H51 | 4:A:426:PX4:H33 | 0.43 | 1.90 | 11 | 1 |
| 4:A:333:PX4:H14 | 4:A:340:PX4:O2 | 0.43 | 2.14 | 9 | 1 |
| 4:A:412:PX4:H36 | 4:A:419:PX4:H28 | 0.43 | 1.90 | 2 | 1 |
| 4:A:353:PX4:H35 | 4:A:366:PX4:H22 | 0.43 | 1.91 | 10 | 1 |
| 4:A:349:PX4:H65 | 4:A:406:PX4:H68 | 0.43 | 1.88 | 5 | 1 |
| 4:A:412:PX4:H58 | 4:A:427:PX4:H30 | 0.43 | 1.90 | 5 | 1 |
| 4:A:384:PX4:O1 | 4:A:385:PX4:H10 | 0.43 | 2.13 | 4 | 1 |
| 4:A:395:PX4:O1 | 4:A:396:PX4:H17 | 0.43 | 2.14 | 7 | 1 |
| 4:A:325:PX4:H49 | 4:A:341:PX4:H19 | 0.43 | 1.89 | 6 | 1 |
| 4:A:345:PX4:H19 | 4:A:346:PX4:H22 | 0.43 | 1.90 | 6 | 1 |
| 4:A:387:PX4:H56 | 4:A:387:PX4:H50 | 0.43 | 1.43 | 6 | 1 |
| 4:A:391:PX4:H26 | 4:A:392:PX4:H46 | 0.43 | 1.89 | 6 | 1 |
| 4:A:333:PX4:H30 | 4:A:339:PX4:H28 | 0.43 | 1.90 | 14 | 1 |
| 4:A:398:PX4:H21 | 4:A:407:PX4:H46 | 0.43 | 1.91 | 14 | 1 |
| 4:A:309:PX4:H28 | 4:A:309:PX4:H62 | 0.43 | 1.89 | 3 | 1 |
| 4:A:331:PX4:H17 | 4:A:340:PX4:H5 | 0.43 | 1.89 | 3 | 1 |
| 4:A:346:PX4:O6 | 4:A:362:PX4:H15 | 0.43 | 2.14 | 3 | 1 |
| 4:A:330:PX4:H31 | 4:A:348:PX4:H30 | 0.43 | 1.89 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:334:PX4:H51 | 4:A:334:PX4:H56 | 0.43 | 1.42 | 11 | 1 |
| 4:A:356:PX4:H62 | 4:A:397:PX4:H71 | 0.43 | 1.90 | 11 | 1 |
| 4:A:381:PX4:H16 | 4:A:388:PX4:H12 | 0.43 | 1.90 | 2 | 1 |
| 4:A:326:PX4:H61 | 4:A:334:PX4:H35 | 0.43 | 1.89 | 10 | 1 |
| 4:A:391:PX4:H23 | 4:A:392:PX4:H14 | 0.43 | 1.89 | 10 | 1 |
| 4:A:345:PX4:H71 | 4:A:403:PX4:H36 | 0.43 | 1.91 | 10 | 1 |
| 4:A:330:PX4:H5 | 4:A:344:PX4:H16 | 0.43 | 1.91 | 4 | 1 |
| 4:A:314:PX4:H33 | 4:A:362:PX4:H16 | 0.43 | 1.89 | 7 | 1 |
| 4:A:403:PX4:H3 | 4:A:427:PX4:H49 | 0.43 | 1.90 | 7 | 1 |
| 1:A:116:TYR:CD1 | 1:A:138:PHE:CE2 | 0.43 | 3.06 | 8 | 1 |
| 4:A:395:PX4:H9 | 4:A:411:PX4:O2 | 0.43 | 2.14 | 14 | 1 |
| 4:A:308:PX4:H14 | 4:A:311:PX4:O8 | 0.43 | 2.14 | 3 | 1 |
| 4:A:350:PX4:H61 | 4:A:363:PX4:H23 | 0.43 | 1.89 | 3 | 1 |
| 4:A:326:PX4:H47 | 4:A:334:PX4:H60 | 0.43 | 1.90 | 1 | 1 |
| 4:A:373:PX4:H28 | 4:A:381:PX4:H57 | 0.43 | 1.91 | 1 | 1 |
| 4:A:339:PX4:H68 | 4:A:339:PX4:H62 | 0.43 | 1.44 | 13 | 1 |
| 4:A:391:PX4:H37 | 4:A:393:PX4:H72 | 0.43 | 1.89 | 13 | 1 |
| 4:A:314:PX4:H44 | 4:A:355:PX4:H46 | 0.43 | 1.90 | 11 | 1 |
| 4:A:325:PX4:H32 | 4:A:332:PX4:H28 | 0.43 | 1.90 | 9 | 1 |
| 4:A:379:PX4:H71 | 4:A:379:PX4:H65 | 0.43 | 1.55 | 2 | 1 |
| 4:A:335:PX4:H42 | 4:A:343:PX4:H64 | 0.43 | 1.89 | 10 | 1 |
| 4:A:354:PX4:H65 | 4:A:360:PX4:H24 | 0.43 | 1.89 | 5 | 1 |
| 4:A:403:PX4:H32 | 4:A:404:PX4:H21 | 0.43 | 1.91 | 7 | 1 |
| 4:A:327:PX4:O3 | 4:A:327:PX4:H10 | 0.43 | 2.14 | 6 | 1 |
| 4:A:376:PX4:H36 | 4:A:376:PX4:H42 | 0.43 | 1.68 | 6 | 1 |
| 4:A:386:PX4:H17 | 4:A:394:PX4:O8 | 0.43 | 2.13 | 6 | 1 |
| 4:A:337:PX4:H45 | 4:A:338:PX4:H52 | 0.43 | 1.91 | 8 | 1 |
| 4:A:371:PX4:H46 | 4:A:371:PX4:H16 | 0.43 | 1.75 | 3 | 2 |
| 4:A:378:PX4:H19 | 4:A:426:PX4:H28 | 0.43 | 1.90 | 3 | 1 |
| 4:A:325:PX4:H28 | 4:A:407:PX4:H41 | 0.43 | 1.90 | 1 | 1 |
| 4:A:412:PX4:H51 | 4:A:419:PX4:H16 | 0.43 | 1.91 | 12 | 1 |
| 4:A:404:PX4:H71 | 4:A:404:PX4:H19 | 0.43 | 1.89 | 13 | 1 |
| 4:A:314:PX4:H71 | 4:A:364:PX4:H39 | 0.43 | 1.91 | 2 | 1 |
| 4:A:367:PX4:H20 | 4:A:424:PX4:H16 | 0.43 | 1.91 | 10 | 1 |
| 4:A:372:PX4:H54 | 4:A:379:PX4:H53 | 0.43 | 1.90 | 5 | 1 |
| 4:A:328:PX4:H56 | 4:A:354:PX4:H72 | 0.43 | 1.90 | 7 | 1 |
| 1:A:207:SER:O | 4:A:321:PX4:H9 | 0.43 | 2.13 | 6 | 1 |
| 4:A:314:PX4:H47 | 4:A:349:PX4:H19 | 0.43 | 1.91 | 8 | 1 |
| 4:A:377:PX4:H72 | 4:A:425:PX4:O2 | 0.43 | 2.13 | 8 | 1 |
| 4:A:314:PX4:H38 | 4:A:355:PX4:H57 | 0.43 | 1.91 | 3 | 1 |
| 4:A:403:PX4:H47 | 4:A:427:PX4:H47 | 0.43 | 1.90 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:353:PX4:H58 | 4:A:360:PX4:H61 | 0.43 | 1.91 | 11 | 1 |
| 4:A:393:PX4:H17 | 4:A:401:PX4:H22 | 0.43 | 1.91 | 11 | 1 |
| 4:A:348:PX4:H60 | 4:A:348:PX4:H67 | 0.42 | 1.52 | 9 | 1 |
| 4:A:395:PX4:H62 | 4:A:413:PX4:O8 | 0.42 | 2.14 | 2 | 1 |
| 4:A:378:PX4:H23 | 4:A:378:PX4:H30 | 0.42 | 1.54 | 4 | 1 |
| 4:A:388:PX4:H63 | 4:A:397:PX4:H63 | 0.42 | 1.89 | 4 | 1 |
| 4:A:320:PX4:H17 | 4:A:359:PX4:C29 | 0.42 | 2.43 | 7 | 1 |
| 4:A:335:PX4:H41 | 4:A:335:PX4:H36 | 0.42 | 1.61 | 7 | 1 |
| 4:A:418:PX4:H33 | 4:A:418:PX4:H40 | 0.42 | 1.61 | 3 | 1 |
| 4:A:419:PX4:H60 | 4:A:427:PX4:H25 | 0.42 | 1.91 | 1 | 1 |
| 4:A:316:PX4:O2 | 4:A:364:PX4:H12 | 0.42 | 2.13 | 12 | 1 |
| 4:A:349:PX4:H16 | 4:A:350:PX4:H30 | 0.42 | 1.90 | 9 | 1 |
| 4:A:317:PX4:H55 | 4:A:324:PX4:C10 | 0.42 | 2.42 | 2 | 1 |
| 4:A:412:PX4:H17 | 4:A:419:PX4:H20 | 0.42 | 1.89 | 5 | 1 |
| 4:A:315:PX4:H3 | 4:A:361:PX4:O1 | 0.42 | 2.14 | 6 | 1 |
| 4:A:342:PX4:H52 | 4:A:351:PX4:H27 | 0.42 | 1.91 | 8 | 1 |
| 4:A:344:PX4:H37 | 4:A:344:PX4:H45 | 0.42 | 1.62 | 3 | 1 |
| 4:A:398:PX4:H41 | 4:A:415:PX4:H20 | 0.42 | 1.90 | 1 | 1 |
| 4:A:308:PX4:H66 | 4:A:308:PX4:H61 | 0.42 | 1.59 | 12 | 1 |
| 4:A:308:PX4:H34 | 4:A:311:PX4:H65 | 0.42 | 1.89 | 12 | 1 |
| 4:A:330:PX4:C22 | 4:A:344:PX4:H45 | 0.42 | 2.40 | 12 | 1 |
| 4:A:376:PX4:H62 | 4:A:385:PX4:H30 | 0.42 | 1.90 | 12 | 1 |
| 4:A:354:PX4:H22 | 4:A:362:PX4:H21 | 0.42 | 1.90 | 13 | 1 |
| 4:A:392:PX4:O6 | 4:A:392:PX4:H10 | 0.42 | 2.13 | 13 | 1 |
| 4:A:331:PX4:H28 | 4:A:347:PX4:H51 | 0.42 | 1.91 | 11 | 1 |
| 4:A:333:PX4:H16 | 4:A:340:PX4:H15 | 0.42 | 1.90 | 9 | 1 |
| 4:A:351:PX4:H54 | 4:A:358:PX4:H22 | 0.42 | 1.90 | 9 | 1 |
| 4:A:314:PX4:H26 | 4:A:314:PX4:H19 | 0.42 | 1.66 | 10 | 1 |
| 4:A:314:PX4:O8 | 4:A:314:PX4:H15 | 0.42 | 2.13 | 5 | 1 |
| 4:A:310:PX4:H16 | 4:A:363:PX4:O6 | 0.42 | 2.14 | 5 | 1 |
| 4:A:380:PX4:O4 | 4:A:381:PX4:H15 | 0.42 | 2.14 | 4 | 1 |
| 4:A:429:PX4:H54 | 4:A:429:PX4:H27 | 0.42 | 1.91 | 7 | 1 |
| 4:A:378:PX4:H60 | 4:A:410:PX4:H70 | 0.42 | 1.90 | 8 | 1 |
| 4:A:310:PX4:H36 | 4:A:351:PX4:H65 | 0.42 | 1.91 | 14 | 1 |
| 4:A:332:PX4:H28 | 4:A:334:PX4:H53 | 0.42 | 1.90 | 14 | 1 |
| 4:A:369:PX4:H58 | 4:A:424:PX4:H50 | 0.42 | 1.91 | 1 | 1 |
| 4:A:317:PX4:H1 | 4:A:317:PX4:O6 | 0.42 | 2.14 | 13 | 1 |
| 4:A:361:PX4:C33 | 4:A:412:PX4:H40 | 0.42 | 2.44 | 11 | 1 |
| 4:A:423:PX4:H26 | 4:A:423:PX4:H57 | 0.42 | 1.91 | 11 | 1 |
| 4:A:320:PX4:H21 | 4:A:359:PX4:H60 | 0.42 | 1.91 | 9 | 1 |
| 4:A:361:PX4:H29 | 4:A:361:PX4:H24 | 0.42 | 1.61 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:391:PX4:H67 | 4:A:401:PX4:H33 | 0.42 | 1.91 | 9 | 1 |
| 4:A:316:PX4:H71 | 4:A:333:PX4:H67 | 0.42 | 1.92 | 2 | 1 |
| 4:A:358:PX4:H70 | 4:A:401:PX4:H37 | 0.42 | 1.91 | 10 | 1 |
| 4:A:357:PX4:H66 | 4:A:357:PX4:H61 | 0.42 | 1.65 | 5 | 1 |
| 4:A:382:PX4:H22 | 4:A:428:PX4:C16 | 0.42 | 2.42 | 5 | 1 |
| 4:A:416:PX4:H48 | 4:A:425:PX4:H48 | 0.42 | 1.91 | 5 | 1 |
| 4:A:355:PX4:H55 | 4:A:355:PX4:H49 | 0.42 | 1.69 | 4 | 1 |
| 4:A:332:PX4:H66 | 4:A:349:PX4:H67 | 0.42 | 1.91 | 8 | 1 |
| 4:A:412:PX4:H20 | 4:A:428:PX4:H49 | 0.42 | 1.90 | 14 | 1 |
| 4:A:381:PX4:H61 | 4:A:381:PX4:H40 | 0.42 | 1.91 | 3 | 1 |
| 4:A:346:PX4:H25 | 4:A:354:PX4:H31 | 0.42 | 1.90 | 12 | 1 |
| 4:A:356:PX4:H42 | 4:A:356:PX4:H35 | 0.42 | 1.71 | 11 | 1 |
| 4:A:412:PX4:H24 | 4:A:430:PX4:H58 | 0.42 | 1.92 | 9 | 1 |
| 4:A:335:PX4:H6 | 4:A:344:PX4:O6 | 0.42 | 2.13 | 2 | 1 |
| 4:A:315:PX4:O3 | 4:A:361:PX4:H4 | 0.42 | 2.15 | 10 | 1 |
| 4:A:369:PX4:H48 | 4:A:377:PX4:H67 | 0.42 | 1.91 | 10 | 1 |
| 4:A:387:PX4:H17 | 4:A:411:PX4:H61 | 0.42 | 1.90 | 10 | 1 |
| 4:A:308:PX4:H16 | 4:A:311:PX4:C10 | 0.42 | 2.44 | 5 | 1 |
| 4:A:356:PX4:H16 | 4:A:356:PX4:O3 | 0.42 | 2.15 | 5 | 1 |
| 4:A:307:PX4:H16 | 4:A:307:PX4:H46 | 0.42 | 1.64 | 4 | 2 |
| 4:A:406:PX4:O1 | 4:A:414:PX4:H3 | 0.42 | 2.15 | 4 | 1 |
| 4:A:312:PX4:H59 | 4:A:359:PX4:H30 | 0.42 | 1.91 | 7 | 1 |
| 4:A:325:PX4:H64 | 4:A:341:PX4:H35 | 0.42 | 1.90 | 7 | 1 |
| 4:A:424:PX4:H17 | 4:A:429:PX4:H21 | 0.42 | 1.92 | 6 | 1 |
| 4:A:330:PX4:H49 | 4:A:343:PX4:H46 | 0.42 | 1.91 | 14 | 1 |
| 4:A:356:PX4:H42 | 4:A:405:PX4:H60 | 0.42 | 1.91 | 3 | 1 |
| 4:A:381:PX4:H54 | 4:A:388:PX4:H57 | 0.42 | 1.90 | 3 | 1 |
| 4:A:415:PX4:H11 | 4:A:422:PX4:H16 | 0.42 | 1.91 | 1 | 1 |
| 4:A:418:PX4:H34 | 4:A:425:PX4:H56 | 0.42 | 1.91 | 1 | 1 |
| 4:A:387:PX4:H17 | 4:A:411:PX4:H57 | 0.42 | 1.91 | 12 | 1 |
| 4:A:395:PX4:H27 | 4:A:405:PX4:H28 | 0.42 | 1.91 | 13 | 1 |
| 4:A:334:PX4:H22 | 4:A:334:PX4:H27 | 0.42 | 1.65 | 11 | 1 |
| 4:A:317:PX4:H66 | 4:A:342:PX4:H66 | 0.42 | 1.91 | 2 | 1 |
| 4:A:406:PX4:H33 | 4:A:414:PX4:H34 | 0.42 | 1.91 | 2 | 1 |
| 4:A:404:PX4:H54 | 4:A:405:PX4:H39 | 0.42 | 1.91 | 5 | 1 |
| 4:A:372:PX4:H29 | 4:A:420:PX4:H55 | 0.42 | 1.92 | 4 | 1 |
| 4:A:367:PX4:O6 | 4:A:423:PX4:H11 | 0.42 | 2.15 | 6 | 1 |
| 4:A:326:PX4:H44 | 4:A:416:PX4:H41 | 0.42 | 1.91 | 8 | 1 |
| 4:A:350:PX4:O2 | 4:A:363:PX4:H7 | 0.42 | 2.14 | 8 | 1 |
| 4:A:384:PX4:H3 | 4:A:385:PX4:H18 | 0.42 | 1.91 | 14 | 1 |
| 4:A:337:PX4:H20 | 4:A:346:PX4:H63 | 0.42 | 1.92 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:354:PX4:H50 | 4:A:360:PX4:H18 | 0.42 | 1.90 | 11 | 1 |
| 4:A:342:PX4:H37 | 4:A:352:PX4:H33 | 0.42 | 1.90 | 9 | 1 |
| 4:A:346:PX4:O4 | 4:A:362:PX4:H11 | 0.42 | 2.15 | 10 | 1 |
| 4:A:381:PX4:H53 | 4:A:397:PX4:H46 | 0.42 | 1.90 | 10 | 1 |
| 4:A:382:PX4:H22 | 4:A:428:PX4:H34 | 0.42 | 1.92 | 10 | 1 |
| 4:A:406:PX4:H17 | 4:A:414:PX4:H22 | 0.42 | 1.92 | 10 | 1 |
| 4:A:391:PX4:H71 | 4:A:415:PX4:H45 | 0.42 | 1.92 | 10 | 1 |
| 4:A:326:PX4:O6 | 4:A:350:PX4:H5 | 0.42 | 2.14 | 6 | 1 |
| 4:A:332:PX4:H25 | 4:A:334:PX4:H49 | 0.42 | 1.90 | 14 | 1 |
| 4:A:334:PX4:H29 | 4:A:414:PX4:H69 | 0.42 | 1.91 | 11 | 1 |
| 4:A:338:PX4:H68 | 4:A:348:PX4:H58 | 0.42 | 1.90 | 11 | 1 |
| 4:A:349:PX4:O6 | 4:A:349:PX4:H7 | 0.42 | 2.15 | 11 | 1 |
| 4:A:321:PX4:H47 | 4:A:354:PX4:H20 | 0.42 | 1.91 | 2 | 1 |
| 4:A:331:PX4:H62 | 4:A:397:PX4:H59 | 0.42 | 1.92 | 10 | 1 |
| 4:A:307:PX4:H58 | 4:A:314:PX4:H17 | 0.42 | 1.92 | 5 | 1 |
| 4:A:337:PX4:O6 | 4:A:345:PX4:H49 | 0.42 | 2.15 | 5 | 1 |
| 4:A:347:PX4:H56 | 4:A:356:PX4:H56 | 0.42 | 1.92 | 5 | 1 |
| 4:A:416:PX4:H17 | 4:A:425:PX4:O8 | 0.42 | 2.14 | 5 | 1 |
| 4:A:402:PX4:H33 | 4:A:402:PX4:H28 | 0.42 | 1.57 | 4 | 1 |
| 4:A:391:PX4:H66 | 4:A:408:PX4:H57 | 0.42 | 1.92 | 4 | 1 |
| 4:A:384:PX4:H30 | 4:A:384:PX4:H57 | 0.42 | 1.91 | 7 | 1 |
| 4:A:344:PX4:H27 | 4:A:348:PX4:H21 | 0.42 | 1.92 | 6 | 1 |
| 4:A:398:PX4:H40 | 4:A:414:PX4:C16 | 0.42 | 2.45 | 6 | 1 |
| 4:A:370:PX4:H36 | 4:A:402:PX4:H40 | 0.42 | 1.92 | 8 | 1 |
| 4:A:371:PX4:H36 | 4:A:379:PX4:H60 | 0.42 | 1.91 | 3 | 1 |
| 4:A:375:PX4:H19 | 4:A:429:PX4:H45 | 0.42 | 1.90 | 3 | 1 |
| 4:A:338:PX4:H65 | 4:A:338:PX4:H58 | 0.42 | 1.68 | 13 | 1 |
| 4:A:333:PX4:O8 | 4:A:340:PX4:H15 | 0.42 | 2.15 | 11 | 1 |
| 4:A:363:PX4:H47 | 4:A:364:PX4:H33 | 0.42 | 1.91 | 9 | 1 |
| 4:A:367:PX4:O1 | 4:A:423:PX4:H3 | 0.42 | 2.15 | 2 | 1 |
| 4:A:395:PX4:H70 | 4:A:421:PX4:H58 | 0.42 | 1.91 | 10 | 1 |
| 4:A:353:PX4:H41 | 4:A:353:PX4:H35 | 0.42 | 1.58 | 4 | 1 |
| 4:A:375:PX4:H3 | 4:A:429:PX4:H17 | 0.42 | 1.91 | 4 | 1 |
| 4:A:382:PX4:H14 | 4:A:382:PX4:O6 | 0.42 | 2.14 | 4 | 1 |
| 4:A:324:PX4:H23 | 4:A:342:PX4:H55 | 0.42 | 1.91 | 7 | 1 |
| 4:A:388:PX4:H28 | 4:A:411:PX4:H16 | 0.42 | 1.91 | 7 | 1 |
| 4:A:337:PX4:H43 | 4:A:380:PX4:H39 | 0.42 | 1.91 | 6 | 1 |
| 4:A:354:PX4:H30 | 4:A:362:PX4:H17 | 0.42 | 1.90 | 3 | 1 |
| 4:A:372:PX4:H61 | 4:A:379:PX4:H59 | 0.42 | 1.91 | 3 | 1 |
| 4:A:308:PX4:H7 | 4:A:308:PX4:O3 | 0.42 | 2.15 | 12 | 1 |
| 4:A:318:PX4:H56 | 4:A:328:PX4:H33 | 0.42 | 1.90 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:335:PX4:H17 | 4:A:343:PX4:O1 | 0.42 | 2.15 | 12 | 1 |
| 4:A:317:PX4:H41 | 4:A:385:PX4:H65 | 0.42 | 1.92 | 13 | 1 |
| 4:A:325:PX4:H62 | 4:A:342:PX4:H70 | 0.42 | 1.90 | 13 | 1 |
| 4:A:332:PX4:H54 | 4:A:407:PX4:H70 | 0.42 | 1.90 | 13 | 1 |
| 4:A:391:PX4:H17 | 4:A:408:PX4:O5 | 0.42 | 2.15 | 13 | 1 |
| 4:A:403:PX4:H52 | 4:A:403:PX4:H47 | 0.42 | 1.50 | 11 | 1 |
| 4:A:408:PX4:H50 | 4:A:409:PX4:H19 | 0.42 | 1.92 | 11 | 1 |
| 4:A:372:PX4:H29 | 4:A:420:PX4:H26 | 0.42 | 1.91 | 2 | 1 |
| 4:A:322:PX4:C27 | 4:A:336:PX4:H32 | 0.42 | 2.45 | 10 | 1 |
| 4:A:354:PX4:H32 | 4:A:354:PX4:H25 | 0.42 | 1.63 | 10 | 1 |
| 4:A:333:PX4:H23 | 4:A:340:PX4:H24 | 0.42 | 1.91 | 5 | 1 |
| 4:A:364:PX4:H69 | 4:A:364:PX4:H62 | 0.42 | 1.69 | 5 | 1 |
| 4:A:376:PX4:H26 | 4:A:399:PX4:C25 | 0.42 | 2.45 | 4 | 1 |
| 4:A:373:PX4:H22 | 4:A:397:PX4:O3 | 0.42 | 2.14 | 7 | 1 |
| 4:A:334:PX4:C35 | 4:A:352:PX4:H32 | 0.42 | 2.45 | 6 | 1 |
| 4:A:395:PX4:H40 | 4:A:397:PX4:H65 | 0.42 | 1.92 | 6 | 1 |
| 4:A:398:PX4:H48 | 4:A:405:PX4:H49 | 0.42 | 1.92 | 6 | 1 |
| 4:A:383:PX4:H13 | 4:A:399:PX4:O1 | 0.42 | 2.15 | 6 | 1 |
| 4:A:350:PX4:H36 | 4:A:415:PX4:H71 | 0.42 | 1.92 | 6 | 1 |
| 4:A:308:PX4:H69 | 4:A:426:PX4:H70 | 0.42 | 1.91 | 14 | 1 |
| 4:A:306:PX4:H40 | 4:A:329:PX4:H40 | 0.42 | 1.91 | 3 | 1 |
| 4:A:316:PX4:H34 | 4:A:320:PX4:C19 | 0.42 | 2.43 | 3 | 1 |
| 4:A:424:PX4:H47 | 4:A:429:PX4:H19 | 0.42 | 1.91 | 1 | 1 |
| 4:A:388:PX4:H6 | 4:A:396:PX4:O8 | 0.42 | 2.15 | 12 | 1 |
| 4:A:413:PX4:H17 | 4:A:430:PX4:C8 | 0.42 | 2.45 | 12 | 1 |
| 4:A:424:PX4:H48 | 4:A:424:PX4:H55 | 0.42 | 1.64 | 13 | 1 |
| 4:A:393:PX4:H10 | 4:A:393:PX4:O6 | 0.41 | 2.14 | 9 | 1 |
| 4:A:340:PX4:H35 | 4:A:397:PX4:H60 | 0.41 | 1.91 | 10 | 1 |
| 4:A:363:PX4:H62 | 4:A:363:PX4:H57 | 0.41 | 1.56 | 10 | 1 |
| 4:A:389:PX4:H68 | 4:A:390:PX4:H38 | 0.41 | 1.92 | 10 | 1 |
| 4:A:318:PX4:H39 | 4:A:359:PX4:H36 | 0.41 | 1.92 | 5 | 1 |
| 4:A:398:PX4:H51 | 4:A:405:PX4:C23 | 0.41 | 2.45 | 4 | 1 |
| 4:A:405:PX4:H58 | 4:A:414:PX4:H26 | 0.41 | 1.91 | 4 | 1 |
| 4:A:346:PX4:H24 | 4:A:360:PX4:H55 | 0.41 | 1.92 | 14 | 1 |
| 4:A:403:PX4:H48 | 4:A:419:PX4:H9 | 0.41 | 1.91 | 14 | 1 |
| 4:A:371:PX4:O8 | 4:A:377:PX4:H3 | 0.41 | 2.15 | 1 | 1 |
| 4:A:378:PX4:H28 | 4:A:420:PX4:H57 | 0.41 | 1.92 | 1 | 1 |
| 4:A:308:PX4:H41 | 4:A:410:PX4:H45 | 0.41 | 1.91 | 12 | 1 |
| 4:A:423:PX4:H40 | 4:A:430:PX4:H36 | 0.41 | 1.92 | 12 | 1 |
| 4:A:322:PX4:H37 | 4:A:361:PX4:H25 | 0.41 | 1.91 | 13 | 1 |
| 4:A:410:PX4:H57 | 4:A:417:PX4:H69 | 0.41 | 1.91 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:369:PX4:C19 | 4:A:416:PX4:H63 | 0.41 | 2.45 | 11 | 1 |
| 4:A:403:PX4:H49 | 4:A:404:PX4:H28 | 0.41 | 1.90 | 5 | 1 |
| 4:A:345:PX4:H68 | 4:A:345:PX4:H45 | 0.41 | 1.91 | 4 | 1 |
| 4:A:308:PX4:H32 | 4:A:364:PX4:H52 | 0.41 | 1.91 | 4 | 1 |
| 4:A:378:PX4:H47 | 4:A:410:PX4:H19 | 0.41 | 1.93 | 7 | 1 |
| 4:A:347:PX4:H20 | 4:A:348:PX4:O3 | 0.41 | 2.14 | 6 | 1 |
| 4:A:416:PX4:H22 | 4:A:425:PX4:H50 | 0.41 | 1.92 | 6 | 1 |
| 4:A:421:PX4:H35 | 4:A:430:PX4:H48 | 0.41 | 1.92 | 6 | 1 |
| 4:A:352:PX4:H31 | 4:A:352:PX4:H38 | 0.41 | 1.60 | 14 | 1 |
| 4:A:398:PX4:H68 | 4:A:398:PX4:H63 | 0.41 | 1.73 | 14 | 1 |
| 4:A:349:PX4:H27 | 4:A:356:PX4:H30 | 0.41 | 1.92 | 3 | 1 |
| 4:A:309:PX4:H23 | 4:A:320:PX4:H49 | 0.41 | 1.92 | 1 | 1 |
| 4:A:410:PX4:H14 | 4:A:418:PX4:H40 | 0.41 | 1.92 | 1 | 1 |
| 4:A:372:PX4:H39 | 4:A:420:PX4:H34 | 0.41 | 1.92 | 12 | 1 |
| 4:A:308:PX4:H67 | 4:A:359:PX4:H70 | 0.41 | 1.91 | 13 | 1 |
| 4:A:308:PX4:H63 | 4:A:308:PX4:H68 | 0.41 | 1.64 | 11 | 1 |
| 4:A:337:PX4:H25 | 4:A:337:PX4:H5 | 0.41 | 1.92 | 11 | 1 |
| 4:A:335:PX4:H39 | 4:A:344:PX4:H39 | 0.41 | 1.92 | 11 | 1 |
| 4:A:373:PX4:H66 | 4:A:381:PX4:H44 | 0.41 | 1.92 | 10 | 1 |
| 4:A:314:PX4:H34 | 4:A:356:PX4:H41 | 0.41 | 1.91 | 8 | 1 |
| 4:A:376:PX4:H65 | 4:A:392:PX4:H35 | 0.41 | 1.92 | 14 | 1 |
| 4:A:313:PX4:H62 | 4:A:329:PX4:H32 | 0.41 | 1.90 | 1 | 1 |
| 4:A:383:PX4:O6 | 4:A:392:PX4:H3 | 0.41 | 2.14 | 1 | 1 |
| 4:A:421:PX4:H34 | 4:A:423:PX4:H23 | 0.41 | 1.93 | 12 | 1 |
| 4:A:322:PX4:H17 | 4:A:361:PX4:H56 | 0.41 | 1.92 | 13 | 1 |
| 4:A:366:PX4:H55 | 4:A:366:PX4:H60 | 0.41 | 1.70 | 9 | 1 |
| 4:A:372:PX4:O2 | 4:A:420:PX4:H9 | 0.41 | 2.15 | 9 | 1 |
| 4:A:420:PX4:H57 | 4:A:420:PX4:H50 | 0.41 | 1.68 | 9 | 1 |
| 4:A:367:PX4:H20 | 4:A:424:PX4:H22 | 0.41 | 1.93 | 2 | 1 |
| 4:A:341:PX4:H29 | 4:A:341:PX4:H24 | 0.41 | 1.63 | 10 | 1 |
| 4:A:389:PX4:H60 | 4:A:398:PX4:H17 | 0.41 | 1.93 | 5 | 1 |
| 4:A:393:PX4:H16 | 4:A:401:PX4:H18 | 0.41 | 1.91 | 5 | 1 |
| 4:A:348:PX4:H37 | 4:A:357:PX4:H36 | 0.41 | 1.92 | 7 | 1 |
| 4:A:421:PX4:H41 | 4:A:423:PX4:H35 | 0.41 | 1.91 | 7 | 1 |
| 4:A:337:PX4:H24 | 4:A:346:PX4:H69 | 0.41 | 1.91 | 6 | 1 |
| 4:A:347:PX4:H68 | 4:A:390:PX4:H39 | 0.41 | 1.92 | 6 | 1 |
| 4:A:352:PX4:H13 | 4:A:352:PX4:H2 | 0.41 | 1.76 | 6 | 1 |
| 4:A:346:PX4:H27 | 4:A:353:PX4:H58 | 0.41 | 1.93 | 6 | 1 |
| 4:A:316:PX4:O2 | 4:A:364:PX4:H11 | 0.41 | 2.15 | 8 | 1 |
| 4:A:380:PX4:H59 | 4:A:380:PX4:H25 | 0.41 | 1.91 | 8 | 1 |
| 4:A:403:PX4:H26 | 4:A:404:PX4:H21 | 0.41 | 1.92 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:367:PX4:H63 | 4:A:367:PX4:H68 | 0.41 | 1.51 | 14 | 1 |
| 4:A:407:PX4:H29 | 4:A:408:PX4:H41 | 0.41 | 1.90 | 14 | 1 |
| 4:A:331:PX4:H8 | 4:A:340:PX4:O1 | 0.41 | 2.14 | 3 | 1 |
| 4:A:378:PX4:H35 | 4:A:378:PX4:H42 | 0.41 | 1.61 | 3 | 1 |
| 4:A:368:PX4:H46 | 4:A:429:PX4:H20 | 0.41 | 1.90 | 1 | 1 |
| 4:A:337:PX4:H61 | 4:A:353:PX4:H48 | 0.41 | 1.93 | 9 | 1 |
| 4:A:413:PX4:H9 | 4:A:430:PX4:O1 | 0.41 | 2.16 | 2 | 1 |
| 4:A:325:PX4:H27 | 4:A:334:PX4:H21 | 0.41 | 1.93 | 5 | 1 |
| 1:A:244:ASP:OD1 | 4:A:349:PX4:H3 | 0.41 | 2.15 | 5 | 1 |
| 4:A:405:PX4:H48 | 4:A:406:PX4:H52 | 0.41 | 1.92 | 4 | 1 |
| 4:A:369:PX4:O1 | 4:A:425:PX4:H1 | 0.41 | 2.15 | 4 | 1 |
| 4:A:406:PX4:H34 | 4:A:406:PX4:H39 | 0.41 | 1.55 | 7 | 1 |
| 1:A:214:LEU:HD22 | 1:A:243:VAL:CG2 | 0.41 | 2.45 | 8 | 1 |
| 4:A:347:PX4:O1 | 4:A:348:PX4:H3 | 0.41 | 2.15 | 8 | 1 |
| 4:A:362:PX4:H21 | 4:A:362:PX4:H28 | 0.41 | 1.65 | 8 | 1 |
| 4:A:306:PX4:H37 | 4:A:367:PX4:H72 | 0.41 | 1.92 | 14 | 1 |
| 4:A:392:PX4:H56 | 4:A:392:PX4:H63 | 0.41 | 1.65 | 14 | 1 |
| 4:A:332:PX4:H38 | 4:A:407:PX4:H61 | 0.41 | 1.93 | 14 | 1 |
| 4:A:314:PX4:H35 | 4:A:314:PX4:H41 | 0.41 | 1.64 | 3 | 1 |
| 4:A:359:PX4:H47 | 4:A:359:PX4:H53 | 0.41 | 1.64 | 3 | 1 |
| 4:A:340:PX4:H43 | 4:A:389:PX4:H27 | 0.41 | 1.93 | 12 | 1 |
| 4:A:423:PX4:H42 | 4:A:423:PX4:H36 | 0.41 | 1.54 | 12 | 1 |
| 4:A:360:PX4:H30 | 4:A:366:PX4:H61 | 0.41 | 1.91 | 9 | 1 |
| 4:A:398:PX4:H42 | 4:A:408:PX4:H26 | 0.41 | 1.92 | 9 | 1 |
| 4:A:308:PX4:H14 | 4:A:311:PX4:H16 | 0.41 | 1.92 | 2 | 1 |
| 4:A:408:PX4:H32 | 4:A:415:PX4:H42 | 0.41 | 1.92 | 2 | 1 |
| 4:A:355:PX4:H30 | 4:A:356:PX4:H51 | 0.41 | 1.91 | 10 | 1 |
| 4:A:385:PX4:H67 | 4:A:392:PX4:H26 | 0.41 | 1.90 | 5 | 1 |
| 1:A:138:PHE:CD1 | 1:A:149:PHE:CD1 | 0.41 | 3.08 | 6 | 2 |
| 4:A:308:PX4:H65 | 4:A:308:PX4:H72 | 0.41 | 1.59 | 4 | 1 |
| 4:A:369:PX4:O1 | 4:A:425:PX4:H13 | 0.41 | 2.16 | 4 | 1 |
| 4:A:383:PX4:H65 | 4:A:407:PX4:H27 | 0.41 | 1.92 | 6 | 1 |
| 4:A:420:PX4:H67 | 4:A:426:PX4:H38 | 0.41 | 1.92 | 8 | 1 |
| 4:A:367:PX4:H60 | 4:A:429:PX4:H41 | 0.41 | 1.91 | 8 | 1 |
| 4:A:338:PX4:H68 | 4:A:338:PX4:H63 | 0.41 | 1.58 | 14 | 1 |
| 4:A:344:PX4:H49 | 4:A:344:PX4:H54 | 0.41 | 1.71 | 14 | 1 |
| 4:A:337:PX4:H65 | 4:A:345:PX4:H71 | 0.41 | 1.92 | 14 | 1 |
| 4:A:345:PX4:O4 | 4:A:346:PX4:H10 | 0.41 | 2.15 | 3 | 1 |
| 4:A:321:PX4:H61 | 4:A:361:PX4:H57 | 0.41 | 1.93 | 1 | 1 |
| 4:A:418:PX4:H64 | 4:A:418:PX4:H72 | 0.41 | 1.59 | 12 | 1 |
| 4:A:388:PX4:H3 | 4:A:395:PX4:O1 | 0.41 | 2.15 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:350:PX4:H60 | 4:A:400:PX4:H44 | 0.41 | 1.93 | 11 | 1 |
| 4:A:311:PX4:H17 | 4:A:359:PX4:H50 | 0.41 | 1.93 | 2 | 1 |
| 4:A:382:PX4:H29 | 4:A:382:PX4:H36 | 0.41 | 1.73 | 2 | 1 |
| 4:A:416:PX4:H40 | 4:A:421:PX4:H70 | 0.41 | 1.92 | 5 | 1 |
| 4:A:323:PX4:H19 | 4:A:333:PX4:H47 | 0.41 | 1.92 | 4 | 1 |
| 4:A:363:PX4:H38 | 4:A:365:PX4:H30 | 0.41 | 1.92 | 4 | 1 |
| 4:A:391:PX4:H48 | 4:A:391:PX4:H54 | 0.41 | 1.60 | 4 | 1 |
| 4:A:319:PX4:H60 | 4:A:324:PX4:H59 | 0.41 | 1.92 | 7 | 1 |
| 4:A:380:PX4:H59 | 4:A:388:PX4:H40 | 0.41 | 1.91 | 7 | 1 |
| 4:A:377:PX4:H44 | 4:A:377:PX4:H38 | 0.41 | 1.75 | 6 | 1 |
| 4:A:395:PX4:H56 | 4:A:402:PX4:H50 | 0.41 | 1.91 | 6 | 1 |
| 4:A:381:PX4:H42 | 4:A:381:PX4:H60 | 0.41 | 1.92 | 8 | 1 |
| 4:A:392:PX4:H65 | 4:A:392:PX4:H72 | 0.41 | 1.73 | 14 | 1 |
| 4:A:409:PX4:H37 | 4:A:410:PX4:H53 | 0.41 | 1.93 | 3 | 1 |
| 4:A:308:PX4:H23 | 4:A:311:PX4:H54 | 0.41 | 1.92 | 1 | 1 |
| 4:A:338:PX4:H38 | 4:A:338:PX4:H45 | 0.41 | 1.58 | 11 | 1 |
| 4:A:415:PX4:H55 | 4:A:421:PX4:H56 | 0.41 | 1.93 | 2 | 1 |
| 4:A:407:PX4:H17 | 4:A:414:PX4:O8 | 0.41 | 2.16 | 10 | 1 |
| 4:A:395:PX4:H54 | 4:A:395:PX4:H61 | 0.41 | 1.72 | 5 | 1 |
| 4:A:307:PX4:H10 | 4:A:322:PX4:O8 | 0.41 | 2.16 | 4 | 1 |
| 4:A:428:PX4:H38 | 4:A:428:PX4:H44 | 0.41 | 1.78 | 4 | 1 |
| 4:A:332:PX4:H14 | 4:A:356:PX4:H9 | 0.41 | 1.92 | 7 | 1 |
| 4:A:388:PX4:H34 | 4:A:388:PX4:H39 | 0.41 | 1.63 | 6 | 1 |
| 4:A:421:PX4:H52 | 4:A:421:PX4:H59 | 0.41 | 1.65 | 6 | 1 |
| 4:A:352:PX4:H16 | 4:A:358:PX4:H47 | 0.41 | 1.93 | 8 | 1 |
| 4:A:328:PX4:H20 | 4:A:328:PX4:H25 | 0.41 | 1.67 | 14 | 1 |
| 4:A:349:PX4:H45 | 4:A:355:PX4:H45 | 0.41 | 1.93 | 13 | 1 |
| 4:A:378:PX4:H63 | 4:A:418:PX4:H62 | 0.41 | 1.93 | 13 | 1 |
| 4:A:398:PX4:H21 | 4:A:407:PX4:H22 | 0.41 | 1.93 | 13 | 1 |
| 4:A:400:PX4:H56 | 4:A:409:PX4:H34 | 0.41 | 1.93 | 13 | 1 |
| 4:A:309:PX4:O8 | 4:A:316:PX4:H46 | 0.41 | 2.16 | 11 | 1 |
| 4:A:367:PX4:H42 | 4:A:423:PX4:H36 | 0.41 | 1.90 | 11 | 1 |
| 4:A:315:PX4:H24 | 4:A:322:PX4:H36 | 0.41 | 1.92 | 9 | 1 |
| 4:A:416:PX4:H48 | 4:A:425:PX4:H53 | 0.41 | 1.92 | 9 | 1 |
| 4:A:363:PX4:H28 | 4:A:365:PX4:H21 | 0.41 | 1.92 | 9 | 1 |
| 4:A:391:PX4:H47 | 4:A:408:PX4:H16 | 0.41 | 1.93 | 9 | 1 |
| 4:A:429:PX4:H33 | 4:A:429:PX4:C27 | 0.41 | 2.46 | 9 | 1 |
| 4:A:314:PX4:H47 | 4:A:350:PX4:H37 | 0.41 | 1.91 | 2 | 1 |
| 4:A:337:PX4:H45 | 4:A:338:PX4:H56 | 0.41 | 1.93 | 2 | 1 |
| 4:A:375:PX4:H67 | 4:A:375:PX4:H60 | 0.41 | 1.66 | 2 | 1 |
| 4:A:376:PX4:H46 | 4:A:384:PX4:H3 | 0.41 | 1.93 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:404:PX4:H52 | 4:A:404:PX4:H59 | 0.41 | 1.53 | 2 | 1 |
| 4:A:366:PX4:H68 | 4:A:419:PX4:H38 | 0.41 | 1.93 | 10 | 1 |
| 4:A:326:PX4:H29 | 4:A:350:PX4:H51 | 0.41 | 1.92 | 5 | 1 |
| 4:A:415:PX4:H5 | 4:A:421:PX4:H14 | 0.41 | 1.92 | 5 | 1 |
| 4:A:316:PX4:H26 | 4:A:364:PX4:H47 | 0.41 | 1.92 | 5 | 1 |
| 4:A:345:PX4:H17 | 4:A:346:PX4:H6 | 0.41 | 1.93 | 5 | 1 |
| 4:A:306:PX4:O2 | 4:A:329:PX4:H12 | 0.41 | 2.15 | 4 | 1 |
| 4:A:314:PX4:H42 | 4:A:362:PX4:H21 | 0.41 | 1.91 | 4 | 1 |
| 4:A:404:PX4:H63 | 4:A:404:PX4:H68 | 0.41 | 1.65 | 7 | 1 |
| 4:A:375:PX4:H47 | 4:A:429:PX4:H40 | 0.41 | 1.92 | 6 | 1 |
| 4:A:372:PX4:H52 | 4:A:372:PX4:H47 | 0.41 | 1.71 | 8 | 1 |
| 4:A:423:PX4:H4 | 4:A:430:PX4:O8 | 0.41 | 2.16 | 8 | 1 |
| 4:A:331:PX4:O6 | 4:A:331:PX4:H7 | 0.41 | 2.16 | 14 | 1 |
| 4:A:424:PX4:H25 | 4:A:424:PX4:H32 | 0.41 | 1.37 | 14 | 1 |
| 4:A:312:PX4:H39 | 4:A:365:PX4:H37 | 0.41 | 1.93 | 3 | 1 |
| 4:A:363:PX4:H55 | 4:A:363:PX4:H60 | 0.41 | 1.65 | 3 | 1 |
| 4:A:358:PX4:H35 | 4:A:365:PX4:H31 | 0.41 | 1.91 | 3 | 1 |
| 4:A:375:PX4:H18 | 4:A:382:PX4:O6 | 0.41 | 2.16 | 3 | 1 |
| 4:A:330:PX4:H16 | 4:A:343:PX4:H2 | 0.41 | 1.93 | 1 | 1 |
| 4:A:345:PX4:H69 | 4:A:388:PX4:H35 | 0.41 | 1.92 | 1 | 1 |
| 4:A:348:PX4:H68 | 4:A:348:PX4:H63 | 0.41 | 1.63 | 1 | 1 |
| 4:A:306:PX4:H56 | 4:A:354:PX4:C13 | 0.41 | 2.46 | 1 | 1 |
| 4:A:335:PX4:H23 | 4:A:343:PX4:H53 | 0.41 | 1.91 | 12 | 1 |
| 4:A:390:PX4:H63 | 4:A:397:PX4:H40 | 0.41 | 1.92 | 12 | 1 |
| 4:A:383:PX4:H20 | 4:A:392:PX4:C14 | 0.41 | 2.46 | 12 | 1 |
| 4:A:325:PX4:H9 | 4:A:341:PX4:O6 | 0.41 | 2.15 | 13 | 1 |
| 4:A:307:PX4:H41 | 4:A:361:PX4:H42 | 0.41 | 1.92 | 13 | 1 |
| 4:A:338:PX4:H62 | 4:A:362:PX4:H62 | 0.41 | 1.93 | 13 | 1 |
| 4:A:382:PX4:H67 | 4:A:428:PX4:H20 | 0.41 | 1.93 | 9 | 1 |
| 4:A:388:PX4:H15 | 4:A:396:PX4:H18 | 0.41 | 1.92 | 9 | 1 |
| 4:A:424:PX4:H56 | 4:A:425:PX4:H31 | 0.41 | 1.93 | 9 | 1 |
| 4:A:349:PX4:H60 | 4:A:349:PX4:H66 | 0.41 | 1.58 | 10 | 1 |
| 4:A:388:PX4:H51 | 4:A:396:PX4:C25 | 0.41 | 2.45 | 10 | 1 |
| 4:A:325:PX4:H45 | 4:A:334:PX4:H40 | 0.41 | 1.93 | 4 | 1 |
| 4:A:330:PX4:H19 | 4:A:330:PX4:C3 | 0.41 | 2.46 | 7 | 1 |
| 4:A:354:PX4:H21 | 4:A:362:PX4:C5 | 0.41 | 2.46 | 7 | 1 |
| 4:A:332:PX4:O3 | 4:A:356:PX4:H4 | 0.41 | 2.16 | 7 | 1 |
| 4:A:341:PX4:H32 | 4:A:383:PX4:H70 | 0.41 | 1.93 | 6 | 1 |
| 4:A:309:PX4:H27 | 4:A:318:PX4:H28 | 0.41 | 1.93 | 8 | 1 |
| 4:A:319:PX4:H19 | 4:A:342:PX4:H50 | 0.41 | 1.92 | 14 | 1 |
| 4:A:326:PX4:H64 | 4:A:391:PX4:H43 | 0.41 | 1.92 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:345:PX4:H4 | 4:A:353:PX4:O4 | 0.41 | 2.16 | 14 | 1 |
| 4:A:405:PX4:H45 | 4:A:405:PX4:H37 | 0.41 | 1.61 | 14 | 1 |
| 4:A:326:PX4:H27 | 4:A:350:PX4:H21 | 0.41 | 1.92 | 3 | 1 |
| 4:A:311:PX4:H71 | 4:A:316:PX4:H38 | 0.41 | 1.93 | 12 | 1 |
| 4:A:369:PX4:H71 | 4:A:369:PX4:H65 | 0.41 | 1.47 | 12 | 1 |
| 4:A:353:PX4:H31 | 4:A:366:PX4:H25 | 0.41 | 1.93 | 11 | 1 |
| 4:A:313:PX4:H18 | 4:A:318:PX4:C24 | 0.40 | 2.36 | 9 | 1 |
| 4:A:316:PX4:O4 | 4:A:364:PX4:H5 | 0.40 | 2.16 | 2 | 1 |
| 4:A:389:PX4:H61 | 4:A:389:PX4:H66 | 0.40 | 1.60 | 10 | 1 |
| 4:A:314:PX4:H64 | 4:A:314:PX4:H59 | 0.40 | 1.39 | 4 | 1 |
| 4:A:350:PX4:H56 | 4:A:363:PX4:H52 | 0.40 | 1.92 | 4 | 1 |
| 4:A:334:PX4:H65 | 4:A:363:PX4:H69 | 0.40 | 1.93 | 4 | 1 |
| 4:A:371:PX4:H65 | 4:A:417:PX4:H65 | 0.40 | 1.92 | 4 | 1 |
| 4:A:366:PX4:H41 | 4:A:366:PX4:H36 | 0.40 | 1.64 | 7 | 1 |
| 1:A:214:LEU:H | 1:A:214:LEU:HD23 | 0.40 | 1.75 | 6 | 1 |
| 4:A:358:PX4:H27 | 4:A:364:PX4:H42 | 0.40 | 1.92 | 6 | 1 |
| 4:A:416:PX4:H35 | 4:A:421:PX4:H66 | 0.40 | 1.92 | 8 | 1 |
| 4:A:313:PX4:H15 | 4:A:360:PX4:O6 | 0.40 | 2.16 | 14 | 1 |
| 4:A:404:PX4:H8 | 4:A:412:PX4:O6 | 0.40 | 2.17 | 14 | 1 |
| 4:A:387:PX4:H38 | 4:A:387:PX4:H31 | 0.40 | 1.72 | 1 | 1 |
| 4:A:403:PX4:O8 | 4:A:419:PX4:H8 | 0.40 | 2.15 | 1 | 1 |
| 4:A:326:PX4:H55 | 4:A:326:PX4:H60 | 0.40 | 1.78 | 12 | 1 |
| 4:A:380:PX4:H31 | 4:A:381:PX4:H60 | 0.40 | 1.92 | 12 | 1 |
| 4:A:427:PX4:H37 | 4:A:427:PX4:H32 | 0.40 | 1.63 | 12 | 1 |
| 4:A:322:PX4:H69 | 4:A:322:PX4:H62 | 0.40 | 1.62 | 13 | 1 |
| 4:A:378:PX4:H17 | 4:A:410:PX4:O6 | 0.40 | 2.15 | 13 | 1 |
| 4:A:384:PX4:H17 | 4:A:385:PX4:H20 | 0.40 | 1.93 | 13 | 1 |
| 4:A:384:PX4:H46 | 4:A:386:PX4:H49 | 0.40 | 1.93 | 11 | 1 |
| 4:A:315:PX4:H43 | 4:A:425:PX4:H32 | 0.40 | 1.92 | 2 | 1 |
| 4:A:308:PX4:H51 | 4:A:363:PX4:H19 | 0.40 | 1.92 | 10 | 1 |
| 4:A:308:PX4:H25 | 4:A:311:PX4:H23 | 0.40 | 1.93 | 10 | 1 |
| 4:A:323:PX4:H58 | 4:A:323:PX4:H65 | 0.40 | 1.68 | 5 | 1 |
| 4:A:330:PX4:H14 | 4:A:338:PX4:H19 | 0.40 | 1.91 | 7 | 1 |
| 4:A:377:PX4:H62 | 4:A:416:PX4:H55 | 0.40 | 1.92 | 6 | 1 |
| 4:A:334:PX4:H59 | 4:A:334:PX4:H64 | 0.40 | 1.36 | 8 | 1 |
| 4:A:352:PX4:H7 | 4:A:352:PX4:H15 | 0.40 | 1.93 | 14 | 1 |
| 4:A:308:PX4:H41 | 4:A:316:PX4:H39 | 0.40 | 1.92 | 3 | 1 |
| 4:A:419:PX4:H71 | 4:A:427:PX4:H64 | 0.40 | 1.93 | 3 | 1 |
| 4:A:327:PX4:H43 | 4:A:374:PX4:H66 | 0.40 | 1.93 | 12 | 1 |
| 4:A:389:PX4:H52 | 4:A:389:PX4:H59 | 0.40 | 1.59 | 13 | 1 |
| 4:A:391:PX4:H31 | 4:A:408:PX4:H23 | 0.40 | 1.91 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:332:PX4:H45 | 4:A:407:PX4:H53 | 0.40 | 1.93 | 13 | 1 |
| 4:A:368:PX4:H20 | 4:A:377:PX4:H57 | 0.40 | 1.92 | 11 | 1 |
| 4:A:428:PX4:H65 | 4:A:430:PX4:H48 | 0.40 | 1.93 | 11 | 1 |
| 4:A:372:PX4:H38 | 4:A:372:PX4:H32 | 0.40 | 1.63 | 5 | 1 |
| 4:A:323:PX4:H14 | 4:A:323:PX4:H9 | 0.40 | 1.92 | 4 | 1 |
| 4:A:319:PX4:O2 | 4:A:324:PX4:H4 | 0.40 | 2.16 | 7 | 1 |
| 4:A:401:PX4:H38 | 4:A:401:PX4:H44 | 0.40 | 1.72 | 6 | 1 |
| 4:A:317:PX4:O5 | 4:A:351:PX4:H23 | 0.40 | 2.17 | 8 | 1 |
| 4:A:405:PX4:H58 | 4:A:414:PX4:H30 | 0.40 | 1.93 | 8 | 1 |
| 4:A:417:PX4:H65 | 4:A:417:PX4:H58 | 0.40 | 1.62 | 14 | 1 |
| 4:A:321:PX4:H45 | 4:A:360:PX4:H69 | 0.40 | 1.93 | 1 | 1 |
| 4:A:383:PX4:H55 | 4:A:399:PX4:H17 | 0.40 | 1.92 | 13 | 1 |
| 4:A:404:PX4:H2 | 4:A:412:PX4:O1 | 0.40 | 2.16 | 13 | 1 |
| 1:A:109:TRP:CH2 | 1:A:158:ASP:HB3 | 0.40 | 2.51 | 11 | 1 |
| 4:A:348:PX4:H56 | 4:A:355:PX4:H72 | 0.40 | 1.93 | 11 | 1 |
| 4:A:388:PX4:H25 | 4:A:388:PX4:H32 | 0.40 | 1.65 | 9 | 1 |
| 4:A:410:PX4:H40 | 4:A:410:PX4:H61 | 0.40 | 1.92 | 2 | 1 |
| 4:A:375:PX4:H37 | 4:A:375:PX4:H32 | 0.40 | 1.68 | 10 | 1 |
| 4:A:412:PX4:H16 | 4:A:428:PX4:H16 | 0.40 | 1.93 | 10 | 1 |
| 4:A:345:PX4:H33 | 4:A:353:PX4:H61 | 0.40 | 1.94 | 5 | 1 |
| 4:A:416:PX4:H47 | 4:A:416:PX4:H52 | 0.40 | 1.75 | 5 | 1 |
| 4:A:410:PX4:O2 | 4:A:416:PX4:H4 | 0.40 | 2.17 | 8 | 1 |
| 4:A:394:PX4:H65 | 4:A:394:PX4:H71 | 0.40 | 1.66 | 14 | 1 |
| 4:A:326:PX4:H34 | 4:A:406:PX4:H36 | 0.40 | 1.93 | 3 | 1 |
| 4:A:321:PX4:H63 | 4:A:321:PX4:H68 | 0.40 | 1.68 | 12 | 1 |
| 4:A:402:PX4:H39 | 4:A:402:PX4:H34 | 0.40 | 1.45 | 12 | 1 |
| 4:A:336:PX4:H28 | 4:A:361:PX4:H63 | 0.40 | 1.93 | 13 | 1 |
| 4:A:378:PX4:H67 | 4:A:418:PX4:H66 | 0.40 | 1.93 | 13 | 1 |
| 4:A:380:PX4:H20 | 4:A:381:PX4:H6 | 0.40 | 1.93 | 13 | 1 |
| 4:A:395:PX4:H15 | 4:A:396:PX4:H15 | 0.40 | 1.93 | 13 | 1 |
| 4:A:378:PX4:H47 | 4:A:418:PX4:H46 | 0.40 | 1.92 | 13 | 1 |
| 4:A:307:PX4:C12 | 4:A:314:PX4:H16 | 0.40 | 2.47 | 11 | 1 |
| 4:A:362:PX4:H54 | 4:A:362:PX4:H60 | 0.40 | 1.39 | 11 | 1 |
| 4:A:381:PX4:H10 | 4:A:381:PX4:H14 | 0.40 | 1.93 | 11 | 1 |
| 4:A:345:PX4:H17 | 4:A:346:PX4:H10 | 0.40 | 1.91 | 2 | 1 |
| 4:A:316:PX4:H60 | 4:A:320:PX4:H36 | 0.40 | 1.93 | 5 | 1 |
| 4:A:344:PX4:H38 | 4:A:347:PX4:H38 | 0.40 | 1.93 | 5 | 1 |
| 4:A:429:PX4:H53 | 4:A:429:PX4:H29 | 0.40 | 1.93 | 5 | 1 |
| 4:A:320:PX4:H20 | 4:A:359:PX4:H58 | 0.40 | 1.94 | 4 | 1 |
| 4:A:353:PX4:H35 | 4:A:353:PX4:H30 | 0.40 | 1.62 | 7 | 1 |
| 4:A:319:PX4:H38 | 4:A:319:PX4:H44 | 0.40 | 1.70 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:385:PX4:O1 | 4:A:392:PX4:H8 | 0.40 | 2.17 | 8 | 1 |
| 4:A:355:PX4:C10 | 4:A:362:PX4:H51 | 0.40 | 2.47 | 14 | 1 |
| 4:A:374:PX4:H20 | 4:A:374:PX4:H25 | 0.40 | 1.49 | 14 | 1 |
| 4:A:374:PX4:H34 | 4:A:374:PX4:H27 | 0.40 | 1.72 | 3 | 1 |
| 4:A:364:PX4:H32 | 4:A:364:PX4:H25 | 0.40 | 1.68 | 1 | 1 |
| 4:A:380:PX4:H33 | 4:A:380:PX4:H28 | 0.40 | 1.75 | 1 | 1 |
| 4:A:398:PX4:H60 | 4:A:405:PX4:H29 | 0.40 | 1.94 | 13 | 1 |
| 4:A:319:PX4:H58 | 4:A:324:PX4:H30 | 0.40 | 1.94 | 11 | 1 |
| 4:A:332:PX4:H39 | 4:A:334:PX4:H57 | 0.40 | 1.92 | 11 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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 | A | 158/164 (96%) | 145±3 (92±2%) | 12±3 (8±2%) | 1±1 (1±0%) | 33 | 77 |
| All | All | 2212/2296 (96%) | 2030 (92%) | 168 (8%) | 14 (1%) | 33 | 77 |

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 171 | PHE | 5 |
| 1 | A | 175 | ASP | 3 |
| 1 | A | 107 | PRO | 2 |
| 1 | A | 213 | PHE | 1 |
| 1 | A | 179 | GLY | 1 |
| 1 | A | 146 | PRO | 1 |
| 1 | A | 183 | HIS | 1 |

6.3.2 Protein sidechains [i](#)

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 | A | 129/131 (98%) | 123±2 (95±2%) | 6±2 (5±2%) | 33 | 78 |
| All | All | 1806/1834 (98%) | 1716 (95%) | 90 (5%) | 33 | 78 |

All 25 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 | A | 244 | ASP | 14 |
| 1 | A | 101 | ARG | 14 |
| 1 | A | 199 | GLU | 9 |
| 1 | A | 222 | HIS | 8 |
| 1 | A | 249 | ARG | 7 |
| 1 | A | 214 | LEU | 6 |
| 1 | A | 175 | ASP | 5 |
| 1 | A | 243 | VAL | 4 |
| 1 | A | 142 | SER | 3 |
| 1 | A | 170 | ASP | 3 |
| 1 | A | 198 | ASP | 2 |
| 1 | A | 129 | ASP | 2 |
| 1 | A | 122 | THR | 1 |
| 1 | A | 200 | ASP | 1 |
| 1 | A | 139 | GLN | 1 |
| 1 | A | 115 | THR | 1 |
| 1 | A | 140 | VAL | 1 |
| 1 | A | 168 | HIS | 1 |
| 1 | A | 205 | THR | 1 |
| 1 | A | 156 | MET | 1 |
| 1 | A | 146 | PRO | 1 |
| 1 | A | 162 | VAL | 1 |
| 1 | A | 134 | ILE | 1 |
| 1 | A | 108 | VAL | 1 |
| 1 | A | 103 | MET | 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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 for Mogul analysis.

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 |
| 4 | PX4 | A | 306 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 307 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 308 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 309 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 310 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 311 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 312 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 313 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 314 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 315 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 316 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 317 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 318 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 319 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 320 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 321 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 322 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 323 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 324 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 325 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 326 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 327 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 328 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 329 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 330 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 331 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 332 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 333 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 334 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 335 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 336 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 337 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 338 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 339 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 340 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 341 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 342 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 343 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 344 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 345 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 346 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 347 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 348 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 349 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 350 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 351 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 352 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 353 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 354 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 355 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 356 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 357 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 358 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 359 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 360 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 361 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 362 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 363 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 364 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 365 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 366 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 367 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 368 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 369 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 370 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 371 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 372 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 373 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 374 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 375 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 376 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 377 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 378 | - | 45,45,45 | 0.62±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 379 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 380 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 381 | - | 45,45,45 | 0.62±0.03 | 0±0 (0±0%) |
| 4 | PX4 | A | 382 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 383 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 384 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 385 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 386 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 387 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 388 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 389 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 390 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 391 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 392 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 393 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 394 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 395 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 396 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 397 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 398 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 399 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 400 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 401 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 402 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 403 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 404 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 405 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 406 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 407 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 408 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 409 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 410 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 411 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 412 | - | 45,45,45 | 0.62±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 413 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 414 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 415 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 416 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 417 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 418 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 419 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 420 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 421 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 422 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 423 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 424 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 425 | - | 45,45,45 | 0.64±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 426 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 427 | - | 45,45,45 | 0.63±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 428 | - | 45,45,45 | 0.64±0.02 | 0±0 (0±0%) |
| 4 | PX4 | A | 429 | - | 45,45,45 | 0.62±0.01 | 0±0 (0±0%) |
| 4 | PX4 | A | 430 | - | 45,45,45 | 0.63±0.01 | 0±0 (0±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 |
| 4 | PX4 | A | 306 | - | 50,53,53 | 1.48±0.07 | 0±0 (0±0%) |
| 4 | PX4 | A | 307 | - | 50,53,53 | 1.57±0.20 | 0±0 (0±0%) |
| 4 | PX4 | A | 308 | - | 50,53,53 | 1.50±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 309 | - | 50,53,53 | 1.50±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 310 | - | 50,53,53 | 1.47±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 311 | - | 50,53,53 | 1.54±0.21 | 0±1 (0±1%) |
| 4 | PX4 | A | 312 | - | 50,53,53 | 1.47±0.18 | 0±1 (0±1%) |
| 4 | PX4 | A | 313 | - | 50,53,53 | 1.50±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 314 | - | 50,53,53 | 1.47±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 315 | - | 50,53,53 | 1.41±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 316 | - | 50,53,53 | 1.43±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 317 | - | 50,53,53 | 1.43±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 318 | - | 50,53,53 | 1.43±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 319 | - | 50,53,53 | 1.51±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 320 | - | 50,53,53 | 1.45±0.16 | 0±1 (0±1%) |
| 4 | PX4 | A | 321 | - | 50,53,53 | 1.43±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 322 | - | 50,53,53 | 1.49±0.17 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 323 | - | 50,53,53 | 1.41±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 324 | - | 50,53,53 | 1.42±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 325 | - | 50,53,53 | 1.50±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 326 | - | 50,53,53 | 1.44±0.20 | 0±0 (0±0%) |
| 4 | PX4 | A | 327 | - | 50,53,53 | 1.55±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 328 | - | 50,53,53 | 1.49±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 329 | - | 50,53,53 | 1.50±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 330 | - | 50,53,53 | 1.45±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 331 | - | 50,53,53 | 1.51±0.14 | 0±1 (0±1%) |
| 4 | PX4 | A | 332 | - | 50,53,53 | 1.46±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 333 | - | 50,53,53 | 1.50±0.17 | 1±1 (1±1%) |
| 4 | PX4 | A | 334 | - | 50,53,53 | 1.51±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 335 | - | 50,53,53 | 1.48±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 336 | - | 50,53,53 | 1.48±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 337 | - | 50,53,53 | 1.45±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 338 | - | 50,53,53 | 1.52±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 339 | - | 50,53,53 | 1.44±0.24 | 0±1 (0±1%) |
| 4 | PX4 | A | 340 | - | 50,53,53 | 1.56±0.10 | 0±0 (0±0%) |
| 4 | PX4 | A | 341 | - | 50,53,53 | 1.48±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 342 | - | 50,53,53 | 1.50±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 343 | - | 50,53,53 | 1.45±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 344 | - | 50,53,53 | 1.51±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 345 | - | 50,53,53 | 1.43±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 346 | - | 50,53,53 | 1.45±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 347 | - | 50,53,53 | 1.47±0.20 | 0±0 (0±0%) |
| 4 | PX4 | A | 348 | - | 50,53,53 | 1.48±0.16 | 0±1 (0±1%) |
| 4 | PX4 | A | 349 | - | 50,53,53 | 1.51±0.12 | 0±1 (0±1%) |
| 4 | PX4 | A | 350 | - | 50,53,53 | 1.41±0.11 | 0±0 (0±0%) |
| 4 | PX4 | A | 351 | - | 50,53,53 | 1.49±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 352 | - | 50,53,53 | 1.49±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 353 | - | 50,53,53 | 1.49±0.11 | 0±0 (0±0%) |
| 4 | PX4 | A | 354 | - | 50,53,53 | 1.55±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 355 | - | 50,53,53 | 1.46±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 356 | - | 50,53,53 | 1.49±0.20 | 0±0 (0±0%) |
| 4 | PX4 | A | 357 | - | 50,53,53 | 1.47±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 358 | - | 50,53,53 | 1.44±0.15 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 359 | - | 50,53,53 | 1.52±0.14 | 1±1 (1±1%) |
| 4 | PX4 | A | 360 | - | 50,53,53 | 1.49±0.12 | 0±1 (0±1%) |
| 4 | PX4 | A | 361 | - | 50,53,53 | 1.52±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 362 | - | 50,53,53 | 1.48±0.08 | 0±0 (0±0%) |
| 4 | PX4 | A | 363 | - | 50,53,53 | 1.45±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 364 | - | 50,53,53 | 1.53±0.21 | 0±0 (0±0%) |
| 4 | PX4 | A | 365 | - | 50,53,53 | 1.48±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 366 | - | 50,53,53 | 1.50±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 367 | - | 50,53,53 | 1.49±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 368 | - | 50,53,53 | 1.49±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 369 | - | 50,53,53 | 1.37±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 370 | - | 50,53,53 | 1.47±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 371 | - | 50,53,53 | 1.67±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 372 | - | 50,53,53 | 1.45±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 373 | - | 50,53,53 | 1.58±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 374 | - | 50,53,53 | 1.45±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 375 | - | 50,53,53 | 1.50±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 376 | - | 50,53,53 | 1.48±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 377 | - | 50,53,53 | 1.52±0.20 | 0±1 (0±1%) |
| 4 | PX4 | A | 378 | - | 50,53,53 | 1.43±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 379 | - | 50,53,53 | 1.53±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 380 | - | 50,53,53 | 1.46±0.16 | 0±1 (0±1%) |
| 4 | PX4 | A | 381 | - | 50,53,53 | 1.56±0.13 | 0±1 (0±1%) |
| 4 | PX4 | A | 382 | - | 50,53,53 | 1.44±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 383 | - | 50,53,53 | 1.42±0.11 | 0±0 (0±0%) |
| 4 | PX4 | A | 384 | - | 50,53,53 | 1.47±0.22 | 0±0 (0±0%) |
| 4 | PX4 | A | 385 | - | 50,53,53 | 1.52±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 386 | - | 50,53,53 | 1.46±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 387 | - | 50,53,53 | 1.52±0.16 | 0±1 (0±1%) |
| 4 | PX4 | A | 388 | - | 50,53,53 | 1.43±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 389 | - | 50,53,53 | 1.53±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 390 | - | 50,53,53 | 1.46±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 391 | - | 50,53,53 | 1.49±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 392 | - | 50,53,53 | 1.53±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 393 | - | 50,53,53 | 1.54±0.14 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | PX4 | A | 394 | - | 50,53,53 | 1.50±0.16 | 0±1 (0±1%) |
| 4 | PX4 | A | 395 | - | 50,53,53 | 1.49±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 396 | - | 50,53,53 | 1.53±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 397 | - | 50,53,53 | 1.51±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 398 | - | 50,53,53 | 1.45±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 399 | - | 50,53,53 | 1.46±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 400 | - | 50,53,53 | 1.47±0.19 | 0±1 (0±1%) |
| 4 | PX4 | A | 401 | - | 50,53,53 | 1.56±0.15 | 0±1 (0±1%) |
| 4 | PX4 | A | 402 | - | 50,53,53 | 1.42±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 403 | - | 50,53,53 | 1.49±0.14 | 0±1 (0±1%) |
| 4 | PX4 | A | 404 | - | 50,53,53 | 1.53±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 405 | - | 50,53,53 | 1.48±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 406 | - | 50,53,53 | 1.43±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 407 | - | 50,53,53 | 1.44±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 408 | - | 50,53,53 | 1.49±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 409 | - | 50,53,53 | 1.50±0.10 | 0±0 (0±0%) |
| 4 | PX4 | A | 410 | - | 50,53,53 | 1.47±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 411 | - | 50,53,53 | 1.46±0.11 | 0±0 (0±0%) |
| 4 | PX4 | A | 412 | - | 50,53,53 | 1.40±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 413 | - | 50,53,53 | 1.49±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 414 | - | 50,53,53 | 1.52±0.14 | 0±0 (0±0%) |
| 4 | PX4 | A | 415 | - | 50,53,53 | 1.54±0.17 | 0±1 (0±1%) |
| 4 | PX4 | A | 416 | - | 50,53,53 | 1.46±0.17 | 0±0 (0±0%) |
| 4 | PX4 | A | 417 | - | 50,53,53 | 1.53±0.16 | 0±0 (0±0%) |
| 4 | PX4 | A | 418 | - | 50,53,53 | 1.48±0.15 | 0±0 (0±0%) |
| 4 | PX4 | A | 419 | - | 50,53,53 | 1.50±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 420 | - | 50,53,53 | 1.47±0.13 | 0±1 (0±1%) |
| 4 | PX4 | A | 421 | - | 50,53,53 | 1.46±0.14 | 0±1 (0±1%) |
| 4 | PX4 | A | 422 | - | 50,53,53 | 1.50±0.13 | 0±0 (0±0%) |
| 4 | PX4 | A | 423 | - | 50,53,53 | 1.46±0.12 | 0±0 (0±0%) |
| 4 | PX4 | A | 424 | - | 50,53,53 | 1.41±0.18 | 0±0 (0±0%) |
| 4 | PX4 | A | 425 | - | 50,53,53 | 1.44±0.11 | 0±0 (0±0%) |
| 4 | PX4 | A | 426 | - | 50,53,53 | 1.45±0.14 | 0±1 (0±1%) |
| 4 | PX4 | A | 427 | - | 50,53,53 | 1.61±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 428 | - | 50,53,53 | 1.52±0.11 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Counts | Bond angles | |
|-----|------|-------|-----|------|----------|-------------|------------|
| | | | | | | RMSZ | #Z>2 |
| 4 | PX4 | A | 429 | - | 50,53,53 | 1.47±0.19 | 0±0 (0±0%) |
| 4 | PX4 | A | 430 | - | 50,53,53 | 1.56±0.15 | 0±0 (0±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 |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 4 | PX4 | A | 306 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 307 | - | - | 2±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 308 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 309 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 310 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 311 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 312 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 313 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 314 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 315 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 316 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 317 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 318 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 319 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 320 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 321 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 322 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 323 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 324 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 325 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 326 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 327 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 328 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 329 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 330 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 331 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 332 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 333 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 334 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 335 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 336 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 337 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 338 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 4 | PX4 | A | 339 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 340 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 341 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 342 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 343 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 344 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 345 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 346 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 347 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 348 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 349 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 350 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 351 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 352 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 353 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 354 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 355 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 356 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 357 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 358 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 359 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 360 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 361 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 362 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 363 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 364 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 365 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 366 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 367 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 368 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 369 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 370 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 371 | - | - | 2±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 372 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 373 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 374 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 375 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 376 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 377 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 378 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 379 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 380 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 4 | PX4 | A | 381 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 382 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 383 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 384 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 385 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 386 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 387 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 388 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 389 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 390 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 391 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 392 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 393 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 394 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 395 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 396 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 397 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 398 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 399 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 400 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 401 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 402 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 403 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 404 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 405 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 406 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 407 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 408 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 409 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 410 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 411 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 412 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 413 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 414 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 415 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 416 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 417 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 418 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 419 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 420 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 421 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 422 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 4 | PX4 | A | 423 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 424 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 425 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 426 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 427 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 428 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 429 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |
| 4 | PX4 | A | 430 | - | - | 0±0,49,49,49 | 0±0,0,0,0 |

There are no bond-length outliers.

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 |
| 4 | A | 417 | PX4 | O7-C23-C24 | 7.82 | 127.78 | 111.55 | 6 | 2 |
| 4 | A | 427 | PX4 | O5-C8-C7 | 7.40 | 127.26 | 108.66 | 6 | 3 |
| 4 | A | 413 | PX4 | C8-C7-C6 | 7.34 | 95.29 | 111.86 | 8 | 1 |
| 4 | A | 396 | PX4 | C8-C7-C6 | 7.28 | 95.44 | 111.86 | 3 | 6 |
| 4 | A | 427 | PX4 | C8-C7-C6 | 7.12 | 95.79 | 111.86 | 14 | 1 |
| 4 | A | 426 | PX4 | O7-C23-C24 | 7.10 | 126.28 | 111.55 | 7 | 1 |
| 4 | A | 385 | PX4 | O7-C23-C24 | 7.09 | 126.27 | 111.55 | 6 | 1 |
| 4 | A | 353 | PX4 | C8-C7-C6 | 6.98 | 96.10 | 111.86 | 11 | 4 |
| 4 | A | 370 | PX4 | O5-C8-C7 | 6.98 | 126.20 | 108.66 | 1 | 1 |
| 4 | A | 376 | PX4 | C8-C7-C6 | 6.96 | 96.16 | 111.86 | 2 | 1 |
| 4 | A | 388 | PX4 | O5-C8-C7 | 6.94 | 126.09 | 108.66 | 7 | 1 |
| 4 | A | 320 | PX4 | O5-C8-C7 | 6.94 | 126.09 | 108.66 | 7 | 1 |
| 4 | A | 389 | PX4 | C8-C7-C6 | 6.92 | 96.24 | 111.86 | 10 | 1 |
| 4 | A | 349 | PX4 | O7-C23-C24 | 6.91 | 125.89 | 111.55 | 8 | 3 |
| 4 | A | 312 | PX4 | O5-C8-C7 | 6.90 | 126.00 | 108.66 | 5 | 1 |
| 4 | A | 334 | PX4 | O5-C8-C7 | 6.87 | 125.92 | 108.66 | 4 | 1 |
| 4 | A | 424 | PX4 | O7-C23-C24 | 6.87 | 125.82 | 111.55 | 7 | 1 |
| 4 | A | 397 | PX4 | O7-C23-C24 | 6.87 | 125.81 | 111.55 | 13 | 1 |
| 4 | A | 371 | PX4 | O7-C23-C24 | 6.80 | 125.67 | 111.55 | 3 | 4 |
| 4 | A | 310 | PX4 | C8-C7-C6 | 6.76 | 96.60 | 111.86 | 3 | 1 |
| 4 | A | 367 | PX4 | O7-C23-C24 | 6.74 | 125.56 | 111.55 | 5 | 2 |
| 4 | A | 345 | PX4 | O5-C8-C7 | 6.71 | 125.52 | 108.66 | 7 | 1 |
| 4 | A | 428 | PX4 | C8-C7-C6 | 6.70 | 96.74 | 111.86 | 6 | 1 |
| 4 | A | 380 | PX4 | O5-C8-C7 | 6.70 | 125.48 | 108.66 | 11 | 1 |
| 4 | A | 331 | PX4 | C8-C7-C6 | 6.67 | 96.81 | 111.86 | 12 | 2 |
| 4 | A | 401 | PX4 | C8-C7-C6 | 6.66 | 96.84 | 111.86 | 13 | 3 |
| 4 | A | 380 | PX4 | C8-C7-C6 | 6.62 | 96.92 | 111.86 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 429 | PX4 | O5-C8-C7 | 6.61 | 125.26 | 108.66 | 5 | 1 |
| 4 | A | 326 | PX4 | O5-C8-C7 | 6.58 | 125.18 | 108.66 | 6 | 1 |
| 4 | A | 405 | PX4 | O5-C8-C7 | 6.54 | 125.09 | 108.66 | 11 | 1 |
| 4 | A | 335 | PX4 | O5-C8-C7 | 6.54 | 125.09 | 108.66 | 8 | 2 |
| 4 | A | 397 | PX4 | C8-C7-C6 | 6.53 | 97.12 | 111.86 | 3 | 1 |
| 4 | A | 337 | PX4 | C7-O7-C23 | 6.52 | 133.29 | 117.88 | 12 | 1 |
| 4 | A | 333 | PX4 | O5-C8-C7 | 6.45 | 124.85 | 108.66 | 13 | 5 |
| 4 | A | 365 | PX4 | O5-C8-C7 | 6.43 | 124.81 | 108.66 | 6 | 1 |
| 4 | A | 363 | PX4 | O5-C8-C7 | 6.43 | 124.80 | 108.66 | 9 | 2 |
| 4 | A | 361 | PX4 | C8-C7-C6 | 6.41 | 97.41 | 111.86 | 3 | 2 |
| 4 | A | 321 | PX4 | C8-C7-C6 | 6.38 | 97.48 | 111.86 | 13 | 1 |
| 4 | A | 413 | PX4 | O5-C8-C7 | 6.36 | 124.65 | 108.66 | 10 | 1 |
| 4 | A | 339 | PX4 | O5-C8-C7 | 6.36 | 124.64 | 108.66 | 5 | 2 |
| 4 | A | 390 | PX4 | O5-C8-C7 | 6.35 | 124.61 | 108.66 | 6 | 2 |
| 4 | A | 382 | PX4 | C8-C7-C6 | 6.31 | 97.61 | 111.86 | 8 | 1 |
| 4 | A | 377 | PX4 | C8-C7-C6 | 6.31 | 97.62 | 111.86 | 14 | 3 |
| 4 | A | 359 | PX4 | O7-C23-C24 | 6.31 | 124.65 | 111.55 | 7 | 2 |
| 4 | A | 345 | PX4 | C8-C7-C6 | 6.31 | 97.63 | 111.86 | 6 | 2 |
| 4 | A | 360 | PX4 | O5-C8-C7 | 6.27 | 124.41 | 108.66 | 12 | 1 |
| 4 | A | 317 | PX4 | C7-O7-C23 | 6.26 | 132.66 | 117.88 | 5 | 1 |
| 4 | A | 399 | PX4 | O7-C23-C24 | 6.25 | 124.53 | 111.55 | 10 | 1 |
| 4 | A | 389 | PX4 | O7-C23-C24 | 6.25 | 124.53 | 111.55 | 11 | 1 |
| 4 | A | 339 | PX4 | O7-C23-C24 | 6.24 | 124.50 | 111.55 | 3 | 2 |
| 4 | A | 403 | PX4 | O3-P1-O2 | 6.23 | 84.12 | 109.25 | 2 | 1 |
| 4 | A | 427 | PX4 | O7-C23-C24 | 6.22 | 124.47 | 111.55 | 1 | 1 |
| 4 | A | 403 | PX4 | C5-N1-C3 | 6.21 | 93.24 | 108.98 | 7 | 1 |
| 4 | A | 401 | PX4 | O5-C8-C7 | 6.21 | 124.25 | 108.66 | 7 | 1 |
| 4 | A | 425 | PX4 | C8-C7-C6 | 6.20 | 97.86 | 111.86 | 14 | 1 |
| 4 | A | 414 | PX4 | C8-C7-C6 | 6.20 | 97.88 | 111.86 | 6 | 1 |
| 4 | A | 314 | PX4 | O5-C8-C7 | 6.17 | 124.16 | 108.66 | 11 | 1 |
| 4 | A | 353 | PX4 | O5-C8-C7 | 6.17 | 124.15 | 108.66 | 14 | 2 |
| 4 | A | 377 | PX4 | O5-C8-C7 | 6.16 | 124.14 | 108.66 | 11 | 1 |
| 4 | A | 318 | PX4 | C8-C7-C6 | 6.13 | 98.02 | 111.86 | 3 | 3 |
| 4 | A | 421 | PX4 | O5-C8-C7 | 6.10 | 123.98 | 108.66 | 9 | 3 |
| 4 | A | 415 | PX4 | C4-N1-C3 | 6.08 | 93.59 | 108.98 | 14 | 1 |
| 4 | A | 311 | PX4 | C8-C7-C6 | 6.07 | 98.17 | 111.86 | 8 | 1 |
| 4 | A | 401 | PX4 | C5-N1-C3 | 6.07 | 93.61 | 108.98 | 13 | 1 |
| 4 | A | 428 | PX4 | O5-C8-C7 | 6.06 | 123.88 | 108.66 | 1 | 3 |
| 4 | A | 430 | PX4 | C8-C7-C6 | 6.04 | 98.24 | 111.86 | 10 | 1 |
| 4 | A | 386 | PX4 | O7-C23-C24 | 6.02 | 124.04 | 111.55 | 8 | 2 |
| 4 | A | 341 | PX4 | O7-C23-C24 | 6.01 | 124.03 | 111.55 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 375 | PX4 | C8-C7-C6 | 6.00 | 98.33 | 111.86 | 1 | 1 |
| 4 | A | 430 | PX4 | O5-C8-C7 | 5.99 | 123.71 | 108.66 | 8 | 2 |
| 4 | A | 348 | PX4 | O7-C7-C8 | 5.99 | 130.20 | 108.44 | 6 | 1 |
| 4 | A | 418 | PX4 | O7-C23-C24 | 5.97 | 123.95 | 111.55 | 4 | 1 |
| 4 | A | 398 | PX4 | O5-C8-C7 | 5.96 | 123.62 | 108.66 | 11 | 1 |
| 4 | A | 390 | PX4 | O7-C23-C24 | 5.95 | 123.91 | 111.55 | 7 | 2 |
| 4 | A | 327 | PX4 | O7-C23-C24 | 5.94 | 123.89 | 111.55 | 11 | 2 |
| 4 | A | 323 | PX4 | O7-C23-C24 | 5.94 | 123.88 | 111.55 | 8 | 1 |
| 4 | A | 415 | PX4 | C8-C7-C6 | 5.93 | 98.48 | 111.86 | 3 | 2 |
| 4 | A | 311 | PX4 | C5-N1-C3 | 5.92 | 93.99 | 108.98 | 10 | 1 |
| 4 | A | 356 | PX4 | O7-C23-C24 | 5.91 | 123.83 | 111.55 | 3 | 1 |
| 4 | A | 377 | PX4 | C7-O7-C23 | 5.91 | 131.83 | 117.88 | 4 | 1 |
| 4 | A | 368 | PX4 | O5-C8-C7 | 5.90 | 123.49 | 108.66 | 13 | 2 |
| 4 | A | 374 | PX4 | O5-C8-C7 | 5.90 | 123.49 | 108.66 | 10 | 1 |
| 4 | A | 311 | PX4 | O5-C8-C7 | 5.89 | 123.44 | 108.66 | 8 | 2 |
| 4 | A | 355 | PX4 | O5-C8-C7 | 5.88 | 123.44 | 108.66 | 7 | 1 |
| 4 | A | 363 | PX4 | C8-C7-C6 | 5.87 | 98.63 | 111.86 | 11 | 3 |
| 4 | A | 397 | PX4 | O5-C8-C7 | 5.85 | 123.35 | 108.66 | 11 | 3 |
| 4 | A | 418 | PX4 | O5-C8-C7 | 5.84 | 123.33 | 108.66 | 13 | 1 |
| 4 | A | 373 | PX4 | O5-C8-C7 | 5.84 | 123.33 | 108.66 | 4 | 1 |
| 4 | A | 307 | PX4 | O7-C23-C24 | 5.82 | 123.64 | 111.55 | 9 | 1 |
| 4 | A | 422 | PX4 | O5-C8-C7 | 5.82 | 123.29 | 108.66 | 6 | 1 |
| 4 | A | 370 | PX4 | C8-C7-C6 | 5.78 | 98.82 | 111.86 | 7 | 2 |
| 4 | A | 329 | PX4 | O5-C8-C7 | 5.78 | 123.17 | 108.66 | 1 | 1 |
| 4 | A | 394 | PX4 | O5-C8-C7 | 5.78 | 123.17 | 108.66 | 6 | 2 |
| 4 | A | 359 | PX4 | C8-C7-C6 | 5.77 | 98.83 | 111.86 | 5 | 2 |
| 4 | A | 379 | PX4 | C7-O7-C23 | 5.77 | 131.51 | 117.88 | 2 | 1 |
| 4 | A | 423 | PX4 | O5-C9-O6 | 5.77 | 109.23 | 123.55 | 4 | 1 |
| 4 | A | 319 | PX4 | C8-C7-C6 | 5.77 | 98.85 | 111.86 | 6 | 1 |
| 4 | A | 350 | PX4 | C8-C7-C6 | 5.75 | 98.88 | 111.86 | 10 | 3 |
| 4 | A | 327 | PX4 | C8-C7-C6 | 5.75 | 98.89 | 111.86 | 4 | 3 |
| 4 | A | 408 | PX4 | C4-N1-C3 | 5.74 | 123.53 | 108.98 | 14 | 1 |
| 4 | A | 331 | PX4 | O7-C23-C24 | 5.73 | 123.46 | 111.55 | 8 | 1 |
| 4 | A | 306 | PX4 | O7-C23-C24 | 5.73 | 123.46 | 111.55 | 5 | 1 |
| 4 | A | 417 | PX4 | O5-C8-C7 | 5.73 | 123.06 | 108.66 | 14 | 3 |
| 4 | A | 406 | PX4 | O7-C23-C24 | 5.72 | 123.44 | 111.55 | 6 | 1 |
| 4 | A | 400 | PX4 | C8-C7-C6 | 5.72 | 98.95 | 111.86 | 8 | 2 |
| 4 | A | 342 | PX4 | O7-C23-C24 | 5.72 | 123.43 | 111.55 | 14 | 1 |
| 4 | A | 378 | PX4 | O3-P1-O2 | 5.72 | 86.18 | 109.25 | 4 | 1 |
| 4 | A | 351 | PX4 | C8-C7-C6 | 5.72 | 98.96 | 111.86 | 4 | 2 |
| 4 | A | 407 | PX4 | C8-C7-C6 | 5.71 | 98.97 | 111.86 | 11 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 312 | PX4 | C8-C7-C6 | 5.70 | 99.00 | 111.86 | 5 | 1 |
| 4 | A | 416 | PX4 | O7-C23-C24 | 5.70 | 123.38 | 111.55 | 13 | 1 |
| 4 | A | 354 | PX4 | O5-C8-C7 | 5.69 | 122.96 | 108.66 | 1 | 1 |
| 4 | A | 385 | PX4 | C8-C7-C6 | 5.69 | 99.03 | 111.86 | 8 | 3 |
| 4 | A | 392 | PX4 | O5-C8-C7 | 5.68 | 122.93 | 108.66 | 2 | 2 |
| 4 | A | 330 | PX4 | C8-C7-C6 | 5.67 | 99.06 | 111.86 | 13 | 1 |
| 4 | A | 334 | PX4 | C8-C7-C6 | 5.67 | 99.06 | 111.86 | 9 | 1 |
| 4 | A | 411 | PX4 | O5-C8-C7 | 5.67 | 122.89 | 108.66 | 12 | 2 |
| 4 | A | 327 | PX4 | C7-O7-C23 | 5.67 | 131.26 | 117.88 | 6 | 1 |
| 4 | A | 367 | PX4 | C8-C7-C6 | 5.66 | 99.08 | 111.86 | 13 | 1 |
| 4 | A | 381 | PX4 | C7-O7-C23 | 5.66 | 104.49 | 117.88 | 8 | 1 |
| 4 | A | 422 | PX4 | O7-C23-C24 | 5.64 | 123.27 | 111.55 | 10 | 2 |
| 4 | A | 394 | PX4 | C8-C7-C6 | 5.64 | 99.13 | 111.86 | 10 | 2 |
| 4 | A | 371 | PX4 | C8-C7-C6 | 5.63 | 99.15 | 111.86 | 9 | 1 |
| 4 | A | 384 | PX4 | O5-C8-C7 | 5.63 | 122.81 | 108.66 | 13 | 1 |
| 4 | A | 307 | PX4 | C7-O7-C23 | 5.62 | 131.16 | 117.88 | 3 | 1 |
| 4 | A | 375 | PX4 | O7-C23-C24 | 5.62 | 123.23 | 111.55 | 3 | 1 |
| 4 | A | 429 | PX4 | C8-C7-C6 | 5.62 | 99.18 | 111.86 | 14 | 1 |
| 4 | A | 415 | PX4 | O5-C8-C7 | 5.61 | 122.75 | 108.66 | 14 | 1 |
| 4 | A | 320 | PX4 | C8-C7-C6 | 5.61 | 99.21 | 111.86 | 7 | 1 |
| 4 | A | 362 | PX4 | C8-C7-C6 | 5.60 | 99.23 | 111.86 | 10 | 1 |
| 4 | A | 333 | PX4 | C8-C7-C6 | 5.59 | 99.25 | 111.86 | 7 | 3 |
| 4 | A | 343 | PX4 | O7-C23-C24 | 5.59 | 123.15 | 111.55 | 14 | 1 |
| 4 | A | 368 | PX4 | C8-C7-C6 | 5.58 | 99.28 | 111.86 | 11 | 1 |
| 4 | A | 422 | PX4 | C4-N1-C3 | 5.57 | 94.87 | 108.98 | 9 | 1 |
| 4 | A | 313 | PX4 | O5-C8-C7 | 5.56 | 122.62 | 108.66 | 14 | 1 |
| 4 | A | 400 | PX4 | O5-C8-C7 | 5.55 | 122.61 | 108.66 | 7 | 1 |
| 4 | A | 346 | PX4 | C8-C7-C6 | 5.54 | 99.35 | 111.86 | 9 | 1 |
| 4 | A | 386 | PX4 | O5-C8-C7 | 5.54 | 122.58 | 108.66 | 10 | 1 |
| 4 | A | 338 | PX4 | C8-C7-C6 | 5.54 | 99.36 | 111.86 | 14 | 1 |
| 4 | A | 423 | PX4 | O5-C8-C7 | 5.54 | 122.57 | 108.66 | 5 | 1 |
| 4 | A | 387 | PX4 | C8-C7-C6 | 5.53 | 99.38 | 111.86 | 4 | 3 |
| 4 | A | 426 | PX4 | O7-C23-O8 | 5.53 | 109.89 | 123.68 | 7 | 1 |
| 4 | A | 316 | PX4 | O5-C8-C7 | 5.52 | 122.53 | 108.66 | 12 | 2 |
| 4 | A | 387 | PX4 | P1-O3-C1 | 5.52 | 92.70 | 121.60 | 5 | 1 |
| 4 | A | 378 | PX4 | O5-C8-C7 | 5.52 | 122.53 | 108.66 | 12 | 1 |
| 4 | A | 324 | PX4 | C8-C7-C6 | 5.51 | 99.43 | 111.86 | 9 | 1 |
| 4 | A | 346 | PX4 | O7-C23-C24 | 5.51 | 122.99 | 111.55 | 6 | 1 |
| 4 | A | 340 | PX4 | C8-C7-C6 | 5.49 | 99.47 | 111.86 | 11 | 1 |
| 4 | A | 380 | PX4 | O7-C23-C24 | 5.49 | 122.95 | 111.55 | 6 | 2 |
| 4 | A | 339 | PX4 | C8-C7-C6 | 5.48 | 99.49 | 111.86 | 11 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 348 | PX4 | C8-C7-C6 | 5.45 | 99.57 | 111.86 | 6 | 3 |
| 4 | A | 331 | PX4 | O7-C23-O8 | 5.44 | 110.10 | 123.68 | 8 | 1 |
| 4 | A | 317 | PX4 | C8-C7-C6 | 5.44 | 99.59 | 111.86 | 11 | 1 |
| 4 | A | 313 | PX4 | O7-C23-C24 | 5.43 | 122.83 | 111.55 | 7 | 1 |
| 4 | A | 359 | PX4 | O5-C8-C7 | 5.43 | 122.30 | 108.66 | 5 | 3 |
| 4 | A | 347 | PX4 | O5-C8-C7 | 5.42 | 122.28 | 108.66 | 1 | 1 |
| 4 | A | 393 | PX4 | C8-C7-C6 | 5.42 | 99.64 | 111.86 | 2 | 1 |
| 4 | A | 308 | PX4 | O5-C8-C7 | 5.41 | 122.26 | 108.66 | 10 | 2 |
| 4 | A | 404 | PX4 | O5-C8-C7 | 5.41 | 122.24 | 108.66 | 13 | 1 |
| 4 | A | 408 | PX4 | C8-C7-C6 | 5.39 | 99.70 | 111.86 | 11 | 1 |
| 4 | A | 360 | PX4 | C8-C7-C6 | 5.39 | 99.70 | 111.86 | 12 | 1 |
| 4 | A | 379 | PX4 | O5-C8-C7 | 5.38 | 122.19 | 108.66 | 12 | 1 |
| 4 | A | 328 | PX4 | O7-C23-C24 | 5.38 | 122.72 | 111.55 | 10 | 1 |
| 4 | A | 388 | PX4 | C5-N1-C4 | 5.35 | 95.42 | 108.98 | 3 | 1 |
| 4 | A | 375 | PX4 | O5-C8-C7 | 5.35 | 122.11 | 108.66 | 4 | 2 |
| 4 | A | 351 | PX4 | O5-C8-C7 | 5.35 | 122.09 | 108.66 | 14 | 2 |
| 4 | A | 381 | PX4 | O7-C23-C24 | 5.33 | 122.63 | 111.55 | 12 | 2 |
| 4 | A | 342 | PX4 | C8-C7-C6 | 5.33 | 99.84 | 111.86 | 6 | 2 |
| 4 | A | 348 | PX4 | O7-C23-O8 | 5.31 | 110.43 | 123.68 | 5 | 1 |
| 4 | A | 352 | PX4 | C8-C7-C6 | 5.30 | 99.89 | 111.86 | 6 | 1 |
| 4 | A | 335 | PX4 | C8-C7-C6 | 5.30 | 99.90 | 111.86 | 11 | 2 |
| 4 | A | 309 | PX4 | O7-C23-C24 | 5.30 | 122.56 | 111.55 | 13 | 1 |
| 4 | A | 417 | PX4 | C8-C7-C6 | 5.29 | 99.91 | 111.86 | 1 | 1 |
| 4 | A | 392 | PX4 | C8-C7-C6 | 5.29 | 99.93 | 111.86 | 12 | 1 |
| 4 | A | 411 | PX4 | C4-N1-C3 | 5.28 | 122.35 | 108.98 | 1 | 1 |
| 4 | A | 410 | PX4 | C8-C7-C6 | 5.28 | 99.95 | 111.86 | 8 | 2 |
| 4 | A | 409 | PX4 | O5-C8-C7 | 5.26 | 121.88 | 108.66 | 6 | 2 |
| 4 | A | 365 | PX4 | C8-C7-C6 | 5.26 | 100.00 | 111.86 | 5 | 2 |
| 4 | A | 420 | PX4 | O7-C23-C24 | 5.26 | 122.46 | 111.55 | 13 | 1 |
| 4 | A | 344 | PX4 | C8-C7-C6 | 5.24 | 100.03 | 111.86 | 7 | 1 |
| 4 | A | 328 | PX4 | C5-N1-C4 | 5.24 | 95.72 | 108.98 | 5 | 1 |
| 4 | A | 403 | PX4 | O5-C8-C7 | 5.24 | 121.81 | 108.66 | 5 | 1 |
| 4 | A | 364 | PX4 | C7-O7-C23 | 5.24 | 130.25 | 117.88 | 9 | 1 |
| 4 | A | 382 | PX4 | O5-C8-C7 | 5.23 | 121.81 | 108.66 | 7 | 1 |
| 4 | A | 344 | PX4 | C5-N1-C4 | 5.23 | 95.72 | 108.98 | 6 | 1 |
| 4 | A | 391 | PX4 | C8-C7-C6 | 5.23 | 100.07 | 111.86 | 14 | 1 |
| 4 | A | 412 | PX4 | O7-C23-C24 | 5.22 | 122.39 | 111.55 | 7 | 1 |
| 4 | A | 421 | PX4 | C8-C7-C6 | 5.22 | 100.09 | 111.86 | 8 | 1 |
| 4 | A | 408 | PX4 | O5-C8-C7 | 5.21 | 121.75 | 108.66 | 13 | 1 |
| 4 | A | 352 | PX4 | O5-C8-C7 | 5.21 | 121.74 | 108.66 | 1 | 1 |
| 4 | A | 313 | PX4 | O3-P1-O2 | 5.21 | 88.25 | 109.25 | 13 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 410 | PX4 | O3-P1-O2 | 5.20 | 88.28 | 109.25 | 13 | 1 |
| 4 | A | 387 | PX4 | O7-C23-C24 | 5.19 | 122.33 | 111.55 | 12 | 1 |
| 4 | A | 393 | PX4 | O5-C8-C7 | 5.19 | 121.70 | 108.66 | 6 | 2 |
| 4 | A | 319 | PX4 | O5-C8-C7 | 5.19 | 121.70 | 108.66 | 2 | 1 |
| 4 | A | 338 | PX4 | O5-C9-C10 | 5.18 | 126.98 | 111.90 | 12 | 1 |
| 4 | A | 367 | PX4 | O5-C8-C7 | 5.18 | 121.68 | 108.66 | 8 | 1 |
| 4 | A | 425 | PX4 | O7-C23-C24 | 5.18 | 122.31 | 111.55 | 13 | 1 |
| 4 | A | 406 | PX4 | O5-C8-C7 | 5.18 | 121.67 | 108.66 | 9 | 1 |
| 4 | A | 306 | PX4 | O5-C8-C7 | 5.17 | 121.65 | 108.66 | 2 | 1 |
| 4 | A | 402 | PX4 | P1-O3-C1 | 5.17 | 94.57 | 121.60 | 10 | 1 |
| 4 | A | 316 | PX4 | C8-C7-C6 | 5.16 | 100.21 | 111.86 | 9 | 1 |
| 4 | A | 388 | PX4 | C8-C7-C6 | 5.15 | 100.23 | 111.86 | 1 | 1 |
| 4 | A | 361 | PX4 | C7-O7-C23 | 5.15 | 130.04 | 117.88 | 1 | 1 |
| 4 | A | 349 | PX4 | O5-C8-C7 | 5.13 | 121.56 | 108.66 | 1 | 1 |
| 4 | A | 364 | PX4 | O5-C8-C7 | 5.13 | 121.55 | 108.66 | 12 | 1 |
| 4 | A | 371 | PX4 | C7-O7-C23 | 5.13 | 129.99 | 117.88 | 14 | 1 |
| 4 | A | 385 | PX4 | O5-C8-C7 | 5.13 | 121.54 | 108.66 | 13 | 1 |
| 4 | A | 341 | PX4 | O7-C7-C8 | 5.13 | 127.06 | 108.44 | 7 | 1 |
| 4 | A | 384 | PX4 | O7-C23-C24 | 5.12 | 122.19 | 111.55 | 3 | 2 |
| 4 | A | 399 | PX4 | O5-C8-C7 | 5.12 | 121.52 | 108.66 | 2 | 1 |
| 4 | A | 395 | PX4 | O5-C8-C7 | 5.12 | 121.52 | 108.66 | 6 | 1 |
| 4 | A | 349 | PX4 | C7-O7-C23 | 5.12 | 129.97 | 117.88 | 5 | 1 |
| 4 | A | 394 | PX4 | P1-O3-C1 | 5.11 | 94.87 | 121.60 | 12 | 1 |
| 4 | A | 421 | PX4 | O7-C23-C24 | 5.11 | 122.16 | 111.55 | 9 | 1 |
| 4 | A | 395 | PX4 | C8-C7-C6 | 5.10 | 100.35 | 111.86 | 8 | 1 |
| 4 | A | 322 | PX4 | C7-O7-C23 | 5.10 | 129.92 | 117.88 | 6 | 1 |
| 4 | A | 372 | PX4 | O5-C9-O6 | 5.10 | 110.89 | 123.55 | 8 | 1 |
| 4 | A | 381 | PX4 | C8-C7-C6 | 5.09 | 100.37 | 111.86 | 12 | 2 |
| 4 | A | 424 | PX4 | C7-O7-C23 | 5.09 | 129.91 | 117.88 | 13 | 1 |
| 4 | A | 404 | PX4 | O5-C9-C10 | 5.09 | 126.72 | 111.90 | 3 | 1 |
| 4 | A | 346 | PX4 | O5-C8-C7 | 5.09 | 121.44 | 108.66 | 10 | 1 |
| 4 | A | 389 | PX4 | P1-O3-C1 | 5.09 | 94.98 | 121.60 | 6 | 1 |
| 4 | A | 400 | PX4 | O7-C23-C24 | 5.09 | 122.12 | 111.55 | 8 | 1 |
| 4 | A | 348 | PX4 | O5-C8-C7 | 5.09 | 121.44 | 108.66 | 3 | 1 |
| 4 | A | 377 | PX4 | C5-N1-C4 | 5.09 | 96.10 | 108.98 | 10 | 1 |
| 4 | A | 310 | PX4 | O7-C23-C24 | 5.08 | 122.10 | 111.55 | 14 | 1 |
| 4 | A | 420 | PX4 | O5-C8-C7 | 5.08 | 121.41 | 108.66 | 13 | 1 |
| 4 | A | 311 | PX4 | O7-C23-C24 | 5.08 | 122.09 | 111.55 | 7 | 1 |
| 4 | A | 387 | PX4 | O5-C8-C7 | 5.07 | 121.39 | 108.66 | 6 | 1 |
| 4 | A | 404 | PX4 | C8-C7-C6 | 5.07 | 100.42 | 111.86 | 10 | 1 |
| 4 | A | 322 | PX4 | O7-C23-C24 | 5.07 | 122.07 | 111.55 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 410 | PX4 | C7-O7-C23 | 5.05 | 129.82 | 117.88 | 7 | 1 |
| 4 | A | 307 | PX4 | C8-C7-C6 | 5.05 | 100.46 | 111.86 | 12 | 1 |
| 4 | A | 403 | PX4 | O7-C23-C24 | 5.03 | 121.99 | 111.55 | 2 | 1 |
| 4 | A | 366 | PX4 | O5-C8-C7 | 5.03 | 121.28 | 108.66 | 7 | 1 |
| 4 | A | 324 | PX4 | O5-C8-C7 | 5.02 | 121.28 | 108.66 | 5 | 1 |
| 4 | A | 356 | PX4 | C7-O7-C23 | 5.02 | 129.74 | 117.88 | 10 | 1 |
| 4 | A | 365 | PX4 | C7-O7-C23 | 5.01 | 129.71 | 117.88 | 7 | 1 |
| 4 | A | 322 | PX4 | C8-C7-C6 | 5.01 | 100.56 | 111.86 | 10 | 1 |
| 4 | A | 390 | PX4 | O7-C23-O8 | 5.00 | 111.20 | 123.68 | 13 | 1 |
| 4 | A | 331 | PX4 | O5-C8-C7 | 5.00 | 121.22 | 108.66 | 12 | 1 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|---------------|----------------|
| 4 | A | 371 | PX4 | C7-O7-C23-O8 | 14 |
| 4 | A | 371 | PX4 | C7-O7-C23-C24 | 14 |
| 4 | A | 307 | PX4 | C7-O7-C23-C24 | 12 |
| 4 | A | 307 | PX4 | C7-O7-C23-O8 | 11 |

There are no ring outliers.

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 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: 2mlr_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

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 | 1762 |
| Number of shifts mapped to atoms | 1762 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 2 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 160 | -0.25 ± 0.11 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 138 | 0.11 ± 0.14 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 129 | -0.17 ± 0.15 | None needed (< 0.5 ppm) |
| ^{15}N | 154 | -0.70 ± 0.49 | None needed (imprecise) |

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 83%, i.e. 1600 atoms were assigned a chemical shift out of a possible 1936. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 740/786 (94%) | 306/313 (98%) | 284/320 (89%) | 150/153 (98%) |
| Sidechain | 712/887 (80%) | 443/521 (85%) | 260/326 (80%) | 9/40 (22%) |

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| | Total | ¹H | ¹³C | ¹⁵N |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 148/263 (56%) | 79/142 (56%) | 66/109 (61%) | 3/12 (25%) |
| Overall | 1600/1936 (83%) | 828/976 (85%) | 610/755 (81%) | 162/205 (79%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1629 atoms were assigned a chemical shift out of a possible 1968. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone | 757/806 (94%) | 314/321 (98%) | 289/328 (88%) | 154/157 (98%) |
| Sidechain | 724/899 (81%) | 450/528 (85%) | 265/331 (80%) | 9/40 (22%) |
| Aromatic | 148/263 (56%) | 79/142 (56%) | 66/109 (61%) | 3/12 (25%) |
| Overall | 1629/1968 (83%) | 843/991 (85%) | 620/768 (81%) | 166/209 (79%) |

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 226 | LEU | CG | 33.00 | 32.55 – 21.05 | 5.4 |
| 1 | A | 214 | LEU | CG | 33.00 | 32.55 – 21.05 | 5.4 |

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.

Random coil index (RCI) for chain A:

