# Full wwPDB EM Validation Report ⓘ

Oct 19, 2026 – 10:09 PM JST

| | | |
|---|---|---|
| PDB ID | : | 9X17 / pdb_00009x17 |
| EMDB ID | : | EMD-66453 |
| Title | : | Cryo-EM structure of the dITP-bound acive form of the KomBC filament |
| Authors | : | Li, X.; Liu, M.; Jiang, W.X.; Xing, Q.; Ma, L.X.; Huang, F.T. |
| Deposited on | : | 2025-10-01 |
| Resolution | : | 3.21 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

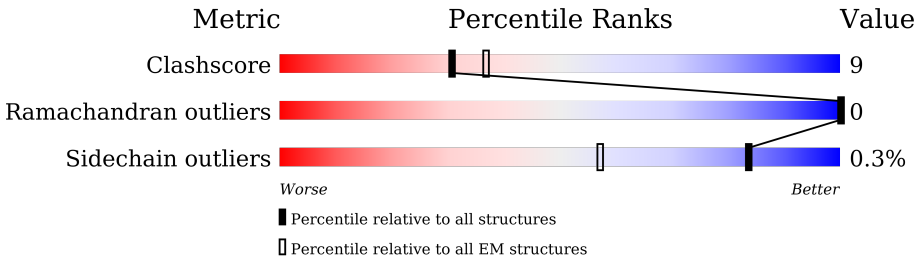
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.51 |

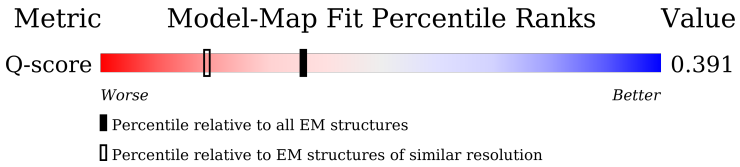
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.21 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 14613 ( 2.71 - 3.71 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AB | 197 | 34% 76% 19% 6% |
| 1 | AC | 197 | 44% 73% 22% 6% |
| 1 | AG | 197 | 27% 77% 17% 6% |
| 1 | AI | 197 | 40% 74% 20% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AN | 197 | 9% 78% 17% 6% |
| 1 | AO | 197 | 5% 78% 16% 6% |
| 1 | AS | 197 | 8% 71% 24% 6% |
| 1 | AU | 197 | 71% 23% 6% |
| 1 | BB | 197 | 75% 19% 6% |
| 1 | BC | 197 | 72% 22% 6% |
| 1 | BG | 197 | 76% 19% 6% |
| 1 | BI | 197 | 75% 20% 6% |
| 1 | BN | 197 | 76% 18% 6% |
| 1 | BO | 197 | 78% 16% 6% |
| 1 | BS | 197 | 69% 25% 6% |
| 1 | BU | 197 | 71% 23% 6% |
| 1 | CB | 197 | 79% 16% 6% |
| 1 | CC | 197 | 74% 21% 6% |
| 1 | CG | 197 | 77% 17% 6% |
| 1 | CI | 197 | 74% 21% 6% |
| 1 | CN | 197 | 5% 76% 18% 6% |
| 1 | CO | 197 | 6% 76% 18% 6% |
| 1 | CS | 197 | 67% 27% 6% |
| 1 | CU | 197 | 6% 71% 23% 6% |
| 1 | DB | 197 | 29% 78% 16% 6% |
| 1 | DC | 197 | 21% 73% 22% 6% |
| 1 | DG | 197 | 29% 77% 18% 6% |
| 1 | DI | 197 | 18% 74% 20% 6% |
| 2 | AD | 264 | 22% 79% 21% |

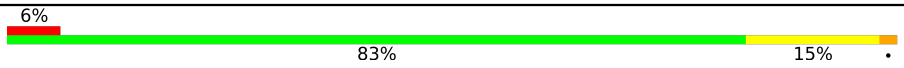
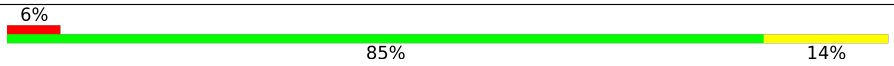
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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | AE | 264 | 10% 91% 9% |
| 2 | AK | 264 | 8% 83% 15% |
| 2 | AL | 264 | 14% 88% 12% |
| 2 | AP | 264 | 86% 14% |
| 2 | AQ | 264 | 86% 14% |
| 2 | AW | 264 | 80% 19% |
| 2 | AX | 264 | 88% 12% |
| 2 | BD | 264 | 79% 21% |
| 2 | BE | 264 | 89% 10% |
| 2 | BK | 264 | 83% 14% |
| 2 | BL | 264 | 89% 11% |
| 2 | BP | 264 | 86% 14% |
| 2 | BQ | 264 | 87% 13% |
| 2 | BW | 264 | 80% 19% |
| 2 | BX | 264 | 87% 13% |
| 2 | CD | 264 | 79% 21% |
| 2 | CE | 264 | 88% 11% |
| 2 | CK | 264 | 83% 14% |
| 2 | CL | 264 | 86% 13% |
| 2 | CP | 264 | 86% 14% |
| 2 | CQ | 264 | 86% 13% |
| 2 | CW | 264 | 80% 19% |
| 2 | CX | 264 | 88% 12% |
| 2 | DD | 264 | 6% 79% 21% |
| 2 | DE | 264 | 11% 89% 10% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | DK | 264 |   |
| 2 | DL | 264 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 3 | Y43 | AB | 201 | X | - | - | - |
| 3 | Y43 | AC | 201 | X | - | - | - |
| 3 | Y43 | AG | 201 | X | - | - | - |
| 3 | Y43 | AI | 201 | X | - | - | - |
| 3 | Y43 | AN | 201 | X | - | - | - |
| 3 | Y43 | AO | 201 | X | - | - | - |
| 3 | Y43 | AS | 201 | X | - | - | - |
| 3 | Y43 | AU | 201 | X | - | - | - |
| 3 | Y43 | BB | 201 | X | - | - | - |
| 3 | Y43 | BC | 201 | X | - | - | - |
| 3 | Y43 | BG | 201 | X | - | - | - |
| 3 | Y43 | BI | 201 | X | - | - | - |
| 3 | Y43 | BN | 201 | X | - | - | - |
| 3 | Y43 | BO | 201 | X | - | - | - |
| 3 | Y43 | BS | 201 | X | - | - | - |
| 3 | Y43 | BU | 201 | X | - | - | - |
| 3 | Y43 | CB | 201 | X | - | - | - |
| 3 | Y43 | CC | 201 | X | - | - | - |
| 3 | Y43 | CG | 201 | X | - | - | - |
| 3 | Y43 | CI | 201 | X | - | - | - |
| 3 | Y43 | CN | 201 | X | - | - | - |
| 3 | Y43 | CO | 201 | X | - | - | - |
| 3 | Y43 | CS | 201 | X | - | - | - |
| 3 | Y43 | CU | 201 | X | - | - | - |
| 3 | Y43 | DB | 201 | X | - | - | - |
| 3 | Y43 | DC | 201 | X | - | - | - |
| 3 | Y43 | DG | 201 | X | - | - | - |
| 3 | Y43 | DI | 201 | X | - | - | - |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 103012 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called KomB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | BC | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BG | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BI | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BN | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BO | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BS | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BU | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CB | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CC | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AB | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CG | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CI | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CN | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CO | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CS | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | CU | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | DB | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | DC | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AC | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | DG | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | DI | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AG | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AI | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AN | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AO | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AS | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | AU | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |
| 1 | BB | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 951 | 251 | 275 | 6 | | |

- Molecule 2 is a protein called KomC.

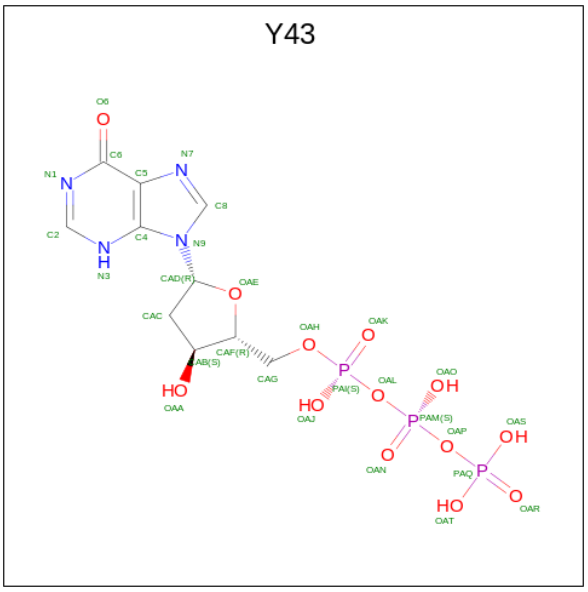
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | BD | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BE | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BK | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BL | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BP | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BQ | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BW | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | BX | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | CD | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CE | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CK | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CL | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CP | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CQ | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CW | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | CX | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | DD | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | DE | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | DK | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | DL | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AD | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AE | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AK | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AL | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AP | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AQ | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AW | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |
| 2 | AX | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2166 | 1403 | 348 | 410 | 5 | | |

- Molecule 3 is 2'-deoxyinosine 5'-triphosphate (CCD ID: Y43) (formula: $C_{10}H_{15}N_4O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | BC | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BG | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BI | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BN | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BO | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BS | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BU | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CB | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CC | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AB | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CG | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CI | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CN | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CO | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | CS | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | CU | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | DB | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | DC | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AC | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | DG | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | DI | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AG | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AI | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AO | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AS | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | AU | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |
| 3 | BB | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 10 | 4 | 13 | 3 | |

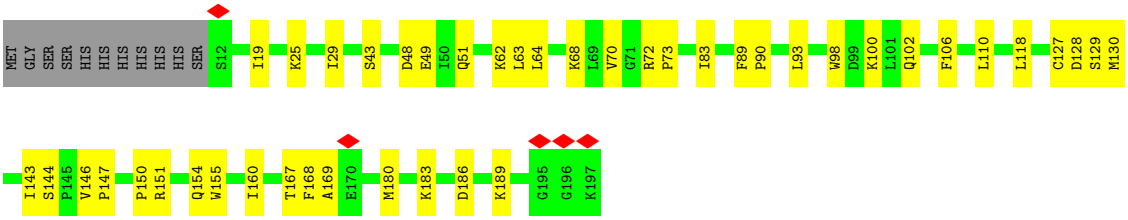
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: KomB

Chain BC:

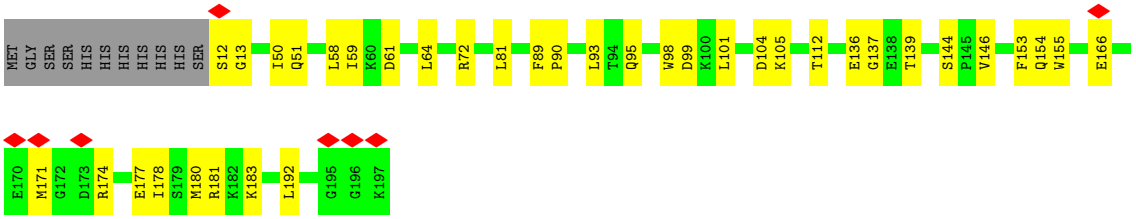



• Molecule 1: KomB

Chain BG:

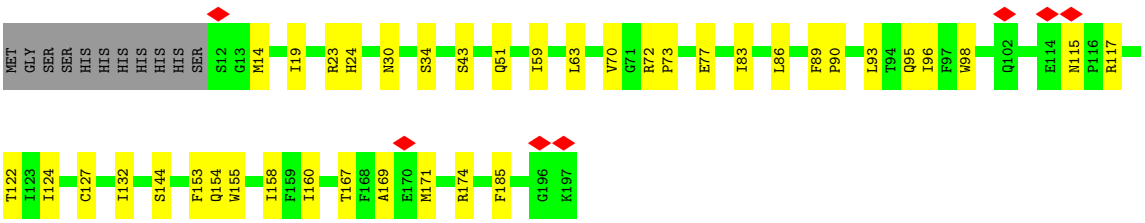



• Molecule 1: KomB

Chain BI:

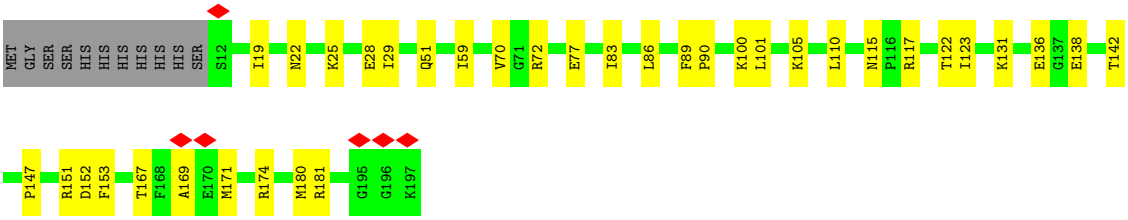



• Molecule 1: KomB

Chain BN:

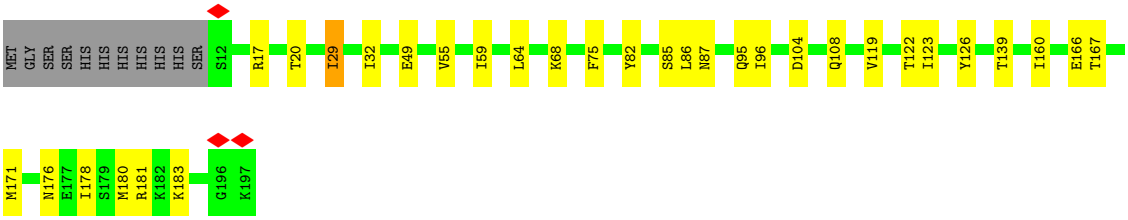





• Molecule 1: KomB

Chain BO:

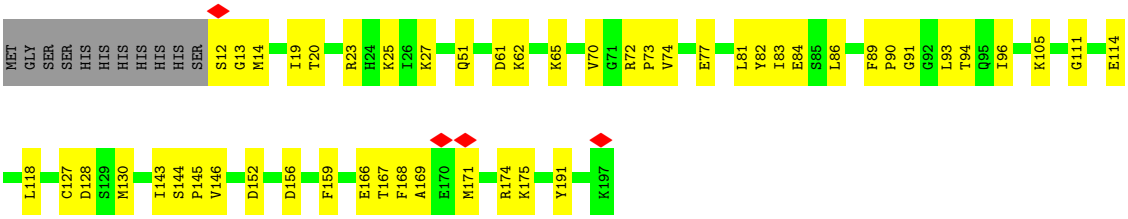



• Molecule 1: KomB

Chain BS:

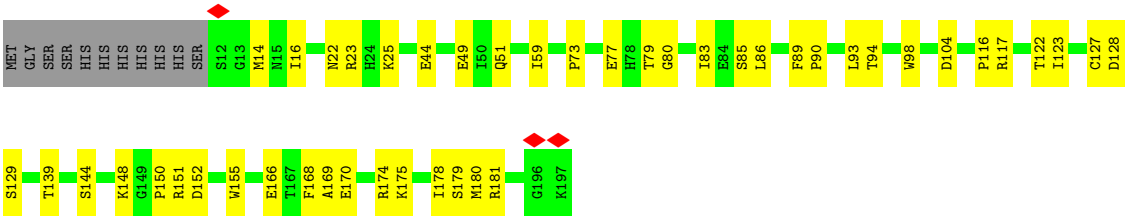



• Molecule 1: KomB

Chain BU:

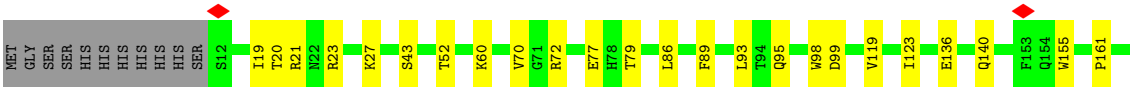


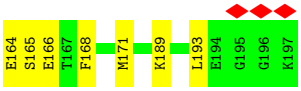




• Molecule 1: KomB

Chain CB:



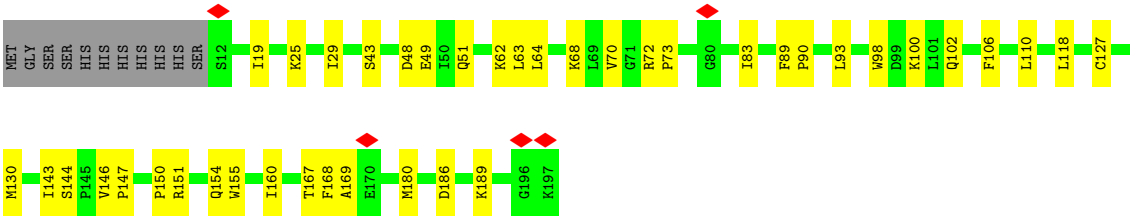






• Molecule 1: KomB

Chain CC:

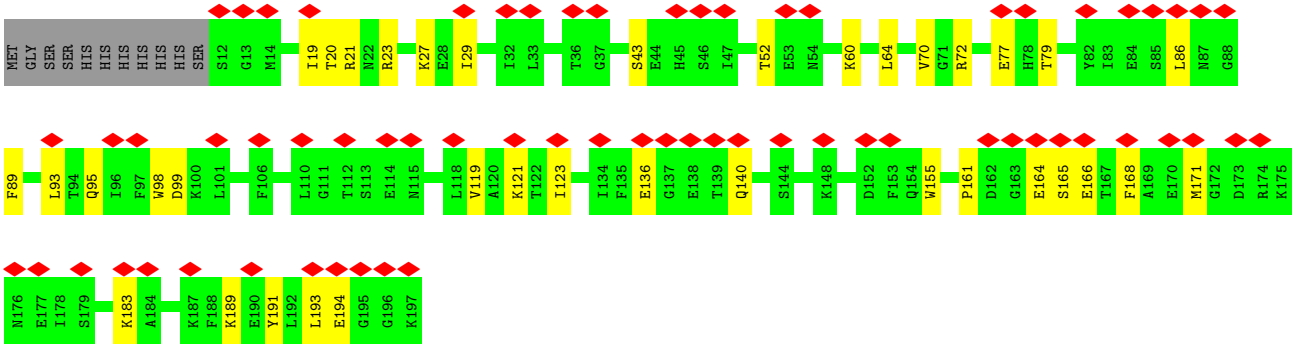



• Molecule 1: KomB

Chain AB:

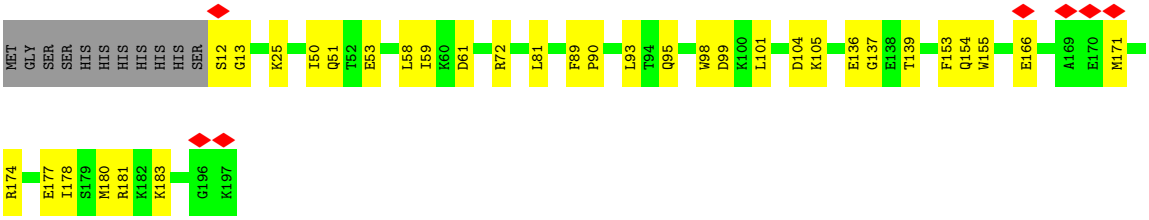



• Molecule 1: KomB

Chain CG:

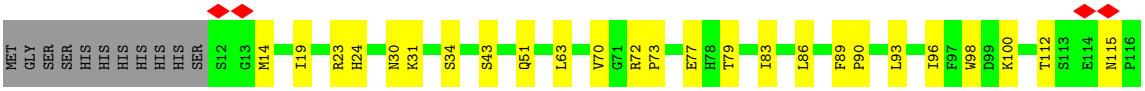


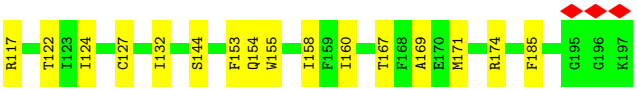




• Molecule 1: KomB

Chain CI:



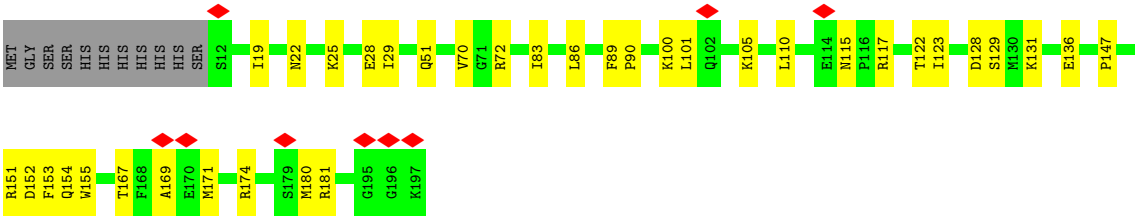






• Molecule 1: KomB

Chain CN:

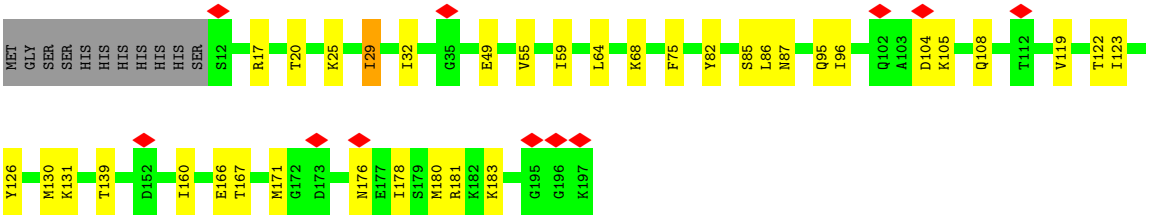



• Molecule 1: KomB

Chain CO:

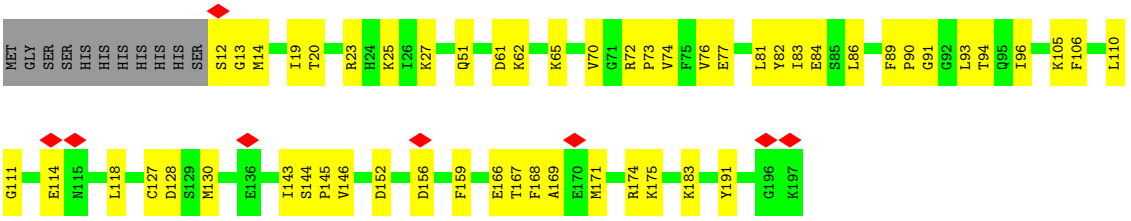



• Molecule 1: KomB

Chain CS:

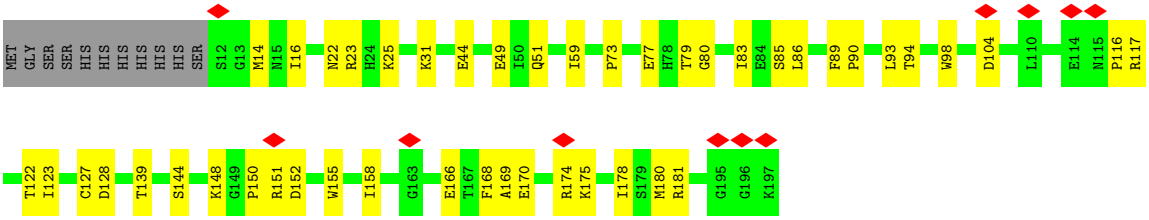



• Molecule 1: KomB

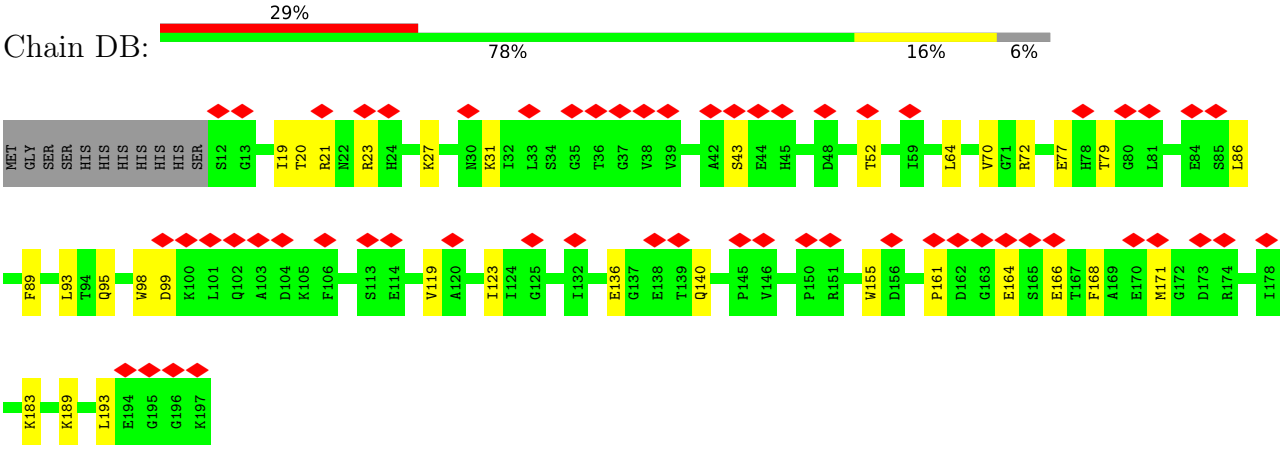
Chain CU:



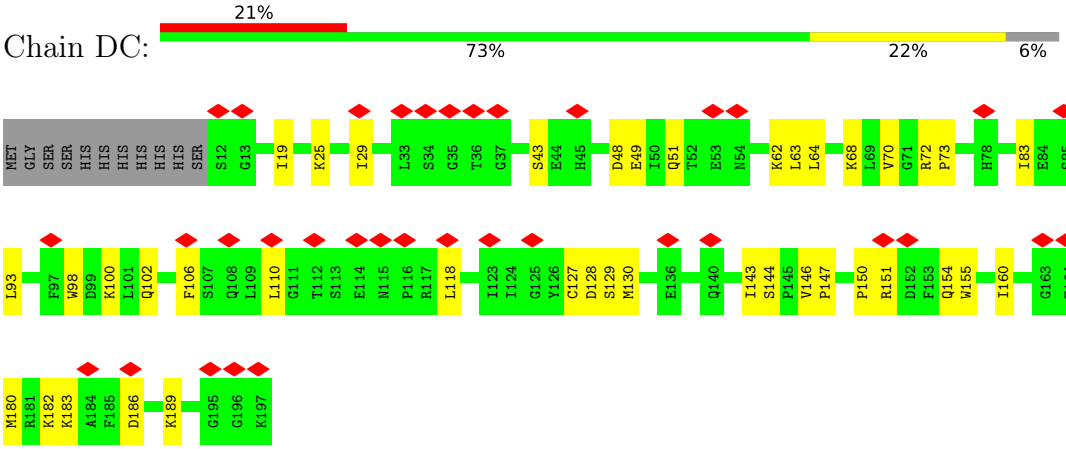

• Molecule 1: KomB

Chain DB:



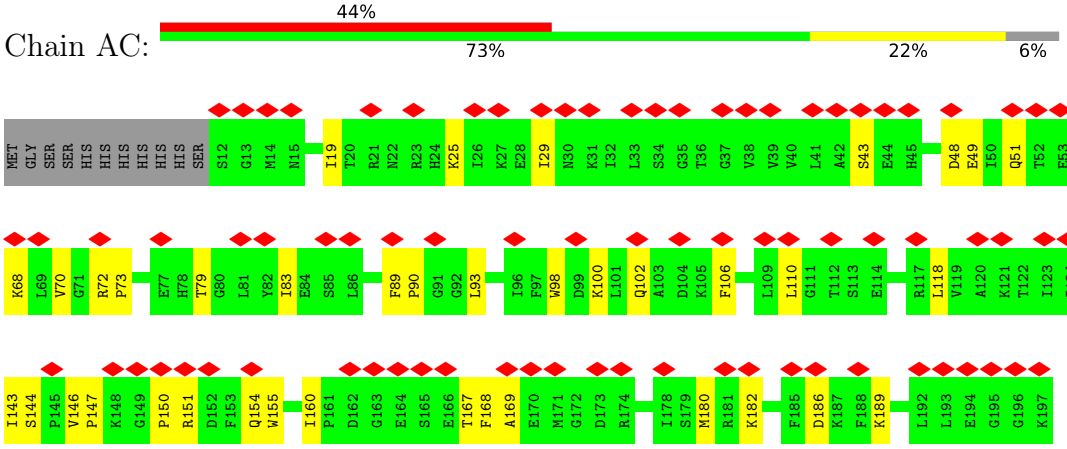

• Molecule 1: KomB

Chain DC:



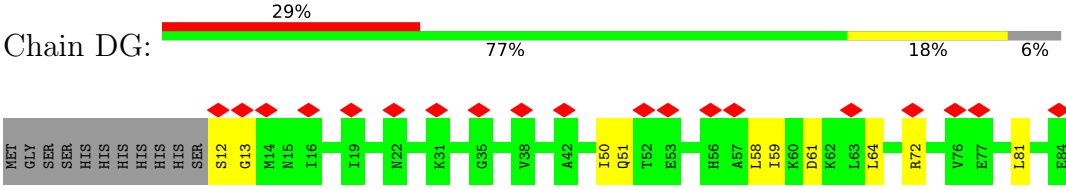

• Molecule 1: KomB

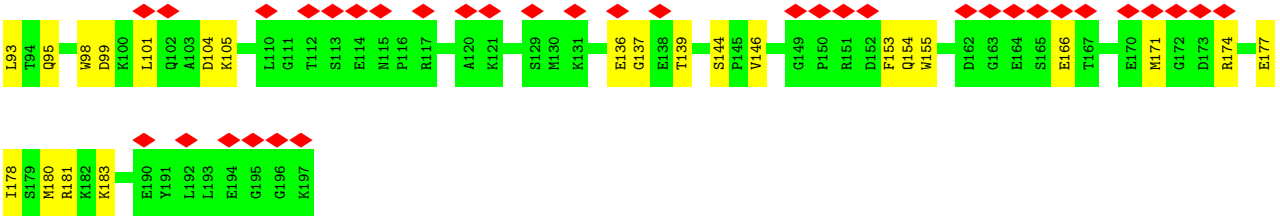
Chain AC:




• Molecule 1: KomB

Chain DG:

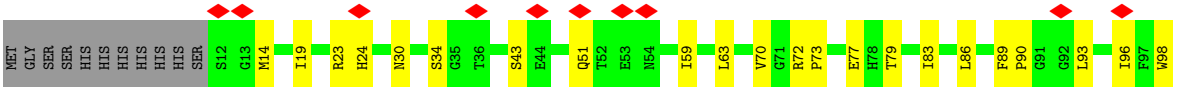


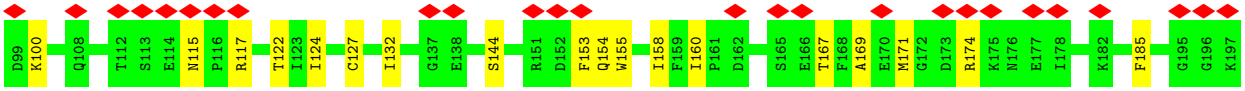



• Molecule 1: KomB

Chain DI:



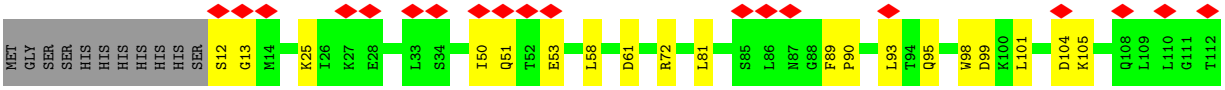



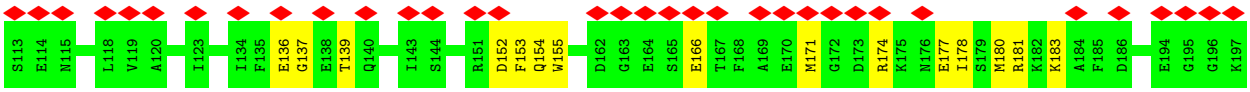




• Molecule 1: KomB

Chain AG:



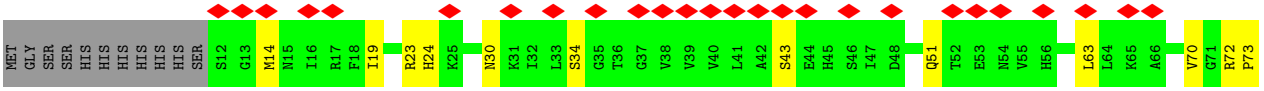



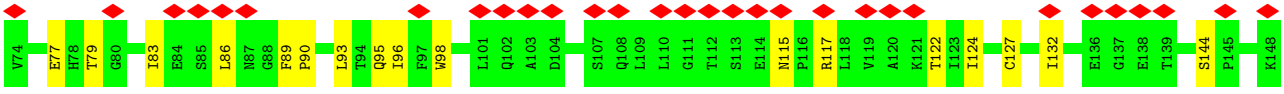




• Molecule 1: KomB

Chain AI:



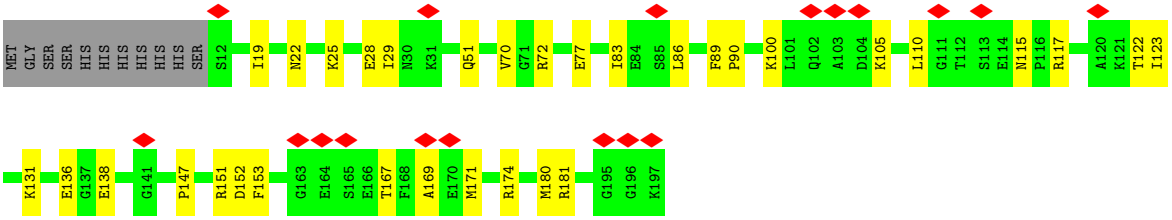




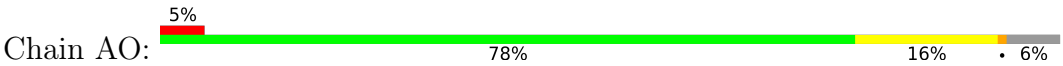
• Molecule 1: KomB

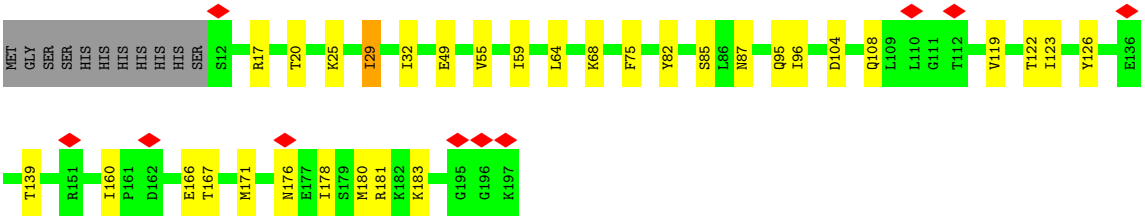
Chain AN:





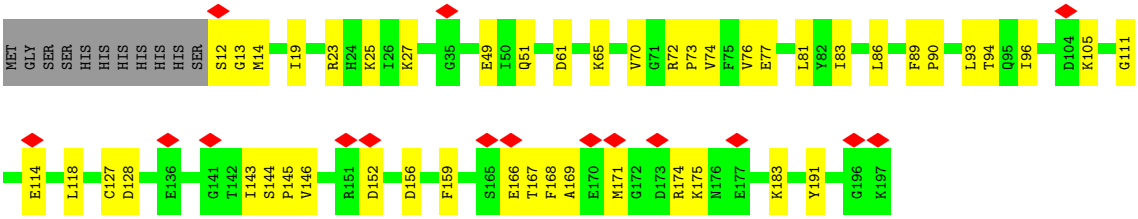

• Molecule 1: KomB



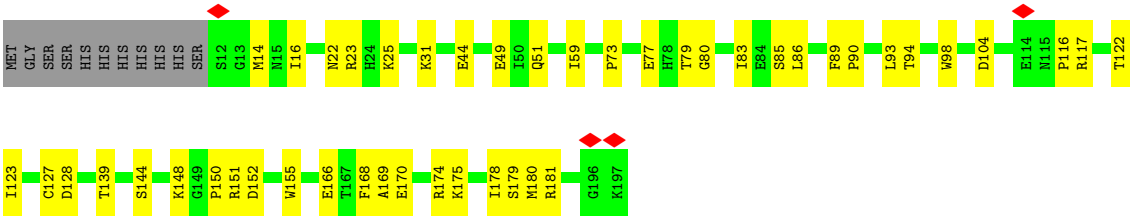

• Molecule 1: KomB



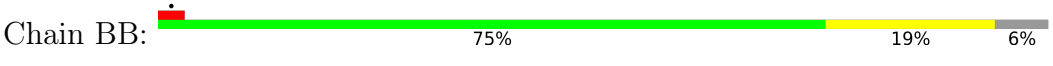



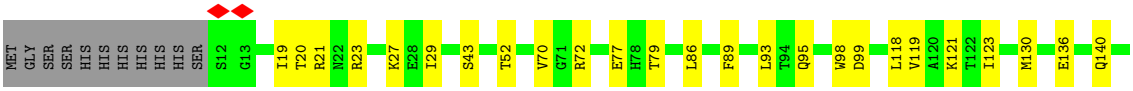

• Molecule 1: KomB

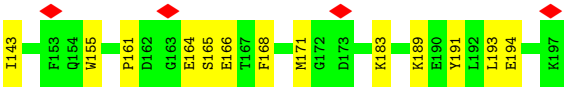



• Molecule 1: KomB



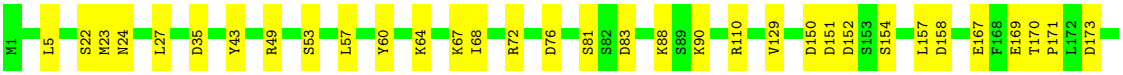



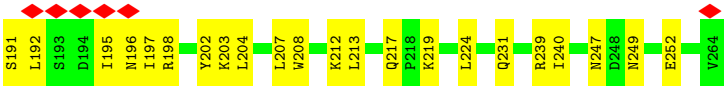



• Molecule 2: KomC

Chain BD:




• Molecule 2: KomC

Chain BE:







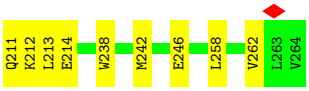
• Molecule 2: KomC

Chain BK:










• Molecule 2: KomC

Chain BL:



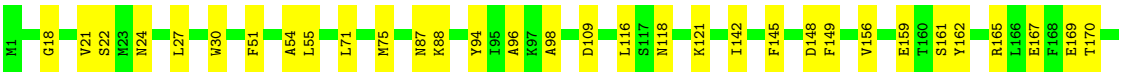


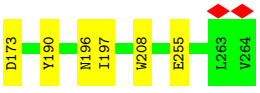


• Molecule 2: KomC

Chain BP:

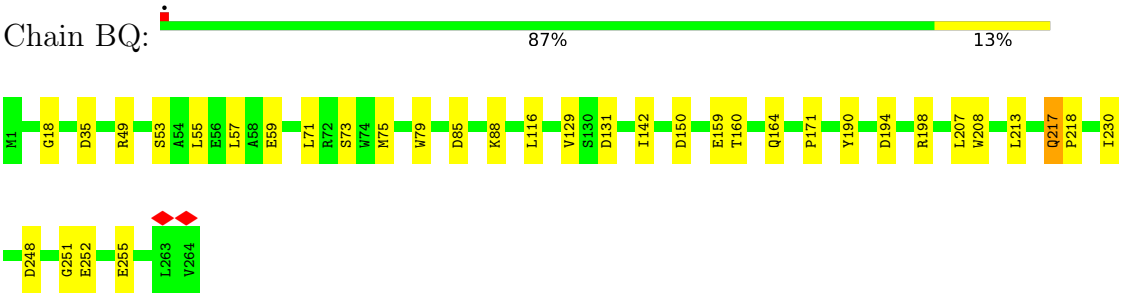


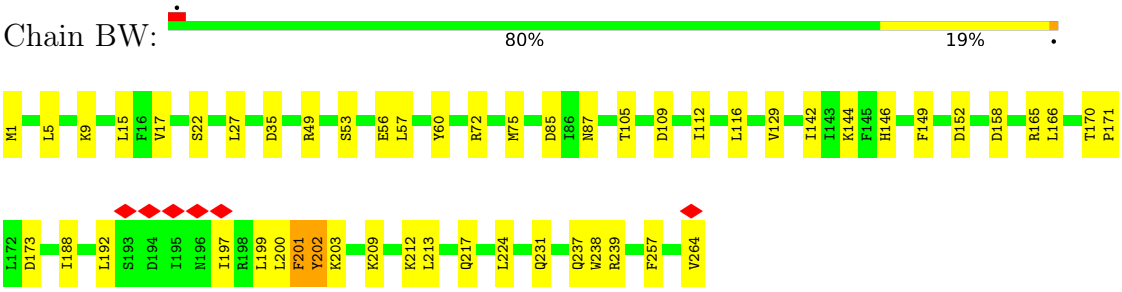
• Molecule 2: KomC

Chain BQ:



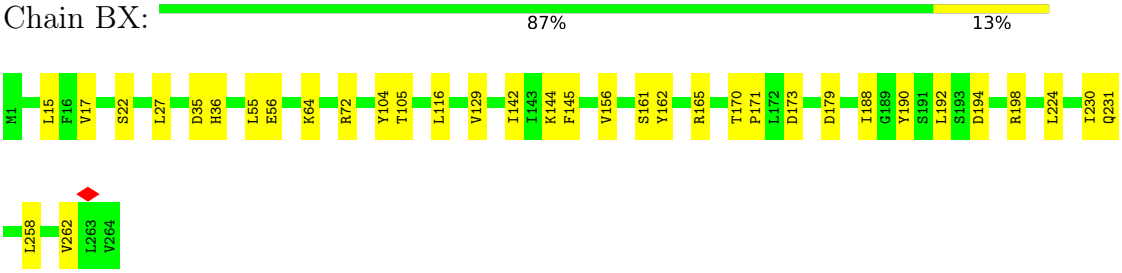

• Molecule 2: KomC

Chain BW:



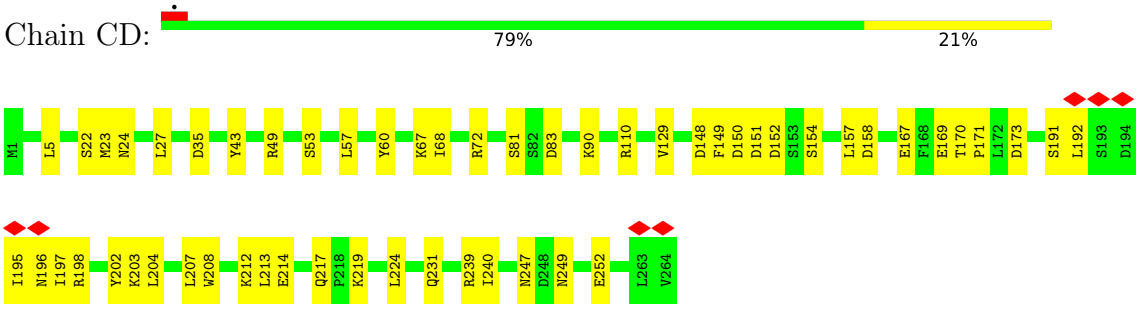

• Molecule 2: KomC

Chain BX:



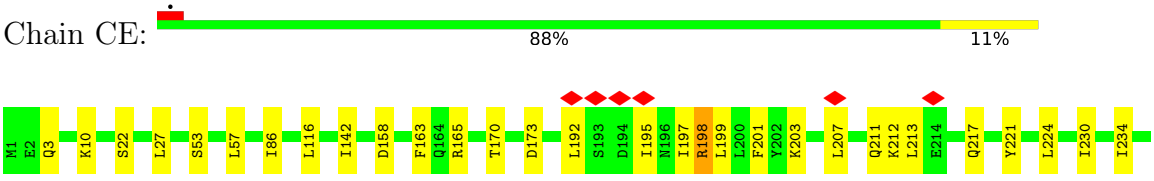

• Molecule 2: KomC

Chain CD:




• Molecule 2: KomC

Chain CE:

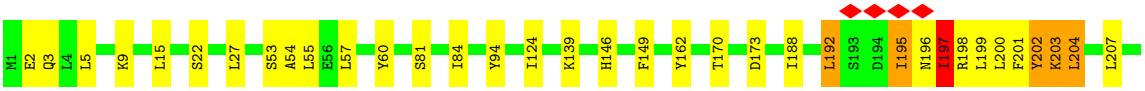


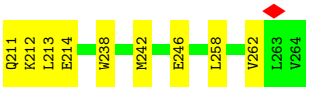



• Molecule 2: KomC

Chain CK:



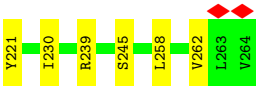

• Molecule 2: KomC

Chain CL:





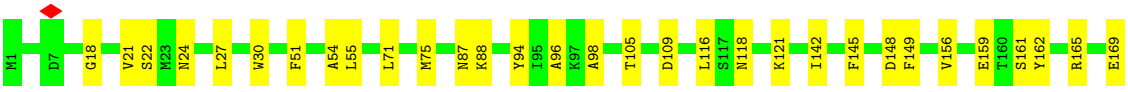


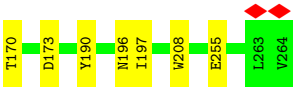



• Molecule 2: KomC

Chain CP:



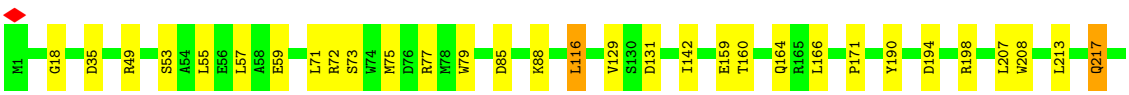



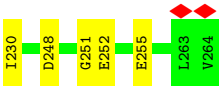




• Molecule 2: KomC

Chain CQ:

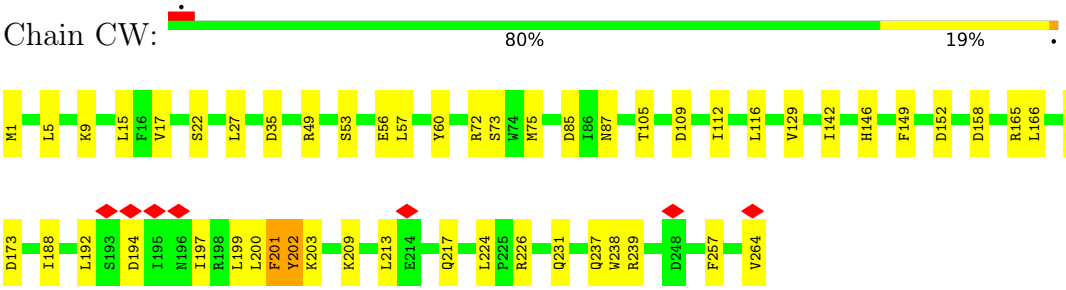


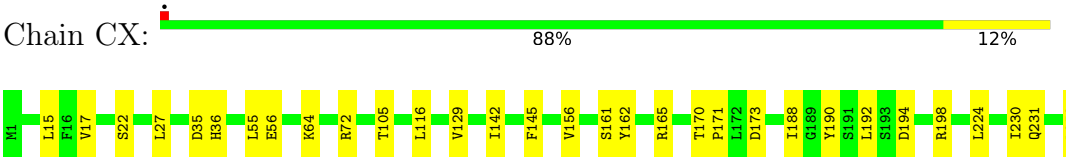

• Molecule 2: KomC

Chain CW:



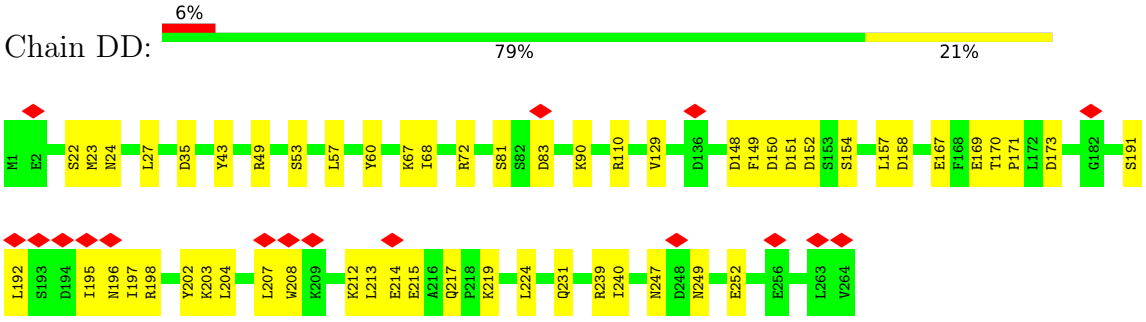

• Molecule 2: KomC

Chain CX:



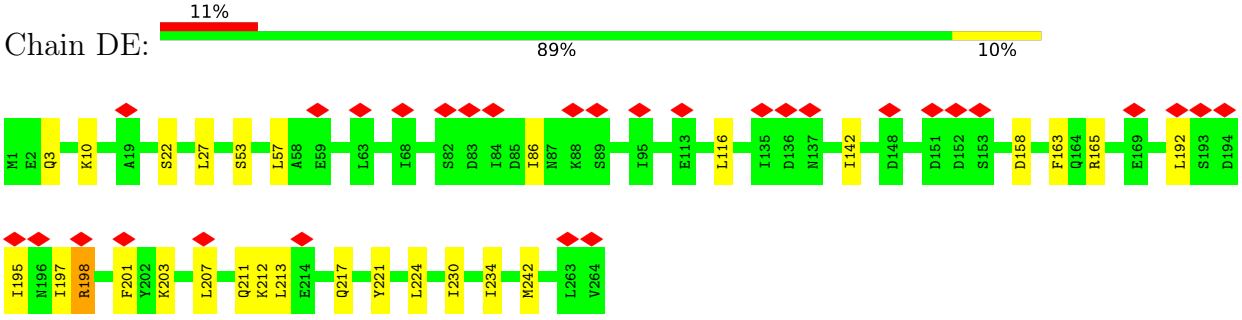

• Molecule 2: KomC

Chain DD:



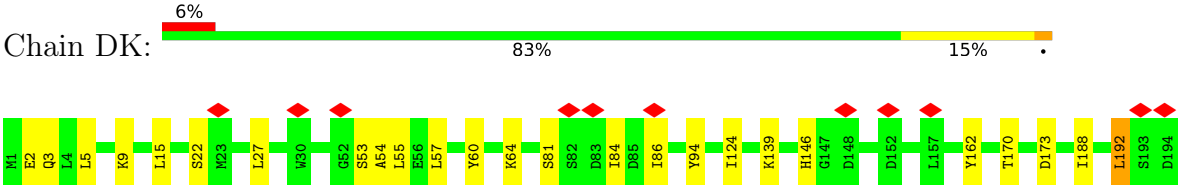

• Molecule 2: KomC

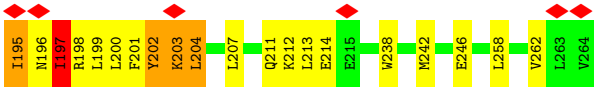
Chain DE:




• Molecule 2: KomC

Chain DK:

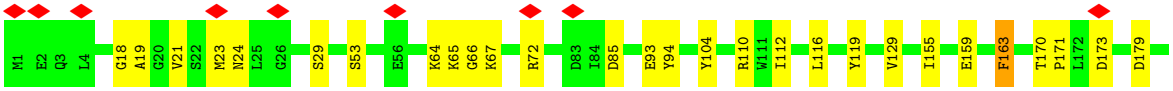





• Molecule 2: KomC

Chain DL:



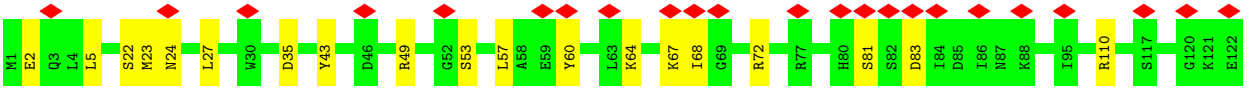


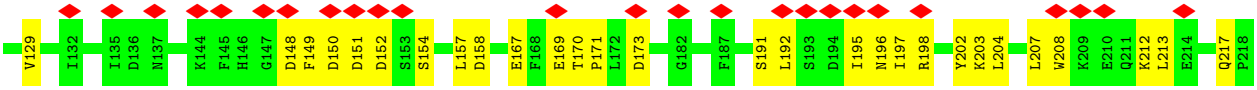


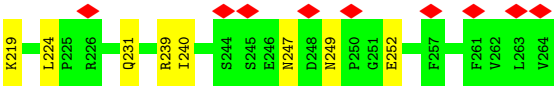
• Molecule 2: KomC

Chain AD:



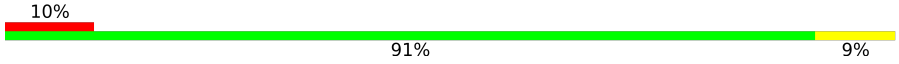



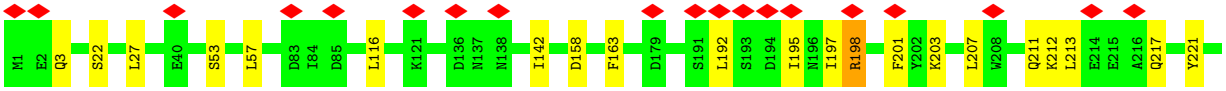



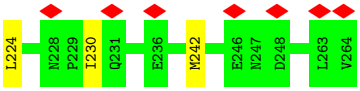




• Molecule 2: KomC

Chain AE:



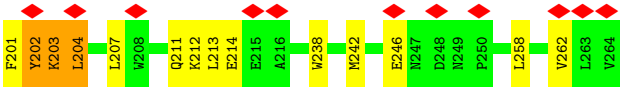




• Molecule 2: KomC

Chain AK:



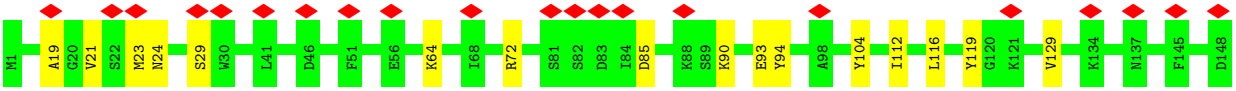


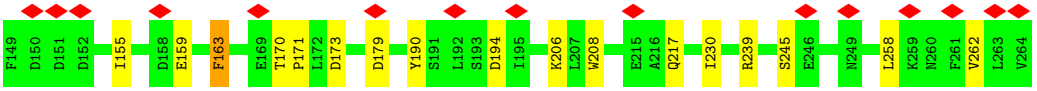




• Molecule 2: KomC

Chain AL:



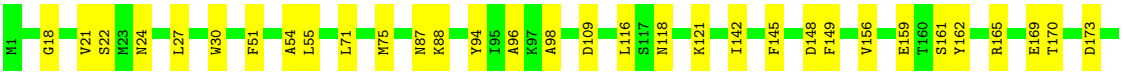



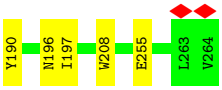




• Molecule 2: KomC

Chain AP:



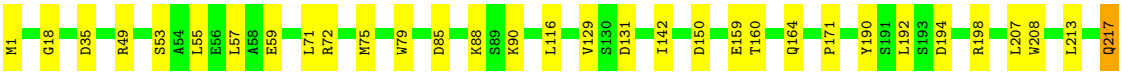



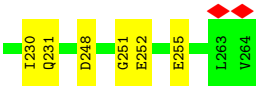




• Molecule 2: KomC

Chain AQ:



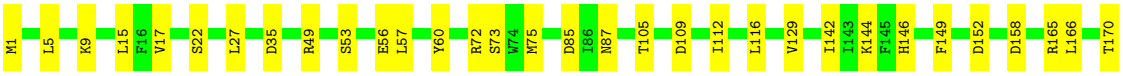



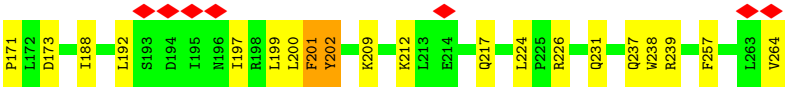




• Molecule 2: KomC

Chain AW:



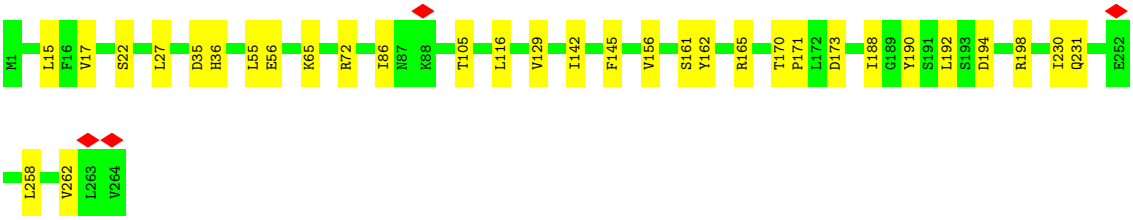




• Molecule 2: KomC

Chain AX:




M1
L15
F16
V17
S22
L27
D35
H36
L55
E56
K65
R72
I86
N87
K88
T105
L116
V129
I142
F145
V156
S161
Y162
R165
T170
P171
L172
D173
I188
G189
Y190
S191
L192
S193
D194
R198
I230
Q231
E252
L258
V262
L263
V264

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 240153 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 30 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.746 | Depositor |
| Minimum map value | -0.451 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.022 | Depositor |
| Recommended contour level | 0.07 | Depositor |
| Map size (Å) | 453.59998, 453.59998, 453.59998 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.756, 0.756, 0.756 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y43

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | AB | 0.12 | 0/1513 | 0.29 | 0/2031 |
| 1 | AC | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | AG | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | AI | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | AN | 0.10 | 0/1513 | 0.26 | 0/2031 |
| 1 | AO | 0.14 | 0/1513 | 0.34 | 0/2031 |
| 1 | AS | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | AU | 0.15 | 0/1513 | 0.36 | 0/2031 |
| 1 | BB | 0.11 | 0/1513 | 0.29 | 0/2031 |
| 1 | BC | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | BG | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | BI | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | BN | 0.10 | 0/1513 | 0.26 | 0/2031 |
| 1 | BO | 0.13 | 0/1513 | 0.34 | 0/2031 |
| 1 | BS | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | BU | 0.14 | 0/1513 | 0.36 | 0/2031 |
| 1 | CB | 0.12 | 0/1513 | 0.29 | 0/2031 |
| 1 | CC | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | CG | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | CI | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 1 | CN | 0.10 | 0/1513 | 0.26 | 0/2031 |
| 1 | CO | 0.14 | 0/1513 | 0.34 | 0/2031 |
| 1 | CS | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | CU | 0.15 | 0/1513 | 0.36 | 0/2031 |
| 1 | DB | 0.12 | 0/1513 | 0.29 | 0/2031 |
| 1 | DC | 0.12 | 0/1513 | 0.28 | 0/2031 |
| 1 | DG | 0.12 | 0/1513 | 0.32 | 0/2031 |
| 1 | DI | 0.11 | 0/1513 | 0.28 | 0/2031 |
| 2 | AD | 0.11 | 0/2218 | 0.26 | 0/2997 |
| 2 | AE | 0.10 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | AK | 0.40 | 2/2218 (0.1%) | 0.59 | 6/2997 (0.2%) |
| 2 | AL | 0.21 | 0/2218 | 0.31 | 1/2997 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | AP | 0.09 | 0/2218 | 0.21 | 0/2997 |
| 2 | AQ | 0.18 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | AW | 0.20 | 0/2218 | 0.34 | 1/2997 (0.0%) |
| 2 | AX | 0.09 | 0/2218 | 0.22 | 0/2997 |
| 2 | BD | 0.10 | 0/2218 | 0.26 | 0/2997 |
| 2 | BE | 0.09 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | BK | 0.40 | 2/2218 (0.1%) | 0.59 | 6/2997 (0.2%) |
| 2 | BL | 0.21 | 0/2218 | 0.31 | 1/2997 (0.0%) |
| 2 | BP | 0.09 | 0/2218 | 0.21 | 0/2997 |
| 2 | BQ | 0.17 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | BW | 0.19 | 0/2218 | 0.34 | 1/2997 (0.0%) |
| 2 | BX | 0.09 | 0/2218 | 0.22 | 0/2997 |
| 2 | CD | 0.11 | 0/2218 | 0.26 | 0/2997 |
| 2 | CE | 0.10 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | CK | 0.40 | 2/2218 (0.1%) | 0.59 | 6/2997 (0.2%) |
| 2 | CL | 0.21 | 0/2218 | 0.31 | 1/2997 (0.0%) |
| 2 | CP | 0.09 | 0/2218 | 0.21 | 0/2997 |
| 2 | CQ | 0.18 | 0/2218 | 0.30 | 1/2997 (0.0%) |
| 2 | CW | 0.20 | 0/2218 | 0.34 | 1/2997 (0.0%) |
| 2 | CX | 0.09 | 0/2218 | 0.22 | 0/2997 |
| 2 | DD | 0.11 | 0/2218 | 0.26 | 0/2997 |
| 2 | DE | 0.10 | 0/2218 | 0.29 | 1/2997 (0.0%) |
| 2 | DK | 0.40 | 2/2218 (0.1%) | 0.59 | 6/2997 (0.2%) |
| 2 | DL | 0.21 | 0/2218 | 0.31 | 1/2997 (0.0%) |
| All | All | 0.17 | 8/104468 (0.0%) | 0.33 | 38/140784 (0.0%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | BK | 203 | LYS | CA-C | -6.44 | 1.45 | 1.52 |
| 2 | DK | 203 | LYS | CA-C | -6.42 | 1.46 | 1.52 |
| 2 | CK | 203 | LYS | CA-C | -6.41 | 1.46 | 1.52 |
| 2 | AK | 203 | LYS | CA-C | -6.41 | 1.46 | 1.52 |
| 2 | BK | 211 | GLN | CA-C | -5.51 | 1.47 | 1.53 |
| 2 | AK | 211 | GLN | CA-C | -5.51 | 1.47 | 1.53 |
| 2 | DK | 211 | GLN | CA-C | -5.50 | 1.47 | 1.53 |
| 2 | CK | 211 | GLN | CA-C | -5.48 | 1.47 | 1.53 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | CK | 213 | LEU | N-CA-C | -10.88 | 100.31 | 112.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | DK | 213 | LEU | N-CA-C | -10.88 | 100.32 | 112.72 |
| 2 | BK | 213 | LEU | N-CA-C | -10.88 | 100.32 | 112.72 |
| 2 | AK | 213 | LEU | N-CA-C | -10.83 | 100.38 | 112.72 |
| 2 | AK | 202 | TYR | N-CA-C | 8.53 | 120.35 | 111.14 |
| 2 | CK | 202 | TYR | N-CA-C | 8.51 | 120.33 | 111.14 |
| 2 | DK | 202 | TYR | N-CA-C | 8.51 | 120.33 | 111.14 |
| 2 | BK | 202 | TYR | N-CA-C | 8.49 | 120.31 | 111.14 |
| 2 | CK | 211 | GLN | N-CA-C | -7.88 | 96.87 | 109.39 |
| 2 | AK | 211 | GLN | N-CA-C | -7.87 | 96.88 | 109.39 |
| 2 | BK | 211 | GLN | N-CA-C | -7.87 | 96.88 | 109.39 |
| 2 | DK | 211 | GLN | N-CA-C | -7.85 | 96.91 | 109.39 |
| 2 | CK | 197 | ILE | N-CA-C | 7.03 | 122.63 | 113.07 |
| 2 | DK | 197 | ILE | N-CA-C | 7.03 | 122.63 | 113.07 |
| 2 | BK | 197 | ILE | N-CA-C | 7.00 | 122.59 | 113.07 |
| 2 | AK | 197 | ILE | N-CA-C | 7.00 | 122.58 | 113.07 |
| 2 | AW | 201 | PHE | N-CA-C | 6.52 | 118.46 | 111.36 |
| 2 | CK | 195 | ILE | N-CA-C | -6.51 | 102.91 | 111.05 |
| 2 | BK | 195 | ILE | N-CA-C | -6.51 | 102.92 | 111.05 |
| 2 | CW | 201 | PHE | N-CA-C | 6.50 | 118.45 | 111.36 |
| 2 | DK | 195 | ILE | N-CA-C | -6.50 | 102.93 | 111.05 |
| 2 | AK | 195 | ILE | N-CA-C | -6.49 | 102.93 | 111.05 |
| 2 | BW | 201 | PHE | N-CA-C | 6.49 | 118.43 | 111.36 |
| 2 | AE | 198 | ARG | N-CA-C | 6.41 | 121.26 | 113.38 |
| 2 | BE | 198 | ARG | N-CA-C | 6.39 | 121.24 | 113.38 |
| 2 | CE | 198 | ARG | N-CA-C | 6.39 | 121.24 | 113.38 |
| 2 | DE | 198 | ARG | N-CA-C | 6.39 | 121.23 | 113.38 |
| 2 | AQ | 217 | GLN | N-CA-C | 5.61 | 118.78 | 110.32 |
| 2 | CQ | 217 | GLN | N-CA-C | 5.59 | 118.75 | 110.32 |
| 2 | BQ | 217 | GLN | N-CA-C | 5.57 | 118.74 | 110.32 |
| 2 | CK | 204 | LEU | N-CA-C | -5.22 | 105.59 | 111.28 |
| 2 | BL | 163 | PHE | N-CA-C | 5.21 | 117.04 | 111.36 |
| 2 | BK | 204 | LEU | N-CA-C | -5.21 | 105.61 | 111.28 |
| 2 | AL | 163 | PHE | N-CA-C | 5.20 | 117.03 | 111.36 |
| 2 | DL | 163 | PHE | N-CA-C | 5.20 | 117.02 | 111.36 |
| 2 | CL | 163 | PHE | N-CA-C | 5.18 | 117.01 | 111.36 |
| 2 | DK | 204 | LEU | N-CA-C | -5.18 | 105.64 | 111.28 |
| 2 | AK | 204 | LEU | N-CA-C | -5.16 | 105.65 | 111.28 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | AB | 1483 | 0 | 1499 | 35 | 0 |
| 1 | AC | 1483 | 0 | 1499 | 40 | 0 |
| 1 | AG | 1483 | 0 | 1499 | 36 | 0 |
| 1 | AI | 1483 | 0 | 1499 | 33 | 0 |
| 1 | AN | 1483 | 0 | 1499 | 25 | 0 |
| 1 | AO | 1483 | 0 | 1499 | 31 | 0 |
| 1 | AS | 1483 | 0 | 1499 | 40 | 0 |
| 1 | AU | 1483 | 0 | 1499 | 39 | 0 |
| 1 | BB | 1483 | 0 | 1499 | 35 | 0 |
| 1 | BC | 1483 | 0 | 1499 | 39 | 0 |
| 1 | BG | 1483 | 0 | 1499 | 39 | 0 |
| 1 | BI | 1483 | 0 | 1499 | 32 | 0 |
| 1 | BN | 1483 | 0 | 1499 | 26 | 0 |
| 1 | BO | 1483 | 0 | 1499 | 30 | 0 |
| 1 | BS | 1483 | 0 | 1499 | 43 | 0 |
| 1 | BU | 1483 | 0 | 1499 | 36 | 0 |
| 1 | CB | 1483 | 0 | 1499 | 29 | 0 |
| 1 | CC | 1483 | 0 | 1499 | 37 | 0 |
| 1 | CG | 1483 | 0 | 1499 | 36 | 0 |
| 1 | CI | 1483 | 0 | 1499 | 33 | 0 |
| 1 | CN | 1483 | 0 | 1499 | 27 | 0 |
| 1 | CO | 1483 | 0 | 1499 | 34 | 0 |
| 1 | CS | 1483 | 0 | 1499 | 44 | 0 |
| 1 | CU | 1483 | 0 | 1499 | 34 | 0 |
| 1 | DB | 1483 | 0 | 1499 | 31 | 0 |
| 1 | DC | 1483 | 0 | 1499 | 41 | 0 |
| 1 | DG | 1483 | 0 | 1499 | 37 | 0 |
| 1 | DI | 1483 | 0 | 1499 | 33 | 0 |
| 2 | AD | 2166 | 0 | 2150 | 50 | 0 |
| 2 | AE | 2166 | 0 | 2150 | 18 | 0 |
| 2 | AK | 2166 | 0 | 2150 | 53 | 0 |
| 2 | AL | 2166 | 0 | 2150 | 27 | 0 |
| 2 | AP | 2166 | 0 | 2150 | 25 | 0 |
| 2 | AQ | 2166 | 0 | 2150 | 31 | 0 |
| 2 | AW | 2166 | 0 | 2150 | 48 | 0 |
| 2 | AX | 2166 | 0 | 2150 | 25 | 0 |
| 2 | BD | 2166 | 0 | 2150 | 54 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | BE | 2166 | 0 | 2150 | 20 | 0 |
| 2 | BK | 2166 | 0 | 2150 | 54 | 0 |
| 2 | BL | 2166 | 0 | 2150 | 24 | 0 |
| 2 | BP | 2166 | 0 | 2150 | 27 | 0 |
| 2 | BQ | 2166 | 0 | 2150 | 27 | 0 |
| 2 | BW | 2166 | 0 | 2150 | 47 | 0 |
| 2 | BX | 2166 | 0 | 2150 | 27 | 0 |
| 2 | CD | 2166 | 0 | 2150 | 52 | 0 |
| 2 | CE | 2166 | 0 | 2150 | 23 | 0 |
| 2 | CK | 2166 | 0 | 2150 | 52 | 0 |
| 2 | CL | 2166 | 0 | 2150 | 30 | 0 |
| 2 | CP | 2166 | 0 | 2150 | 26 | 0 |
| 2 | CQ | 2166 | 0 | 2150 | 29 | 0 |
| 2 | CW | 2166 | 0 | 2150 | 47 | 0 |
| 2 | CX | 2166 | 0 | 2150 | 25 | 0 |
| 2 | DD | 2166 | 0 | 2150 | 52 | 0 |
| 2 | DE | 2166 | 0 | 2150 | 22 | 0 |
| 2 | DK | 2166 | 0 | 2150 | 54 | 0 |
| 2 | DL | 2166 | 0 | 2150 | 34 | 0 |
| 3 | AB | 30 | 0 | 0 | 0 | 0 |
| 3 | AC | 30 | 0 | 0 | 1 | 0 |
| 3 | AG | 30 | 0 | 0 | 1 | 0 |
| 3 | AI | 30 | 0 | 0 | 1 | 0 |
| 3 | AN | 30 | 0 | 0 | 1 | 0 |
| 3 | AO | 30 | 0 | 0 | 1 | 0 |
| 3 | AS | 30 | 0 | 0 | 0 | 0 |
| 3 | AU | 30 | 0 | 0 | 1 | 0 |
| 3 | BB | 30 | 0 | 0 | 0 | 0 |
| 3 | BC | 30 | 0 | 0 | 0 | 0 |
| 3 | BG | 30 | 0 | 0 | 0 | 0 |
| 3 | BI | 30 | 0 | 0 | 0 | 0 |
| 3 | BN | 30 | 0 | 0 | 1 | 0 |
| 3 | BO | 30 | 0 | 0 | 1 | 0 |
| 3 | BS | 30 | 0 | 0 | 2 | 0 |
| 3 | BU | 30 | 0 | 0 | 1 | 0 |
| 3 | CB | 30 | 0 | 0 | 0 | 0 |
| 3 | CC | 30 | 0 | 0 | 0 | 0 |
| 3 | CG | 30 | 0 | 0 | 1 | 0 |
| 3 | CI | 30 | 0 | 0 | 1 | 0 |
| 3 | CN | 30 | 0 | 0 | 1 | 0 |
| 3 | CO | 30 | 0 | 0 | 1 | 0 |
| 3 | CS | 30 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | CU | 30 | 0 | 0 | 1 | 0 |
| 3 | DB | 30 | 0 | 0 | 0 | 0 |
| 3 | DC | 30 | 0 | 0 | 0 | 0 |
| 3 | DG | 30 | 0 | 0 | 0 | 0 |
| 3 | DI | 30 | 0 | 0 | 1 | 0 |
| All | All | 103012 | 0 | 102172 | 1819 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1819) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CD:198:ARG:HG3 | 2:CD:202:TYR:CE2 | 1.74 | 1.21 |
| 2:DD:198:ARG:HG3 | 2:DD:202:TYR:CE2 | 1.74 | 1.21 |
| 2:AD:198:ARG:HG3 | 2:AD:202:TYR:CE2 | 1.74 | 1.21 |
| 2:BD:198:ARG:HG3 | 2:BD:202:TYR:CE2 | 1.74 | 1.19 |
| 2:DK:192:LEU:O | 2:DK:197:ILE:HG12 | 1.43 | 1.18 |
| 2:DK:55:LEU:HD21 | 2:DK:195:ILE:HG22 | 1.20 | 1.17 |
| 2:BK:192:LEU:O | 2:BK:197:ILE:HG12 | 1.43 | 1.17 |
| 2:AK:192:LEU:O | 2:AK:197:ILE:HG12 | 1.43 | 1.17 |
| 2:CK:192:LEU:O | 2:CK:197:ILE:HG12 | 1.43 | 1.16 |
| 2:AK:55:LEU:HD21 | 2:AK:195:ILE:CG2 | 1.73 | 1.16 |
| 2:DK:55:LEU:HD21 | 2:DK:195:ILE:CG2 | 1.73 | 1.16 |
| 2:BK:55:LEU:HD21 | 2:BK:195:ILE:CG2 | 1.73 | 1.15 |
| 2:CK:55:LEU:HD21 | 2:CK:195:ILE:CG2 | 1.73 | 1.15 |
| 2:AK:55:LEU:HD21 | 2:AK:195:ILE:HG22 | 1.20 | 1.15 |
| 2:BK:55:LEU:HD21 | 2:BK:195:ILE:HG22 | 1.19 | 1.14 |
| 2:BX:116:LEU:HD12 | 2:BX:142:ILE:HD11 | 1.29 | 1.13 |
| 2:CX:116:LEU:HD12 | 2:CX:142:ILE:HD11 | 1.29 | 1.11 |
| 2:AX:116:LEU:HD12 | 2:AX:142:ILE:HD11 | 1.29 | 1.11 |
| 2:BD:198:ARG:CG | 2:BD:202:TYR:HE2 | 1.64 | 1.11 |
| 2:CK:55:LEU:HD21 | 2:CK:195:ILE:HG22 | 1.20 | 1.11 |
| 2:DD:198:ARG:CG | 2:DD:202:TYR:HE2 | 1.64 | 1.11 |
| 2:DL:23:MET:HE1 | 2:DL:29:SER:HB3 | 1.31 | 1.11 |
| 2:BD:198:ARG:HG3 | 2:BD:202:TYR:HE2 | 0.93 | 1.10 |
| 2:CD:198:ARG:CG | 2:CD:202:TYR:HE2 | 1.64 | 1.09 |
| 2:AD:198:ARG:CG | 2:AD:202:TYR:HE2 | 1.64 | 1.09 |
| 1:CG:171:MET:HE2 | 1:CG:174:ARG:HH21 | 1.18 | 1.09 |
| 2:DD:198:ARG:HG3 | 2:DD:202:TYR:HE2 | 0.93 | 1.08 |
| 2:CL:23:MET:HE1 | 2:CL:29:SER:HB3 | 1.31 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AL:23:MET:HE1 | 2:AL:29:SER:HB3 | 1.31 | 1.08 |
| 2:CD:198:ARG:HG3 | 2:CD:202:TYR:HE2 | 0.93 | 1.07 |
| 1:CG:171:MET:CE | 1:CG:174:ARG:HE | 1.67 | 1.07 |
| 1:BG:171:MET:HE2 | 1:BG:174:ARG:HH21 | 1.18 | 1.06 |
| 1:AG:171:MET:CE | 1:AG:174:ARG:HE | 1.67 | 1.06 |
| 1:DG:171:MET:CE | 1:DG:174:ARG:HE | 1.67 | 1.06 |
| 1:DG:171:MET:HE2 | 1:DG:174:ARG:HH21 | 1.18 | 1.06 |
| 1:AG:171:MET:HE2 | 1:AG:174:ARG:HH21 | 1.18 | 1.06 |
| 2:BL:23:MET:HE1 | 2:BL:29:SER:HB3 | 1.31 | 1.06 |
| 1:BG:171:MET:CE | 1:BG:174:ARG:HE | 1.67 | 1.05 |
| 2:BX:116:LEU:CD1 | 2:BX:142:ILE:HD11 | 1.85 | 1.05 |
| 2:AD:198:ARG:HG3 | 2:AD:202:TYR:HE2 | 0.93 | 1.05 |
| 2:CX:116:LEU:CD1 | 2:CX:142:ILE:HD11 | 1.85 | 1.05 |
| 2:AX:116:LEU:CD1 | 2:AX:142:ILE:HD11 | 1.85 | 1.04 |
| 1:BI:19:ILE:HD13 | 1:BI:43:SER:OG | 1.58 | 1.04 |
| 1:DI:19:ILE:HD13 | 1:DI:43:SER:OG | 1.58 | 1.04 |
| 2:CK:55:LEU:CD2 | 2:CK:195:ILE:CG2 | 2.35 | 1.04 |
| 2:DK:55:LEU:CD2 | 2:DK:195:ILE:CG2 | 2.35 | 1.04 |
| 1:CG:171:MET:HE2 | 1:CG:174:ARG:NH2 | 1.72 | 1.03 |
| 1:DG:171:MET:HE3 | 1:DG:174:ARG:HE | 1.19 | 1.03 |
| 2:BK:55:LEU:CD2 | 2:BK:195:ILE:CG2 | 2.35 | 1.03 |
| 1:AI:19:ILE:HD13 | 1:AI:43:SER:OG | 1.58 | 1.03 |
| 1:AG:171:MET:HE3 | 1:AG:174:ARG:HE | 1.19 | 1.03 |
| 2:AK:55:LEU:CD2 | 2:AK:195:ILE:CG2 | 2.35 | 1.02 |
| 1:BG:171:MET:HE2 | 1:BG:174:ARG:NH2 | 1.72 | 1.02 |
| 1:DG:171:MET:HE2 | 1:DG:174:ARG:NH2 | 1.72 | 1.02 |
| 1:CG:171:MET:HE3 | 1:CG:174:ARG:HE | 1.19 | 1.02 |
| 1:CI:19:ILE:HD13 | 1:CI:43:SER:OG | 1.58 | 1.02 |
| 1:AG:171:MET:HE2 | 1:AG:174:ARG:NH2 | 1.72 | 1.02 |
| 1:BB:119:VAL:HG22 | 1:BB:140:GLN:HG2 | 1.41 | 1.01 |
| 1:BG:171:MET:HE3 | 1:BG:174:ARG:HE | 1.19 | 1.00 |
| 1:AO:55:VAL:HG11 | 1:AO:123:ILE:HD12 | 1.43 | 1.00 |
| 1:DB:119:VAL:HG22 | 1:DB:140:GLN:HG2 | 1.41 | 1.00 |
| 1:CO:55:VAL:HG11 | 1:CO:123:ILE:HD12 | 1.43 | 1.00 |
| 1:BO:55:VAL:HG11 | 1:BO:123:ILE:HD12 | 1.43 | 0.99 |
| 2:DK:55:LEU:CD2 | 2:DK:195:ILE:HG21 | 1.94 | 0.98 |
| 1:AB:119:VAL:HG22 | 1:AB:140:GLN:HG2 | 1.41 | 0.97 |
| 2:CK:55:LEU:CD2 | 2:CK:195:ILE:HG21 | 1.94 | 0.97 |
| 2:AK:55:LEU:CD2 | 2:AK:195:ILE:HG21 | 1.94 | 0.97 |
| 1:CB:119:VAL:HG22 | 1:CB:140:GLN:HG2 | 1.41 | 0.97 |
| 2:BK:55:LEU:CD2 | 2:BK:195:ILE:HG21 | 1.94 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:191:SER:OG | 2:AD:197:ILE:HD11 | 1.68 | 0.94 |
| 2:BD:191:SER:OG | 2:BD:197:ILE:HD11 | 1.68 | 0.93 |
| 2:BK:54:ALA:HB3 | 2:BK:195:ILE:HD13 | 1.50 | 0.93 |
| 2:CL:129:VAL:HG22 | 2:CL:171:PRO:HG3 | 1.50 | 0.93 |
| 2:AK:54:ALA:HB3 | 2:AK:195:ILE:HD13 | 1.50 | 0.93 |
| 2:DD:191:SER:OG | 2:DD:197:ILE:HD11 | 1.68 | 0.93 |
| 2:CD:191:SER:OG | 2:CD:197:ILE:HD11 | 1.68 | 0.92 |
| 2:DK:54:ALA:HB3 | 2:DK:195:ILE:HD13 | 1.50 | 0.92 |
| 2:BL:129:VAL:HG22 | 2:BL:171:PRO:HG3 | 1.50 | 0.92 |
| 2:AL:129:VAL:HG22 | 2:AL:171:PRO:HG3 | 1.50 | 0.92 |
| 2:DL:129:VAL:HG22 | 2:DL:171:PRO:HG3 | 1.51 | 0.92 |
| 2:CK:54:ALA:HB3 | 2:CK:195:ILE:HD13 | 1.50 | 0.92 |
| 1:BG:171:MET:CE | 1:BG:174:ARG:HH21 | 1.84 | 0.91 |
| 1:DG:171:MET:CE | 1:DG:174:ARG:HH21 | 1.84 | 0.91 |
| 2:BQ:129:VAL:HG22 | 2:BQ:171:PRO:HG3 | 1.54 | 0.90 |
| 2:AQ:129:VAL:HG22 | 2:AQ:171:PRO:HG3 | 1.54 | 0.90 |
| 2:DK:54:ALA:HB3 | 2:DK:195:ILE:CD1 | 2.01 | 0.90 |
| 2:BK:54:ALA:HB3 | 2:BK:195:ILE:CD1 | 2.01 | 0.90 |
| 2:CQ:129:VAL:HG22 | 2:CQ:171:PRO:HG3 | 1.54 | 0.90 |
| 1:CI:19:ILE:HD13 | 1:CI:43:SER:HG | 1.33 | 0.90 |
| 1:CG:171:MET:CE | 1:CG:174:ARG:HH21 | 1.84 | 0.90 |
| 1:AG:171:MET:CE | 1:AG:174:ARG:HH21 | 1.84 | 0.90 |
| 2:AK:54:ALA:HB3 | 2:AK:195:ILE:CD1 | 2.01 | 0.90 |
| 2:CK:54:ALA:HB3 | 2:CK:195:ILE:CD1 | 2.01 | 0.89 |
| 2:AK:55:LEU:CG | 2:AK:195:ILE:CG2 | 2.52 | 0.87 |
| 2:BK:55:LEU:CG | 2:BK:195:ILE:CG2 | 2.52 | 0.87 |
| 2:DK:55:LEU:CG | 2:DK:195:ILE:CG2 | 2.52 | 0.87 |
| 2:CK:55:LEU:CG | 2:CK:195:ILE:CG2 | 2.52 | 0.86 |
| 2:AX:116:LEU:HD12 | 2:AX:142:ILE:CD1 | 2.05 | 0.86 |
| 2:BX:116:LEU:HD12 | 2:BX:142:ILE:CD1 | 2.05 | 0.86 |
| 1:BC:130:MET:HE1 | 2:BD:43:TYR:CE1 | 2.12 | 0.85 |
| 2:CX:116:LEU:HD12 | 2:CX:142:ILE:CD1 | 2.05 | 0.85 |
| 1:CC:130:MET:HE1 | 2:CD:43:TYR:CE1 | 2.12 | 0.85 |
| 1:DC:130:MET:HE1 | 2:DD:43:TYR:CE1 | 2.11 | 0.85 |
| 2:AP:116:LEU:HD12 | 2:AP:142:ILE:HD11 | 1.58 | 0.85 |
| 1:AI:19:ILE:HD13 | 1:AI:43:SER:HG | 1.39 | 0.84 |
| 2:CP:116:LEU:HD12 | 2:CP:142:ILE:HD11 | 1.58 | 0.84 |
| 2:BP:116:LEU:HD12 | 2:BP:142:ILE:HD11 | 1.58 | 0.84 |
| 1:AC:130:MET:HE1 | 2:AD:43:TYR:CE1 | 2.12 | 0.84 |
| 1:CG:171:MET:CE | 1:CG:174:ARG:NE | 2.42 | 0.82 |
| 1:BG:171:MET:CE | 1:BG:174:ARG:NE | 2.42 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DI:19:ILE:CD1 | 1:DI:43:SER:OG | 2.28 | 0.82 |
| 2:BD:197:ILE:O | 2:BD:197:ILE:HG22 | 1.78 | 0.82 |
| 2:DD:197:ILE:HG22 | 2:DD:197:ILE:O | 1.78 | 0.82 |
| 1:DG:171:MET:CE | 1:DG:174:ARG:NE | 2.42 | 0.82 |
| 1:AG:171:MET:CE | 1:AG:174:ARG:NE | 2.42 | 0.82 |
| 1:BO:32:ILE:HG12 | 1:BO:176:ASN:CG | 2.05 | 0.82 |
| 2:CD:197:ILE:O | 2:CD:197:ILE:HG22 | 1.78 | 0.82 |
| 2:AD:197:ILE:HG22 | 2:AD:197:ILE:O | 1.78 | 0.81 |
| 1:CI:19:ILE:CD1 | 1:CI:43:SER:OG | 2.28 | 0.81 |
| 1:BI:19:ILE:CD1 | 1:BI:43:SER:OG | 2.28 | 0.81 |
| 1:AI:19:ILE:CD1 | 1:AI:43:SER:OG | 2.28 | 0.81 |
| 1:AO:32:ILE:HG12 | 1:AO:176:ASN:CG | 2.05 | 0.81 |
| 2:BK:55:LEU:HG | 2:BK:195:ILE:CG2 | 2.11 | 0.80 |
| 2:CL:129:VAL:CG2 | 2:CL:171:PRO:HG3 | 2.11 | 0.80 |
| 2:DL:129:VAL:CG2 | 2:DL:171:PRO:HG3 | 2.11 | 0.80 |
| 2:CK:55:LEU:HG | 2:CK:195:ILE:CG2 | 2.11 | 0.80 |
| 1:CO:32:ILE:HG12 | 1:CO:176:ASN:CG | 2.05 | 0.80 |
| 1:CB:119:VAL:CG2 | 1:CB:140:GLN:HG2 | 2.12 | 0.80 |
| 1:BB:119:VAL:CG2 | 1:BB:140:GLN:HG2 | 2.12 | 0.80 |
| 2:BK:192:LEU:O | 2:BK:197:ILE:CG1 | 2.28 | 0.80 |
| 2:CW:129:VAL:HG22 | 2:CW:171:PRO:HG3 | 1.63 | 0.80 |
| 2:DK:55:LEU:HG | 2:DK:195:ILE:CG2 | 2.11 | 0.80 |
| 2:DK:192:LEU:O | 2:DK:197:ILE:CG1 | 2.28 | 0.79 |
| 1:DB:119:VAL:CG2 | 1:DB:140:GLN:HG2 | 2.12 | 0.79 |
| 2:BL:129:VAL:CG2 | 2:BL:171:PRO:HG3 | 2.11 | 0.79 |
| 2:BW:129:VAL:HG22 | 2:BW:171:PRO:HG3 | 1.63 | 0.79 |
| 1:AB:119:VAL:CG2 | 1:AB:140:GLN:HG2 | 2.12 | 0.79 |
| 2:AL:129:VAL:CG2 | 2:AL:171:PRO:HG3 | 2.11 | 0.79 |
| 2:AK:55:LEU:HG | 2:AK:195:ILE:CG2 | 2.11 | 0.79 |
| 2:AW:129:VAL:HG22 | 2:AW:171:PRO:HG3 | 1.63 | 0.78 |
| 2:AK:192:LEU:O | 2:AK:197:ILE:CG1 | 2.28 | 0.78 |
| 1:CS:90:PRO:HB2 | 1:CS:94:THR:HG22 | 1.64 | 0.78 |
| 1:AB:119:VAL:HG22 | 1:AB:140:GLN:CG | 2.14 | 0.78 |
| 1:BS:90:PRO:HB2 | 1:BS:94:THR:HG22 | 1.64 | 0.78 |
| 2:CK:192:LEU:O | 2:CK:197:ILE:CG1 | 2.28 | 0.77 |
| 1:BB:119:VAL:HG22 | 1:BB:140:GLN:CG | 2.14 | 0.77 |
| 1:CB:119:VAL:HG22 | 1:CB:140:GLN:CG | 2.14 | 0.77 |
| 1:DB:119:VAL:HG22 | 1:DB:140:GLN:CG | 2.14 | 0.77 |
| 1:AS:90:PRO:HB2 | 1:AS:94:THR:HG22 | 1.64 | 0.77 |
| 1:AG:171:MET:HE2 | 1:AG:174:ARG:CZ | 2.15 | 0.77 |
| 2:BW:105:THR:HG21 | 2:BW:112:ILE:HD12 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:171:MET:HE2 | 1:BG:174:ARG:CZ | 2.15 | 0.76 |
| 2:CW:105:THR:HG21 | 2:CW:112:ILE:HD12 | 1.67 | 0.76 |
| 2:AW:105:THR:HG21 | 2:AW:112:ILE:HD12 | 1.67 | 0.76 |
| 2:BD:198:ARG:O | 2:BD:202:TYR:HD2 | 1.68 | 0.76 |
| 2:CD:198:ARG:O | 2:CD:202:TYR:HD2 | 1.68 | 0.76 |
| 2:CP:116:LEU:CD1 | 2:CP:142:ILE:HD11 | 2.16 | 0.76 |
| 2:AD:198:ARG:O | 2:AD:202:TYR:HD2 | 1.69 | 0.76 |
| 1:CG:171:MET:HE3 | 1:CG:174:ARG:NE | 2.00 | 0.76 |
| 2:BP:116:LEU:CD1 | 2:BP:142:ILE:HD11 | 2.16 | 0.76 |
| 1:CG:171:MET:HE2 | 1:CG:174:ARG:CZ | 2.15 | 0.75 |
| 1:DG:171:MET:HE2 | 1:DG:174:ARG:CZ | 2.15 | 0.75 |
| 1:AG:104:ASP:OD1 | 1:AG:105:LYS:N | 2.20 | 0.75 |
| 2:AP:116:LEU:CD1 | 2:AP:142:ILE:HD11 | 2.16 | 0.75 |
| 1:CG:104:ASP:OD1 | 1:CG:105:LYS:N | 2.20 | 0.75 |
| 1:BG:104:ASP:OD1 | 1:BG:105:LYS:N | 2.20 | 0.75 |
| 2:DD:198:ARG:O | 2:DD:202:TYR:HD2 | 1.69 | 0.75 |
| 2:BL:23:MET:CE | 2:BL:29:SER:HB3 | 2.14 | 0.74 |
| 1:DG:104:ASP:OD1 | 1:DG:105:LYS:N | 2.20 | 0.74 |
| 2:CX:17:VAL:HB | 2:CX:105:THR:HG22 | 1.68 | 0.74 |
| 2:DL:23:MET:CE | 2:DL:29:SER:HB3 | 2.14 | 0.74 |
| 2:AX:17:VAL:HB | 2:AX:105:THR:HG22 | 1.68 | 0.74 |
| 2:AD:198:ARG:O | 2:AD:202:TYR:CD2 | 2.41 | 0.74 |
| 2:BD:198:ARG:O | 2:BD:202:TYR:CD2 | 2.41 | 0.73 |
| 2:BK:55:LEU:HG | 2:BK:195:ILE:HG21 | 1.71 | 0.73 |
| 2:DK:55:LEU:HG | 2:DK:195:ILE:HG21 | 1.71 | 0.73 |
| 2:AK:55:LEU:HG | 2:AK:195:ILE:HG21 | 1.71 | 0.73 |
| 2:BX:17:VAL:HB | 2:BX:105:THR:HG22 | 1.68 | 0.73 |
| 2:CK:55:LEU:HG | 2:CK:195:ILE:HG21 | 1.71 | 0.73 |
| 1:BO:55:VAL:CG1 | 1:BO:123:ILE:HD12 | 2.17 | 0.73 |
| 1:BS:51:GLN:CD | 1:BU:93:LEU:HD23 | 2.14 | 0.73 |
| 2:CD:198:ARG:O | 2:CD:202:TYR:CD2 | 2.41 | 0.73 |
| 2:AL:23:MET:CE | 2:AL:29:SER:HB3 | 2.14 | 0.73 |
| 2:BW:129:VAL:CG2 | 2:BW:171:PRO:HG3 | 2.18 | 0.73 |
| 1:AO:55:VAL:CG1 | 1:AO:123:ILE:HD12 | 2.17 | 0.73 |
| 1:CC:186:ASP:OD1 | 1:CC:189:LYS:NZ | 2.22 | 0.73 |
| 1:CS:51:GLN:CD | 1:CU:93:LEU:HD23 | 2.14 | 0.73 |
| 2:CW:129:VAL:CG2 | 2:CW:171:PRO:HG3 | 2.18 | 0.73 |
| 1:DC:186:ASP:OD1 | 1:DC:189:LYS:NZ | 2.22 | 0.73 |
| 1:AS:51:GLN:NE2 | 1:AU:93:LEU:HD23 | 2.04 | 0.73 |
| 1:BC:186:ASP:OD1 | 1:BC:189:LYS:NZ | 2.22 | 0.72 |
| 2:BQ:129:VAL:CG2 | 2:BQ:171:PRO:HG3 | 2.19 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DD:198:ARG:O | 2:DD:202:TYR:CD2 | 2.41 | 0.72 |
| 1:CO:55:VAL:CG1 | 1:CO:123:ILE:HD12 | 2.17 | 0.72 |
| 2:CQ:129:VAL:CG2 | 2:CQ:171:PRO:HG3 | 2.20 | 0.72 |
| 2:AQ:129:VAL:CG2 | 2:AQ:171:PRO:HG3 | 2.20 | 0.72 |
| 2:AW:129:VAL:CG2 | 2:AW:171:PRO:HG3 | 2.18 | 0.72 |
| 2:CK:55:LEU:CG | 2:CK:195:ILE:HG21 | 2.17 | 0.72 |
| 1:AC:186:ASP:OD1 | 1:AC:189:LYS:NZ | 2.22 | 0.72 |
| 1:DI:19:ILE:HD13 | 1:DI:43:SER:HG | 1.54 | 0.72 |
| 2:AQ:207:LEU:HD21 | 2:AX:171:PRO:HG3 | 1.70 | 0.72 |
| 2:CL:23:MET:CE | 2:CL:29:SER:HB3 | 2.14 | 0.72 |
| 1:BS:51:GLN:NE2 | 1:BU:93:LEU:HD23 | 2.04 | 0.72 |
| 2:BQ:207:LEU:HD21 | 2:BX:171:PRO:HG3 | 1.70 | 0.71 |
| 1:CS:51:GLN:NE2 | 1:CU:93:LEU:HD23 | 2.04 | 0.71 |
| 1:AS:51:GLN:CD | 1:AU:93:LEU:HD23 | 2.14 | 0.71 |
| 2:CQ:207:LEU:HD21 | 2:CX:171:PRO:HG3 | 1.70 | 0.71 |
| 2:DL:23:MET:HE1 | 2:DL:29:SER:CB | 2.17 | 0.71 |
| 2:AK:55:LEU:CG | 2:AK:195:ILE:HG21 | 2.18 | 0.71 |
| 1:CC:106:PHE:CZ | 1:CC:110:LEU:HD12 | 2.26 | 0.71 |
| 1:CC:70:VAL:HG12 | 1:CC:72:ARG:H | 1.56 | 0.70 |
| 1:DC:106:PHE:CZ | 1:DC:110:LEU:HD12 | 2.26 | 0.70 |
| 1:BC:106:PHE:CZ | 1:BC:110:LEU:HD12 | 2.26 | 0.70 |
| 2:BK:55:LEU:CG | 2:BK:195:ILE:HG21 | 2.18 | 0.70 |
| 1:CU:83:ILE:HB | 1:CU:86:LEU:HB2 | 1.73 | 0.70 |
| 2:CW:17:VAL:HB | 2:CW:105:THR:HG22 | 1.73 | 0.70 |
| 2:DK:55:LEU:CG | 2:DK:195:ILE:HG21 | 2.17 | 0.70 |
| 2:AW:17:VAL:HB | 2:AW:105:THR:HG22 | 1.73 | 0.70 |
| 2:BL:67:LYS:NZ | 2:AQ:150:ASP:O | 2.24 | 0.70 |
| 1:DC:70:VAL:HG12 | 1:DC:72:ARG:H | 1.56 | 0.70 |
| 1:AC:70:VAL:HG12 | 1:AC:72:ARG:H | 1.56 | 0.70 |
| 2:CP:21:VAL:O | 2:CP:24:ASN:ND2 | 2.25 | 0.70 |
| 2:BW:17:VAL:HB | 2:BW:105:THR:HG22 | 1.73 | 0.70 |
| 1:BU:83:ILE:HB | 1:BU:86:LEU:HB2 | 1.73 | 0.70 |
| 2:BP:21:VAL:O | 2:BP:24:ASN:ND2 | 2.25 | 0.70 |
| 1:CS:83:ILE:HB | 1:CS:86:LEU:HB2 | 1.74 | 0.70 |
| 1:AS:83:ILE:HB | 1:AS:86:LEU:HB2 | 1.74 | 0.70 |
| 1:AC:106:PHE:CZ | 1:AC:110:LEU:HD12 | 2.26 | 0.69 |
| 1:AU:83:ILE:HB | 1:AU:86:LEU:HB2 | 1.73 | 0.69 |
| 2:AP:21:VAL:O | 2:AP:24:ASN:ND2 | 2.25 | 0.69 |
| 1:AS:14:MET:HA | 1:AS:14:MET:HE3 | 1.75 | 0.69 |
| 1:BS:14:MET:HA | 1:BS:14:MET:HE3 | 1.75 | 0.69 |
| 2:BW:116:LEU:HD12 | 2:BW:142:ILE:HD11 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CW:116:LEU:HD12 | 2:CW:142:ILE:HD11 | 1.73 | 0.69 |
| 1:DC:83:ILE:HD13 | 1:DC:110:LEU:CD1 | 2.22 | 0.69 |
| 1:AC:83:ILE:HD13 | 1:AC:110:LEU:CD1 | 2.22 | 0.69 |
| 1:BC:70:VAL:HG12 | 1:BC:72:ARG:H | 1.56 | 0.69 |
| 1:BC:83:ILE:HD13 | 1:BC:110:LEU:CD1 | 2.22 | 0.69 |
| 1:CC:83:ILE:HD13 | 1:CC:110:LEU:CD1 | 2.22 | 0.69 |
| 1:DC:186:ASP:HA | 1:DC:189:LYS:HZ2 | 1.58 | 0.69 |
| 1:BI:19:ILE:HD13 | 1:BI:43:SER:HG | 1.56 | 0.69 |
| 1:BS:83:ILE:HB | 1:BS:86:LEU:HB2 | 1.74 | 0.68 |
| 2:CD:208:TRP:O | 2:CD:217:GLN:NE2 | 2.26 | 0.68 |
| 2:AQ:208:TRP:CZ2 | 2:AQ:217:GLN:HB3 | 2.29 | 0.68 |
| 2:AW:116:LEU:HD12 | 2:AW:142:ILE:HD11 | 1.73 | 0.68 |
| 2:AD:208:TRP:O | 2:AD:217:GLN:NE2 | 2.26 | 0.68 |
| 2:BD:208:TRP:O | 2:BD:217:GLN:NE2 | 2.26 | 0.68 |
| 2:CL:23:MET:HE1 | 2:CL:29:SER:CB | 2.17 | 0.68 |
| 2:CQ:208:TRP:CZ2 | 2:CQ:217:GLN:HB3 | 2.29 | 0.68 |
| 2:DD:208:TRP:O | 2:DD:217:GLN:NE2 | 2.26 | 0.68 |
| 1:CS:14:MET:HA | 1:CS:14:MET:HE3 | 1.75 | 0.68 |
| 1:BO:32:ILE:CG1 | 1:BO:176:ASN:OD1 | 2.42 | 0.68 |
| 1:CO:32:ILE:CG1 | 1:CO:176:ASN:OD1 | 2.42 | 0.68 |
| 1:AO:32:ILE:CG1 | 1:AO:176:ASN:OD1 | 2.42 | 0.68 |
| 1:BC:186:ASP:HA | 1:BC:189:LYS:HZ2 | 1.58 | 0.68 |
| 2:AX:145:PHE:O | 2:AX:165:ARG:NH2 | 2.25 | 0.68 |
| 1:AC:186:ASP:HA | 1:AC:189:LYS:HZ2 | 1.59 | 0.68 |
| 2:BX:145:PHE:O | 2:BX:165:ARG:NH2 | 2.25 | 0.67 |
| 2:CX:145:PHE:O | 2:CX:165:ARG:NH2 | 2.25 | 0.67 |
| 1:DB:70:VAL:HG12 | 1:DB:72:ARG:H | 1.59 | 0.67 |
| 1:AB:70:VAL:HG12 | 1:AB:72:ARG:H | 1.60 | 0.67 |
| 2:BQ:208:TRP:CZ2 | 2:BQ:217:GLN:HB3 | 2.29 | 0.67 |
| 1:AO:55:VAL:HG11 | 1:AO:123:ILE:CD1 | 2.23 | 0.67 |
| 1:BG:171:MET:HE3 | 1:BG:174:ARG:NE | 2.00 | 0.67 |
| 1:CI:144:SER:OG | 1:CI:158:ILE:HA | 1.94 | 0.67 |
| 1:AG:171:MET:HG3 | 1:AG:174:ARG:NH2 | 2.09 | 0.67 |
| 2:BE:198:ARG:HA | 2:BE:201:PHE:HB2 | 1.77 | 0.67 |
| 1:BN:147:PRO:HB2 | 1:BN:151:ARG:HH21 | 1.60 | 0.67 |
| 1:CG:171:MET:HG3 | 1:CG:174:ARG:NH2 | 2.09 | 0.67 |
| 1:DG:171:MET:HG3 | 1:DG:174:ARG:NH2 | 2.09 | 0.67 |
| 2:AL:23:MET:HE1 | 2:AL:29:SER:CB | 2.17 | 0.67 |
| 1:BB:70:VAL:HG12 | 1:BB:72:ARG:H | 1.60 | 0.67 |
| 1:BG:171:MET:HE2 | 1:BG:174:ARG:NE | 2.10 | 0.66 |
| 1:DG:171:MET:HE3 | 1:DG:174:ARG:NE | 2.00 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BG:171:MET:HG3 | 1:BG:174:ARG:NH2 | 2.09 | 0.66 |
| 2:CE:198:ARG:HA | 2:CE:201:PHE:HB2 | 1.77 | 0.66 |
| 1:AG:171:MET:HE3 | 1:AG:174:ARG:NE | 2.00 | 0.66 |
| 1:CB:70:VAL:HG12 | 1:CB:72:ARG:H | 1.60 | 0.66 |
| 1:CN:147:PRO:HB2 | 1:CN:151:ARG:HH21 | 1.60 | 0.66 |
| 1:DG:171:MET:HE2 | 1:DG:174:ARG:NE | 2.11 | 0.66 |
| 2:DE:22:SER:HB3 | 2:DE:27:LEU:HD12 | 1.77 | 0.66 |
| 1:AG:171:MET:HE2 | 1:AG:174:ARG:NE | 2.10 | 0.66 |
| 1:BI:144:SER:OG | 1:BI:158:ILE:HA | 1.94 | 0.66 |
| 2:DE:198:ARG:HA | 2:DE:201:PHE:HB2 | 1.77 | 0.66 |
| 1:DI:144:SER:OG | 1:DI:158:ILE:HA | 1.94 | 0.66 |
| 1:AN:115:ASN:HD21 | 1:AN:117:ARG:HH21 | 1.44 | 0.66 |
| 1:BO:55:VAL:HG11 | 1:BO:123:ILE:CD1 | 2.23 | 0.66 |
| 2:BW:22:SER:HB3 | 2:BW:27:LEU:HD12 | 1.77 | 0.66 |
| 2:AE:22:SER:HB3 | 2:AE:27:LEU:HD12 | 1.77 | 0.66 |
| 2:BL:23:MET:HE1 | 2:BL:29:SER:CB | 2.17 | 0.66 |
| 1:BN:115:ASN:HD21 | 1:BN:117:ARG:HH21 | 1.44 | 0.66 |
| 2:CW:22:SER:HB3 | 2:CW:27:LEU:HD12 | 1.77 | 0.66 |
| 1:CO:55:VAL:HG11 | 1:CO:123:ILE:CD1 | 2.23 | 0.65 |
| 2:BE:22:SER:HB3 | 2:BE:27:LEU:HD12 | 1.77 | 0.65 |
| 1:AI:144:SER:OG | 1:AI:158:ILE:HA | 1.94 | 0.65 |
| 1:AN:167:THR:HG23 | 1:AN:169:ALA:H | 1.61 | 0.65 |
| 1:AB:52:THR:CG2 | 1:AC:48:ASP:OD2 | 2.45 | 0.65 |
| 1:BC:48:ASP:OD2 | 1:BB:52:THR:CG2 | 2.45 | 0.65 |
| 1:CN:167:THR:HG23 | 1:CN:169:ALA:H | 1.61 | 0.65 |
| 1:AN:147:PRO:HB2 | 1:AN:151:ARG:HH21 | 1.60 | 0.65 |
| 1:BG:171:MET:HG3 | 1:BG:174:ARG:HH21 | 1.62 | 0.65 |
| 1:CC:186:ASP:HA | 1:CC:189:LYS:HZ2 | 1.60 | 0.65 |
| 1:CB:52:THR:CG2 | 1:CC:48:ASP:OD2 | 2.45 | 0.65 |
| 1:DB:52:THR:CG2 | 1:DC:48:ASP:OD2 | 2.45 | 0.65 |
| 2:AE:198:ARG:HA | 2:AE:201:PHE:HB2 | 1.77 | 0.65 |
| 2:AD:22:SER:HB3 | 2:AD:27:LEU:HD12 | 1.79 | 0.65 |
| 1:BN:167:THR:HG23 | 1:BN:169:ALA:H | 1.61 | 0.65 |
| 1:CG:171:MET:HG3 | 1:CG:174:ARG:HH21 | 1.62 | 0.65 |
| 1:CG:171:MET:HE2 | 1:CG:174:ARG:NE | 2.10 | 0.64 |
| 2:CW:209:LYS:HD3 | 2:CW:238:TRP:HA | 1.79 | 0.64 |
| 1:AG:171:MET:HG3 | 1:AG:174:ARG:HH21 | 1.62 | 0.64 |
| 1:BN:105:LYS:NZ | 1:BO:85:SER:O | 2.31 | 0.64 |
| 1:BS:105:LYS:NZ | 1:BU:85:SER:O | 2.31 | 0.64 |
| 1:CN:105:LYS:NZ | 1:CO:85:SER:O | 2.31 | 0.64 |
| 1:CS:105:LYS:NZ | 1:CU:85:SER:O | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AN:105:LYS:NZ | 1:AO:85:SER:O | 2.31 | 0.64 |
| 1:AS:105:LYS:NZ | 1:AU:85:SER:O | 2.31 | 0.64 |
| 1:BN:70:VAL:HG12 | 1:BN:72:ARG:H | 1.63 | 0.64 |
| 2:DD:22:SER:HB3 | 2:DD:27:LEU:HD12 | 1.79 | 0.64 |
| 1:AN:70:VAL:HG12 | 1:AN:72:ARG:H | 1.63 | 0.64 |
| 2:DK:81:SER:HB3 | 2:DK:84:ILE:HD12 | 1.79 | 0.64 |
| 2:AW:209:LYS:HD2 | 2:AW:237:GLN:O | 1.98 | 0.64 |
| 2:BQ:73:SER:OG | 2:CL:110:ARG:NH2 | 2.31 | 0.64 |
| 2:CE:22:SER:HB3 | 2:CE:27:LEU:HD12 | 1.77 | 0.64 |
| 1:BG:50:ILE:HD11 | 1:BG:58:LEU:HA | 1.79 | 0.64 |
| 2:BK:81:SER:HB3 | 2:BK:84:ILE:HD12 | 1.79 | 0.64 |
| 2:BW:209:LYS:HD2 | 2:BW:237:GLN:O | 1.98 | 0.64 |
| 2:BX:116:LEU:CD1 | 2:BX:142:ILE:CD1 | 2.71 | 0.64 |
| 1:AG:50:ILE:HD11 | 1:AG:58:LEU:HA | 1.79 | 0.64 |
| 1:CN:115:ASN:HD21 | 1:CN:117:ARG:HH21 | 1.44 | 0.64 |
| 1:DG:50:ILE:HD11 | 1:DG:58:LEU:HA | 1.79 | 0.64 |
| 2:BD:22:SER:HB3 | 2:BD:27:LEU:HD12 | 1.79 | 0.64 |
| 1:CG:50:ILE:HD11 | 1:CG:58:LEU:HA | 1.79 | 0.64 |
| 2:CW:209:LYS:HD2 | 2:CW:237:GLN:O | 1.98 | 0.64 |
| 2:BW:209:LYS:HD3 | 2:BW:238:TRP:HA | 1.79 | 0.63 |
| 2:AK:81:SER:HB3 | 2:AK:84:ILE:HD12 | 1.80 | 0.63 |
| 2:AW:22:SER:HB3 | 2:AW:27:LEU:HD12 | 1.77 | 0.63 |
| 1:BU:22:ASN:HB2 | 1:BU:25:LYS:HD2 | 1.81 | 0.63 |
| 1:CU:22:ASN:HB2 | 1:CU:25:LYS:HD2 | 1.81 | 0.63 |
| 1:DG:171:MET:HG3 | 1:DG:174:ARG:HH21 | 1.62 | 0.63 |
| 2:AW:209:LYS:HD3 | 2:AW:238:TRP:HA | 1.79 | 0.63 |
| 1:AU:22:ASN:HB2 | 1:AU:25:LYS:HD2 | 1.81 | 0.63 |
| 2:DE:192:LEU:HD23 | 2:DE:197:ILE:HD13 | 1.80 | 0.63 |
| 2:AE:116:LEU:HD22 | 2:AE:142:ILE:HD11 | 1.81 | 0.63 |
| 2:AW:9:LYS:HE2 | 2:AW:264:VAL:HG11 | 1.81 | 0.63 |
| 1:CU:23:ARG:NE | 1:CU:44:GLU:OE2 | 2.31 | 0.63 |
| 2:CW:9:LYS:HE2 | 2:CW:264:VAL:HG11 | 1.81 | 0.63 |
| 1:AU:23:ARG:NE | 1:AU:44:GLU:OE2 | 2.31 | 0.63 |
| 2:BE:192:LEU:HD23 | 2:BE:197:ILE:HD13 | 1.80 | 0.63 |
| 2:CK:81:SER:HB3 | 2:CK:84:ILE:HD12 | 1.79 | 0.63 |
| 2:AE:192:LEU:HD23 | 2:AE:197:ILE:HD13 | 1.80 | 0.63 |
| 2:CD:22:SER:HB3 | 2:CD:27:LEU:HD12 | 1.79 | 0.63 |
| 2:CE:192:LEU:HD23 | 2:CE:197:ILE:HD13 | 1.80 | 0.63 |
| 2:AW:209:LYS:CD | 2:AW:237:GLN:O | 2.47 | 0.63 |
| 2:DE:116:LEU:HD22 | 2:DE:142:ILE:HD11 | 1.81 | 0.62 |
| 2:AD:197:ILE:O | 2:AD:197:ILE:CG2 | 2.46 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BU:23:ARG:NE | 1:BU:44:GLU:OE2 | 2.31 | 0.62 |
| 2:BW:209:LYS:CD | 2:BW:237:GLN:O | 2.47 | 0.62 |
| 2:CW:209:LYS:CD | 2:CW:237:GLN:O | 2.47 | 0.62 |
| 1:CN:70:VAL:HG12 | 1:CN:72:ARG:H | 1.63 | 0.62 |
| 1:CB:119:VAL:HG23 | 1:CB:140:GLN:NE2 | 2.15 | 0.62 |
| 1:CO:32:ILE:HG12 | 1:CO:176:ASN:OD1 | 1.98 | 0.62 |
| 2:BE:116:LEU:HD22 | 2:BE:142:ILE:HD11 | 1.81 | 0.62 |
| 2:DD:197:ILE:O | 2:DD:197:ILE:CG2 | 2.46 | 0.62 |
| 2:BQ:251:GLY:O | 2:BQ:255:GLU:HG3 | 2.00 | 0.62 |
| 1:CO:166:GLU:OE2 | 1:CO:171:MET:SD | 2.57 | 0.62 |
| 2:AQ:251:GLY:O | 2:AQ:255:GLU:HG3 | 2.00 | 0.62 |
| 2:BW:75:MET:HE3 | 2:BW:149:PHE:HE1 | 1.65 | 0.62 |
| 1:DB:119:VAL:HG23 | 1:DB:140:GLN:NE2 | 2.15 | 0.62 |
| 1:DG:171:MET:CE | 1:DG:174:ARG:NH2 | 2.52 | 0.62 |
| 2:AW:75:MET:HE3 | 2:AW:149:PHE:HE1 | 1.65 | 0.62 |
| 1:AB:119:VAL:HG23 | 1:AB:140:GLN:NE2 | 2.15 | 0.62 |
| 2:CE:116:LEU:HD22 | 2:CE:142:ILE:HD11 | 1.81 | 0.62 |
| 2:CQ:251:GLY:O | 2:CQ:255:GLU:HG3 | 2.00 | 0.62 |
| 2:AX:129:VAL:CG2 | 2:AX:171:PRO:HG2 | 2.30 | 0.62 |
| 1:AO:166:GLU:OE2 | 1:AO:171:MET:SD | 2.58 | 0.61 |
| 1:BB:119:VAL:HG23 | 1:BB:140:GLN:NE2 | 2.15 | 0.61 |
| 1:BO:166:GLU:OE2 | 1:BO:171:MET:SD | 2.57 | 0.61 |
| 2:BW:9:LYS:HE2 | 2:BW:264:VAL:HG11 | 1.81 | 0.61 |
| 1:CG:101:LEU:HG | 1:CG:105:LYS:HG2 | 1.82 | 0.61 |
| 2:CX:129:VAL:CG2 | 2:CX:171:PRO:HG2 | 2.30 | 0.61 |
| 2:AD:198:ARG:CG | 2:AD:202:TYR:CE2 | 2.55 | 0.61 |
| 1:AG:171:MET:CE | 1:AG:174:ARG:NH2 | 2.52 | 0.61 |
| 2:AQ:35:ASP:OD1 | 2:AQ:49:ARG:NH2 | 2.33 | 0.61 |
| 1:BO:32:ILE:HG12 | 1:BO:176:ASN:OD1 | 1.98 | 0.61 |
| 2:CW:75:MET:HE3 | 2:CW:149:PHE:HE1 | 1.65 | 0.61 |
| 1:DG:101:LEU:HG | 1:DG:105:LYS:HG2 | 1.82 | 0.61 |
| 2:AK:2:GLU:OE2 | 2:AK:2:GLU:N | 2.32 | 0.61 |
| 2:CD:197:ILE:O | 2:CD:197:ILE:CG2 | 2.46 | 0.61 |
| 1:BC:180:MET:N | 1:BC:180:MET:SD | 2.72 | 0.61 |
| 2:BD:198:ARG:CG | 2:BD:202:TYR:CE2 | 2.55 | 0.61 |
| 2:BX:129:VAL:CG2 | 2:BX:171:PRO:HG2 | 2.30 | 0.61 |
| 1:CU:104:ASP:OD1 | 1:CU:151:ARG:NH2 | 2.34 | 0.61 |
| 1:DC:180:MET:SD | 1:DC:180:MET:N | 2.72 | 0.61 |
| 1:AO:32:ILE:HG12 | 1:AO:176:ASN:OD1 | 1.98 | 0.61 |
| 2:BD:249:ASN:ND2 | 2:BD:252:GLU:OE1 | 2.32 | 0.61 |
| 2:BQ:35:ASP:OD1 | 2:BQ:49:ARG:NH2 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:249:ASN:ND2 | 2:AD:252:GLU:OE1 | 2.32 | 0.61 |
| 1:CB:93:LEU:HD23 | 1:CC:93:LEU:HD23 | 1.83 | 0.61 |
| 1:BU:104:ASP:OD1 | 1:BU:151:ARG:NH2 | 2.34 | 0.60 |
| 2:CQ:35:ASP:OD1 | 2:CQ:49:ARG:NH2 | 2.33 | 0.60 |
| 2:CQ:71:LEU:O | 2:CQ:75:MET:HG3 | 2.01 | 0.60 |
| 1:CC:180:MET:N | 1:CC:180:MET:SD | 2.72 | 0.60 |
| 1:AC:130:MET:SD | 2:AD:43:TYR:CZ | 2.94 | 0.60 |
| 1:AU:104:ASP:OD1 | 1:AU:151:ARG:NH2 | 2.34 | 0.60 |
| 1:BG:101:LEU:HG | 1:BG:105:LYS:HG2 | 1.82 | 0.60 |
| 2:BQ:71:LEU:O | 2:BQ:75:MET:HG3 | 2.01 | 0.60 |
| 1:CC:130:MET:SD | 2:CD:43:TYR:CZ | 2.94 | 0.60 |
| 1:DB:93:LEU:HD23 | 1:DC:93:LEU:HD23 | 1.83 | 0.60 |
| 2:DD:249:ASN:ND2 | 2:DD:252:GLU:OE1 | 2.32 | 0.60 |
| 1:AG:95:GLN:NE2 | 1:AG:99:ASP:OD2 | 2.34 | 0.60 |
| 1:BC:93:LEU:HD23 | 1:BB:93:LEU:HD23 | 1.83 | 0.60 |
| 2:BD:197:ILE:O | 2:BD:197:ILE:CG2 | 2.46 | 0.60 |
| 1:BG:95:GLN:NE2 | 1:BG:99:ASP:OD2 | 2.34 | 0.60 |
| 2:CD:249:ASN:ND2 | 2:CD:252:GLU:OE1 | 2.32 | 0.60 |
| 1:CG:95:GLN:NE2 | 1:CG:99:ASP:OD2 | 2.34 | 0.60 |
| 1:AB:93:LEU:HD23 | 1:AC:93:LEU:HD23 | 1.83 | 0.60 |
| 2:DD:72:ARG:NH1 | 2:DD:152:ASP:O | 2.34 | 0.60 |
| 2:AD:72:ARG:NH1 | 2:AD:152:ASP:O | 2.33 | 0.60 |
| 1:BI:171:MET:HB3 | 1:BI:174:ARG:HE | 1.67 | 0.60 |
| 2:BK:15:LEU:HD11 | 2:BK:188:ILE:HD13 | 1.84 | 0.60 |
| 2:CD:72:ARG:NH1 | 2:CD:152:ASP:O | 2.34 | 0.60 |
| 2:CX:116:LEU:CD1 | 2:CX:142:ILE:CD1 | 2.71 | 0.60 |
| 1:DG:95:GLN:NE2 | 1:DG:99:ASP:OD2 | 2.34 | 0.60 |
| 2:AK:15:LEU:HD11 | 2:AK:188:ILE:HD13 | 1.84 | 0.60 |
| 2:AW:158:ASP:OD1 | 2:AW:158:ASP:N | 2.35 | 0.60 |
| 1:DC:130:MET:SD | 2:DD:43:TYR:CZ | 2.94 | 0.60 |
| 2:DD:198:ARG:CG | 2:DD:202:TYR:CE2 | 2.55 | 0.60 |
| 2:DK:15:LEU:HD11 | 2:DK:188:ILE:HD13 | 1.84 | 0.60 |
| 1:AG:101:LEU:HG | 1:AG:105:LYS:HG2 | 1.82 | 0.60 |
| 2:AQ:71:LEU:O | 2:AQ:75:MET:HG3 | 2.01 | 0.60 |
| 1:BC:130:MET:SD | 2:BD:43:TYR:CZ | 2.94 | 0.59 |
| 2:BD:72:ARG:NH1 | 2:BD:152:ASP:O | 2.33 | 0.59 |
| 1:DB:95:GLN:NE2 | 1:DB:99:ASP:OD2 | 2.35 | 0.59 |
| 1:AC:180:MET:N | 1:AC:180:MET:SD | 2.72 | 0.59 |
| 1:CB:95:GLN:NE2 | 1:CB:99:ASP:OD2 | 2.35 | 0.59 |
| 1:CC:144:SER:HB2 | 1:CC:160:ILE:HD11 | 1.84 | 0.59 |
| 2:CK:15:LEU:HD11 | 2:CK:188:ILE:HD13 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DI:171:MET:HB3 | 1:DI:174:ARG:HE | 1.67 | 0.59 |
| 2:BK:246:GLU:OE1 | 2:BK:246:GLU:N | 2.24 | 0.59 |
| 2:DK:55:LEU:HG | 2:DK:195:ILE:HG23 | 1.84 | 0.59 |
| 1:BN:152:ASP:OD1 | 1:BN:153:PHE:N | 2.35 | 0.59 |
| 1:AB:95:GLN:NE2 | 1:AB:99:ASP:OD2 | 2.35 | 0.59 |
| 1:AC:144:SER:HB2 | 1:AC:160:ILE:HD11 | 1.84 | 0.59 |
| 2:AK:162:TYR:OH | 2:AK:196:ASN:HA | 2.02 | 0.59 |
| 2:CK:55:LEU:HG | 2:CK:195:ILE:HG23 | 1.84 | 0.59 |
| 2:CK:246:GLU:OE1 | 2:CK:246:GLU:N | 2.24 | 0.59 |
| 1:CN:152:ASP:OD1 | 1:CN:153:PHE:N | 2.35 | 0.59 |
| 1:AN:152:ASP:OD1 | 1:AN:153:PHE:N | 2.35 | 0.59 |
| 1:BB:95:GLN:NE2 | 1:BB:99:ASP:OD2 | 2.35 | 0.59 |
| 2:BK:55:LEU:HG | 2:BK:195:ILE:HG23 | 1.84 | 0.59 |
| 2:CP:109:ASP:N | 2:CP:109:ASP:OD1 | 2.33 | 0.59 |
| 1:AN:22:ASN:ND2 | 3:AN:201:Y43:OAO | 2.36 | 0.59 |
| 2:BK:162:TYR:OH | 2:BK:196:ASN:HA | 2.02 | 0.59 |
| 1:AI:171:MET:HB3 | 1:AI:174:ARG:HE | 1.67 | 0.59 |
| 2:AK:246:GLU:OE1 | 2:AK:246:GLU:N | 2.24 | 0.59 |
| 1:CC:83:ILE:HD13 | 1:CC:110:LEU:HD11 | 1.84 | 0.59 |
| 1:AB:119:VAL:CG2 | 1:AB:140:GLN:NE2 | 2.66 | 0.59 |
| 1:DB:119:VAL:CG2 | 1:DB:140:GLN:NE2 | 2.66 | 0.59 |
| 1:BN:22:ASN:ND2 | 3:BN:201:Y43:OAO | 2.36 | 0.58 |
| 1:CB:119:VAL:CG2 | 1:CB:140:GLN:NE2 | 2.66 | 0.58 |
| 2:CK:162:TYR:OH | 2:CK:196:ASN:HA | 2.02 | 0.58 |
| 1:DC:144:SER:HB2 | 1:DC:160:ILE:HD11 | 1.85 | 0.58 |
| 2:AK:55:LEU:HG | 2:AK:195:ILE:HG23 | 1.84 | 0.58 |
| 1:AS:171:MET:N | 1:AS:171:MET:SD | 2.76 | 0.58 |
| 2:BD:35:ASP:OD1 | 2:BD:49:ARG:NH2 | 2.34 | 0.58 |
| 1:CN:22:ASN:ND2 | 3:CN:201:Y43:OAO | 2.36 | 0.58 |
| 1:BS:171:MET:N | 1:BS:171:MET:SD | 2.76 | 0.58 |
| 2:CD:195:ILE:CD1 | 2:CE:195:ILE:HD13 | 2.34 | 0.58 |
| 1:CI:171:MET:HB3 | 1:CI:174:ARG:HE | 1.67 | 0.58 |
| 2:DD:195:ILE:CD1 | 2:DE:195:ILE:HD13 | 2.34 | 0.58 |
| 1:AC:83:ILE:HD13 | 1:AC:110:LEU:HD11 | 1.84 | 0.58 |
| 2:AW:209:LYS:CE | 2:AW:238:TRP:HD1 | 2.16 | 0.58 |
| 1:BB:119:VAL:CG2 | 1:BB:140:GLN:NE2 | 2.66 | 0.58 |
| 2:BD:195:ILE:CD1 | 2:BE:195:ILE:HD13 | 2.34 | 0.58 |
| 2:CK:22:SER:HB3 | 2:CK:27:LEU:HD12 | 1.84 | 0.58 |
| 1:CU:25:LYS:NZ | 1:CU:77:GLU:OE2 | 2.37 | 0.58 |
| 1:AU:25:LYS:NZ | 1:AU:77:GLU:OE2 | 2.37 | 0.58 |
| 2:BP:109:ASP:OD1 | 2:BP:109:ASP:N | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BU:25:LYS:NZ | 1:BU:77:GLU:OE2 | 2.37 | 0.58 |
| 2:BW:146:HIS:HE1 | 2:BW:197:ILE:HG23 | 1.69 | 0.58 |
| 2:BW:209:LYS:CE | 2:BW:238:TRP:HD1 | 2.16 | 0.58 |
| 2:CP:208:TRP:CH2 | 2:CW:129:VAL:HG12 | 2.39 | 0.58 |
| 2:DK:162:TYR:OH | 2:DK:196:ASN:HA | 2.02 | 0.58 |
| 2:AW:146:HIS:HE1 | 2:AW:197:ILE:HG23 | 1.69 | 0.58 |
| 2:BP:55:LEU:HD21 | 2:BP:162:TYR:HE1 | 1.68 | 0.58 |
| 2:DK:22:SER:HB3 | 2:DK:27:LEU:HD12 | 1.84 | 0.58 |
| 2:AK:22:SER:HB3 | 2:AK:27:LEU:HD12 | 1.84 | 0.58 |
| 2:AP:208:TRP:CH2 | 2:AW:129:VAL:HG12 | 2.39 | 0.58 |
| 1:BB:77:GLU:OE2 | 1:BB:79:THR:OG1 | 2.21 | 0.58 |
| 1:BC:83:ILE:HD13 | 1:BC:110:LEU:HD11 | 1.84 | 0.58 |
| 2:BK:22:SER:HB3 | 2:BK:27:LEU:HD12 | 1.84 | 0.58 |
| 2:BW:129:VAL:HG22 | 2:BW:171:PRO:CG | 2.34 | 0.58 |
| 1:CS:171:MET:SD | 1:CS:171:MET:N | 2.76 | 0.58 |
| 1:BC:144:SER:HB2 | 1:BC:160:ILE:HD11 | 1.85 | 0.57 |
| 2:CW:146:HIS:HE1 | 2:CW:197:ILE:HG23 | 1.69 | 0.57 |
| 2:AD:195:ILE:CD1 | 2:AE:195:ILE:HD13 | 2.34 | 0.57 |
| 2:AD:195:ILE:HD11 | 2:AE:195:ILE:CD1 | 2.34 | 0.57 |
| 2:AP:109:ASP:N | 2:AP:109:ASP:OD1 | 2.33 | 0.57 |
| 2:BD:195:ILE:HD11 | 2:BE:195:ILE:CD1 | 2.34 | 0.57 |
| 2:CP:165:ARG:NH1 | 2:CP:173:ASP:OD1 | 2.37 | 0.57 |
| 2:BP:165:ARG:NH1 | 2:BP:173:ASP:OD1 | 2.37 | 0.57 |
| 2:BP:208:TRP:CH2 | 2:BW:129:VAL:HG12 | 2.39 | 0.57 |
| 1:AB:77:GLU:OE2 | 1:AB:79:THR:OG1 | 2.21 | 0.57 |
| 1:CN:86:LEU:HD11 | 1:CN:110:LEU:HD11 | 1.85 | 0.57 |
| 2:CW:209:LYS:CE | 2:CW:238:TRP:HD1 | 2.16 | 0.57 |
| 2:AP:94:TYR:HE2 | 2:AP:255:GLU:HG3 | 1.68 | 0.57 |
| 1:DB:77:GLU:OE2 | 1:DB:79:THR:OG1 | 2.21 | 0.57 |
| 2:AP:165:ARG:NH1 | 2:AP:173:ASP:OD1 | 2.37 | 0.57 |
| 2:CP:94:TYR:HE2 | 2:CP:255:GLU:HG3 | 1.68 | 0.57 |
| 1:CS:70:VAL:HG13 | 1:CS:72:ARG:H | 1.69 | 0.57 |
| 2:AW:209:LYS:HD3 | 2:AW:238:TRP:HD1 | 1.69 | 0.57 |
| 1:DI:77:GLU:OE2 | 1:DI:122:THR:OG1 | 2.23 | 0.57 |
| 1:BI:77:GLU:OE2 | 1:BI:122:THR:OG1 | 2.23 | 0.57 |
| 1:CB:77:GLU:OE2 | 1:CB:79:THR:OG1 | 2.21 | 0.57 |
| 1:AC:83:ILE:HD13 | 1:AC:110:LEU:HD13 | 1.85 | 0.57 |
| 2:AP:145:PHE:O | 2:AP:165:ARG:NH2 | 2.38 | 0.57 |
| 1:BO:139:THR:HB | 1:BO:180:MET:HE3 | 1.87 | 0.57 |
| 2:BP:94:TYR:HE2 | 2:BP:255:GLU:HG3 | 1.68 | 0.57 |
| 2:CD:195:ILE:HD11 | 2:CE:195:ILE:CD1 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CG:171:MET:CE | 1:CG:174:ARG:NH2 | 2.52 | 0.57 |
| 2:DD:195:ILE:HD11 | 2:DE:195:ILE:CD1 | 2.34 | 0.57 |
| 1:AN:86:LEU:HD11 | 1:AN:110:LEU:HD11 | 1.85 | 0.57 |
| 1:BC:83:ILE:HD13 | 1:BC:110:LEU:HD13 | 1.85 | 0.57 |
| 1:BN:86:LEU:HD11 | 1:BN:110:LEU:HD11 | 1.85 | 0.57 |
| 2:BP:145:PHE:O | 2:BP:165:ARG:NH2 | 2.38 | 0.57 |
| 1:BS:70:VAL:HG13 | 1:BS:72:ARG:H | 1.69 | 0.57 |
| 2:CK:170:THR:OG1 | 2:CK:173:ASP:OD1 | 2.23 | 0.57 |
| 2:CW:209:LYS:HD3 | 2:CW:238:TRP:HD1 | 1.69 | 0.57 |
| 1:DC:83:ILE:HD13 | 1:DC:110:LEU:HD11 | 1.84 | 0.57 |
| 2:AK:170:THR:OG1 | 2:AK:173:ASP:OD1 | 2.23 | 0.57 |
| 2:AP:55:LEU:HD21 | 2:AP:162:TYR:HE1 | 1.68 | 0.57 |
| 2:BD:192:LEU:HD21 | 2:BD:224:LEU:HD13 | 1.87 | 0.56 |
| 2:CD:192:LEU:HD21 | 2:CD:224:LEU:HD13 | 1.87 | 0.56 |
| 2:DK:170:THR:OG1 | 2:DK:173:ASP:OD1 | 2.23 | 0.56 |
| 1:BG:178:ILE:O | 1:BG:183:LYS:NZ | 2.39 | 0.56 |
| 2:CD:35:ASP:OD1 | 2:CD:49:ARG:NH2 | 2.34 | 0.56 |
| 2:CP:55:LEU:HD21 | 2:CP:162:TYR:HE1 | 1.68 | 0.56 |
| 2:CQ:208:TRP:CE2 | 2:CQ:217:GLN:HB3 | 2.40 | 0.56 |
| 2:DD:192:LEU:HD21 | 2:DD:224:LEU:HD13 | 1.86 | 0.56 |
| 1:AG:178:ILE:O | 1:AG:183:LYS:NZ | 2.39 | 0.56 |
| 1:AS:70:VAL:HG13 | 1:AS:72:ARG:H | 1.69 | 0.56 |
| 2:BK:170:THR:OG1 | 2:BK:173:ASP:OD1 | 2.23 | 0.56 |
| 2:BP:30:TRP:HE1 | 2:BP:54:ALA:HB1 | 1.70 | 0.56 |
| 2:BQ:208:TRP:CE2 | 2:BQ:217:GLN:HB3 | 2.40 | 0.56 |
| 2:BW:209:LYS:HD3 | 2:BW:238:TRP:HD1 | 1.69 | 0.56 |
| 1:CG:178:ILE:O | 1:CG:183:LYS:NZ | 2.39 | 0.56 |
| 1:CO:139:THR:HB | 1:CO:180:MET:HE3 | 1.87 | 0.56 |
| 2:CP:30:TRP:HE1 | 2:CP:54:ALA:HB1 | 1.70 | 0.56 |
| 1:CU:174:ARG:O | 1:CU:178:ILE:HG22 | 2.06 | 0.56 |
| 2:CW:129:VAL:HG22 | 2:CW:171:PRO:CG | 2.34 | 0.56 |
| 1:DC:83:ILE:HD13 | 1:DC:110:LEU:HD13 | 1.85 | 0.56 |
| 2:DD:195:ILE:HD11 | 2:DE:195:ILE:HD13 | 1.88 | 0.56 |
| 1:DG:178:ILE:O | 1:DG:183:LYS:NZ | 2.39 | 0.56 |
| 2:CP:145:PHE:O | 2:CP:165:ARG:NH2 | 2.38 | 0.56 |
| 2:AQ:208:TRP:CE2 | 2:AQ:217:GLN:HB3 | 2.40 | 0.56 |
| 1:CC:83:ILE:HD13 | 1:CC:110:LEU:HD13 | 1.85 | 0.56 |
| 1:CO:55:VAL:CG1 | 1:CO:123:ILE:CD1 | 2.84 | 0.56 |
| 1:AC:147:PRO:HB2 | 1:AC:151:ARG:HH21 | 1.70 | 0.56 |
| 2:AD:192:LEU:HD21 | 2:AD:224:LEU:HD13 | 1.87 | 0.56 |
| 2:CD:195:ILE:HD11 | 2:CE:195:ILE:HD13 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CW:1:MET:HE1 | 2:CW:257:PHE:HE1 | 1.71 | 0.56 |
| 1:AI:77:GLU:OE2 | 1:AI:122:THR:OG1 | 2.23 | 0.56 |
| 1:CC:19:ILE:HG13 | 1:CC:43:SER:HB3 | 1.87 | 0.56 |
| 1:CN:83:ILE:HD12 | 1:CN:86:LEU:HD12 | 1.87 | 0.56 |
| 2:DK:2:GLU:OE2 | 2:DK:2:GLU:N | 2.32 | 0.56 |
| 1:AC:19:ILE:HG13 | 1:AC:43:SER:HB3 | 1.87 | 0.56 |
| 2:DK:201:PHE:CZ | 2:DK:238:TRP:HH2 | 2.24 | 0.56 |
| 1:AN:83:ILE:HD12 | 1:AN:86:LEU:HD12 | 1.87 | 0.56 |
| 1:BC:19:ILE:HG13 | 1:BC:43:SER:HB3 | 1.87 | 0.56 |
| 1:BG:93:LEU:HD13 | 1:BI:93:LEU:HD23 | 1.87 | 0.56 |
| 1:BI:70:VAL:HG12 | 1:BI:72:ARG:H | 1.71 | 0.56 |
| 2:BK:2:GLU:OE2 | 2:BK:2:GLU:N | 2.32 | 0.56 |
| 2:BK:201:PHE:CZ | 2:BK:238:TRP:HH2 | 2.24 | 0.56 |
| 1:BN:83:ILE:HD12 | 1:BN:86:LEU:HD12 | 1.87 | 0.56 |
| 1:BU:174:ARG:O | 1:BU:178:ILE:HG22 | 2.06 | 0.56 |
| 2:AK:201:PHE:CZ | 2:AK:238:TRP:HH2 | 2.24 | 0.56 |
| 2:AW:146:HIS:CE1 | 2:AW:197:ILE:HG23 | 2.41 | 0.56 |
| 1:BC:147:PRO:HB2 | 1:BC:151:ARG:HH21 | 1.70 | 0.56 |
| 2:BD:219:LYS:HG3 | 2:BD:239:ARG:HH21 | 1.71 | 0.56 |
| 1:BS:152:ASP:OD1 | 1:BS:152:ASP:N | 2.38 | 0.56 |
| 2:BW:1:MET:HE1 | 2:BW:257:PHE:HE1 | 1.71 | 0.56 |
| 1:CC:147:PRO:HB2 | 1:CC:151:ARG:HH21 | 1.70 | 0.56 |
| 2:CK:201:PHE:CZ | 2:CK:238:TRP:HH2 | 2.24 | 0.56 |
| 1:DC:147:PRO:HB2 | 1:DC:151:ARG:HH21 | 1.70 | 0.56 |
| 2:DD:35:ASP:OD1 | 2:DD:49:ARG:NH2 | 2.34 | 0.56 |
| 1:DC:19:ILE:HG13 | 1:DC:43:SER:HB3 | 1.87 | 0.55 |
| 1:AS:152:ASP:OD1 | 1:AS:152:ASP:N | 2.38 | 0.55 |
| 2:AW:129:VAL:HG22 | 2:AW:171:PRO:CG | 2.34 | 0.55 |
| 1:AO:139:THR:HB | 1:AO:180:MET:HE3 | 1.87 | 0.55 |
| 2:BK:55:LEU:CD2 | 2:BK:195:ILE:HG22 | 2.08 | 0.55 |
| 1:AC:63:LEU:HD21 | 1:AC:127:CYS:HB2 | 1.88 | 0.55 |
| 2:AD:219:LYS:HG3 | 2:AD:239:ARG:HH21 | 1.71 | 0.55 |
| 2:AL:94:TYR:CD1 | 2:AL:262:VAL:HG11 | 2.42 | 0.55 |
| 2:AP:30:TRP:HE1 | 2:AP:54:ALA:HB1 | 1.70 | 0.55 |
| 2:BD:195:ILE:HD11 | 2:BE:195:ILE:HD13 | 1.88 | 0.55 |
| 2:BK:55:LEU:CG | 2:BK:195:ILE:HG23 | 2.36 | 0.55 |
| 2:BL:94:TYR:CD1 | 2:BL:262:VAL:HG11 | 2.42 | 0.55 |
| 1:CB:98:TRP:CZ3 | 1:CB:155:TRP:HB3 | 2.42 | 0.55 |
| 2:CD:219:LYS:HG3 | 2:CD:239:ARG:HH21 | 1.71 | 0.55 |
| 1:CI:77:GLU:OE2 | 1:CI:122:THR:OG1 | 2.23 | 0.55 |
| 2:CL:104:TYR:OH | 2:CL:179:ASP:OD2 | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DL:104:TYR:OH | 2:DL:179:ASP:OD2 | 2.25 | 0.55 |
| 1:AI:70:VAL:HG12 | 1:AI:72:ARG:H | 1.71 | 0.55 |
| 1:AU:144:SER:OG | 1:AU:148:LYS:NZ | 2.40 | 0.55 |
| 1:BC:63:LEU:HD21 | 1:BC:127:CYS:HB2 | 1.88 | 0.55 |
| 2:BL:104:TYR:OH | 2:BL:179:ASP:OD2 | 2.25 | 0.55 |
| 1:DC:63:LEU:HD21 | 1:DC:127:CYS:HB2 | 1.88 | 0.55 |
| 1:DI:70:VAL:HG12 | 1:DI:72:ARG:H | 1.71 | 0.55 |
| 2:DL:94:TYR:CD1 | 2:DL:262:VAL:HG11 | 2.42 | 0.55 |
| 2:AL:104:TYR:OH | 2:AL:179:ASP:OD2 | 2.25 | 0.55 |
| 1:BB:98:TRP:CZ3 | 1:BB:155:TRP:HB3 | 2.42 | 0.55 |
| 1:CG:93:LEU:HD13 | 1:CI:93:LEU:HD23 | 1.87 | 0.55 |
| 2:DK:246:GLU:OE1 | 2:DK:246:GLU:N | 2.24 | 0.55 |
| 1:AU:174:ARG:O | 1:AU:178:ILE:HG22 | 2.06 | 0.55 |
| 1:BU:144:SER:OG | 1:BU:148:LYS:NZ | 2.40 | 0.55 |
| 1:CS:152:ASP:OD1 | 1:CS:152:ASP:N | 2.38 | 0.55 |
| 1:DB:98:TRP:CZ3 | 1:DB:155:TRP:HB3 | 2.42 | 0.55 |
| 1:DG:93:LEU:HD13 | 1:DI:93:LEU:HD23 | 1.87 | 0.55 |
| 2:AD:195:ILE:HD11 | 2:AE:195:ILE:HD13 | 1.88 | 0.55 |
| 2:CL:94:TYR:CD1 | 2:CL:262:VAL:HG11 | 2.42 | 0.55 |
| 1:CS:171:MET:HB2 | 1:CS:174:ARG:HB3 | 1.89 | 0.55 |
| 2:AD:35:ASP:OD1 | 2:AD:49:ARG:NH2 | 2.34 | 0.55 |
| 2:AX:258:LEU:O | 2:AX:262:VAL:HG12 | 2.07 | 0.55 |
| 1:BS:19:ILE:HD12 | 1:BS:74:VAL:HG21 | 1.88 | 0.55 |
| 2:BW:72:ARG:NE | 2:BW:152:ASP:OD1 | 2.40 | 0.55 |
| 2:BW:146:HIS:CE1 | 2:BW:197:ILE:HG23 | 2.41 | 0.55 |
| 2:CD:198:ARG:CG | 2:CD:202:TYR:CE2 | 2.55 | 0.55 |
| 2:CW:72:ARG:NE | 2:CW:152:ASP:OD1 | 2.40 | 0.55 |
| 1:AC:130:MET:SD | 2:AD:43:TYR:CE2 | 3.00 | 0.55 |
| 2:BX:258:LEU:O | 2:BX:262:VAL:HG12 | 2.07 | 0.55 |
| 2:CK:2:GLU:OE2 | 2:CK:2:GLU:N | 2.32 | 0.55 |
| 2:AK:55:LEU:CG | 2:AK:195:ILE:HG23 | 2.36 | 0.55 |
| 1:AO:32:ILE:CG1 | 1:AO:176:ASN:CG | 2.80 | 0.55 |
| 1:BC:130:MET:SD | 2:BD:43:TYR:CE2 | 3.00 | 0.54 |
| 1:BO:32:ILE:CG1 | 1:BO:176:ASN:CG | 2.80 | 0.54 |
| 2:CW:146:HIS:CE1 | 2:CW:197:ILE:HG23 | 2.41 | 0.54 |
| 1:CC:63:LEU:HD21 | 1:CC:127:CYS:HB2 | 1.88 | 0.54 |
| 1:CC:98:TRP:NE1 | 1:CC:154:GLN:OE1 | 2.40 | 0.54 |
| 1:AB:52:THR:HG22 | 1:AC:48:ASP:OD2 | 2.08 | 0.54 |
| 2:CP:156:VAL:HA | 2:CP:161:SER:HB3 | 1.90 | 0.54 |
| 1:DC:130:MET:SD | 2:DD:43:TYR:CE2 | 3.00 | 0.54 |
| 1:BC:48:ASP:OD2 | 1:BB:52:THR:HG22 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BC:49:GLU:OE2 | 1:BC:62:LYS:NZ | 2.40 | 0.54 |
| 1:BS:171:MET:HB2 | 1:BS:174:ARG:HB3 | 1.89 | 0.54 |
| 1:CC:49:GLU:OE2 | 1:CC:62:LYS:NZ | 2.40 | 0.54 |
| 1:CC:130:MET:SD | 2:CD:43:TYR:CE2 | 3.00 | 0.54 |
| 1:CI:70:VAL:HG12 | 1:CI:72:ARG:H | 1.71 | 0.54 |
| 2:DK:55:LEU:CG | 2:DK:195:ILE:HG23 | 2.35 | 0.54 |
| 2:BP:156:VAL:HA | 2:BP:161:SER:HB3 | 1.90 | 0.54 |
| 1:CB:52:THR:HG22 | 1:CC:48:ASP:OD2 | 2.08 | 0.54 |
| 1:CU:144:SER:OG | 1:CU:148:LYS:NZ | 2.40 | 0.54 |
| 2:CX:258:LEU:O | 2:CX:262:VAL:HG12 | 2.07 | 0.54 |
| 1:AC:49:GLU:OE2 | 1:AC:62:LYS:NZ | 2.40 | 0.54 |
| 1:AB:98:TRP:CZ3 | 1:AB:155:TRP:HB3 | 2.42 | 0.54 |
| 2:CW:158:ASP:OD1 | 2:CW:158:ASP:N | 2.35 | 0.54 |
| 1:DB:52:THR:HG22 | 1:DC:48:ASP:OD2 | 2.08 | 0.54 |
| 1:AG:93:LEU:HD13 | 1:AI:93:LEU:HD23 | 1.88 | 0.54 |
| 2:CK:55:LEU:CG | 2:CK:195:ILE:HG23 | 2.36 | 0.54 |
| 2:DD:219:LYS:HG3 | 2:DD:239:ARG:HH21 | 1.71 | 0.54 |
| 2:AP:156:VAL:HA | 2:AP:161:SER:HB3 | 1.90 | 0.54 |
| 1:BC:98:TRP:NE1 | 1:BC:154:GLN:OE1 | 2.41 | 0.54 |
| 1:DC:49:GLU:OE2 | 1:DC:62:LYS:NZ | 2.40 | 0.54 |
| 1:AS:171:MET:HB2 | 1:AS:174:ARG:HB3 | 1.89 | 0.54 |
| 2:BX:192:LEU:O | 2:BX:198:ARG:NH1 | 2.40 | 0.54 |
| 1:CO:32:ILE:CG1 | 1:CO:176:ASN:CG | 2.80 | 0.54 |
| 2:DD:213:LEU:HG | 2:DD:217:GLN:HG2 | 1.90 | 0.54 |
| 2:AW:1:MET:HE1 | 2:AW:257:PHE:HE1 | 1.71 | 0.54 |
| 1:BS:166:GLU:N | 1:BS:166:GLU:OE1 | 2.41 | 0.54 |
| 1:BU:14:MET:HG3 | 1:BU:16:ILE:HD11 | 1.90 | 0.54 |
| 2:BD:213:LEU:HG | 2:BD:217:GLN:HG2 | 1.90 | 0.54 |
| 2:BQ:75:MET:O | 2:BQ:79:TRP:HB2 | 2.08 | 0.54 |
| 1:CN:19:ILE:HD11 | 1:CN:70:VAL:HG23 | 1.90 | 0.54 |
| 1:CS:19:ILE:HD12 | 1:CS:74:VAL:HG21 | 1.88 | 0.54 |
| 2:AD:213:LEU:HG | 2:AD:217:GLN:HG2 | 1.90 | 0.54 |
| 2:CW:209:LYS:CE | 2:CW:238:TRP:CD1 | 2.91 | 0.53 |
| 1:AU:166:GLU:HG2 | 1:AU:170:GLU:HG3 | 1.90 | 0.53 |
| 2:AW:209:LYS:CE | 2:AW:238:TRP:CD1 | 2.91 | 0.53 |
| 1:BU:166:GLU:HG2 | 1:BU:170:GLU:HG3 | 1.90 | 0.53 |
| 2:BW:158:ASP:OD1 | 2:BW:158:ASP:N | 2.35 | 0.53 |
| 2:CD:213:LEU:HG | 2:CD:217:GLN:HG2 | 1.90 | 0.53 |
| 2:BK:94:TYR:CB | 2:BK:262:VAL:HG21 | 2.39 | 0.53 |
| 1:BN:19:ILE:HD11 | 1:BN:70:VAL:HG23 | 1.90 | 0.53 |
| 2:BW:209:LYS:CE | 2:BW:238:TRP:CD1 | 2.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CG:171:MET:CG | 1:CG:174:ARG:HH21 | 2.21 | 0.53 |
| 1:CI:171:MET:HE2 | 1:CI:174:ARG:HE | 1.72 | 0.53 |
| 2:CK:94:TYR:CB | 2:CK:262:VAL:HG21 | 2.38 | 0.53 |
| 1:CS:166:GLU:OE1 | 1:CS:166:GLU:N | 2.41 | 0.53 |
| 1:AC:118:LEU:HG | 1:AC:143:ILE:HD11 | 1.90 | 0.53 |
| 1:DI:171:MET:HE2 | 1:DI:174:ARG:HE | 1.72 | 0.53 |
| 2:DK:55:LEU:CD2 | 2:DK:195:ILE:HG22 | 2.08 | 0.53 |
| 1:BG:171:MET:CG | 1:BG:174:ARG:HH21 | 2.21 | 0.53 |
| 1:BI:171:MET:HE2 | 1:BI:174:ARG:HE | 1.73 | 0.53 |
| 2:BX:190:TYR:OH | 2:BX:194:ASP:OD2 | 2.22 | 0.53 |
| 2:AK:94:TYR:CB | 2:AK:262:VAL:HG21 | 2.39 | 0.53 |
| 1:BC:118:LEU:HG | 1:BC:143:ILE:HD11 | 1.90 | 0.53 |
| 1:CU:166:GLU:HG2 | 1:CU:170:GLU:HG3 | 1.90 | 0.53 |
| 1:AC:98:TRP:NE1 | 1:AC:154:GLN:OE1 | 2.41 | 0.53 |
| 1:AU:14:MET:HG3 | 1:AU:16:ILE:HD11 | 1.90 | 0.53 |
| 1:CN:122:THR:HG22 | 1:CN:180:MET:HG2 | 1.90 | 0.53 |
| 1:DG:171:MET:CG | 1:DG:174:ARG:HH21 | 2.21 | 0.53 |
| 2:DK:94:TYR:CB | 2:DK:262:VAL:HG21 | 2.39 | 0.53 |
| 2:CD:170:THR:OG1 | 2:CD:173:ASP:OD1 | 2.25 | 0.53 |
| 1:AI:171:MET:HE2 | 1:AI:174:ARG:HE | 1.72 | 0.53 |
| 1:AO:75:PHE:HB3 | 1:AO:126:TYR:HD1 | 1.74 | 0.53 |
| 1:AS:19:ILE:HD12 | 1:AS:74:VAL:HG21 | 1.88 | 0.53 |
| 1:CB:19:ILE:HD13 | 1:CB:43:SER:HB3 | 1.90 | 0.53 |
| 2:CD:151:ASP:HB3 | 2:CD:154:SER:HB2 | 1.91 | 0.53 |
| 2:DD:151:ASP:HB3 | 2:DD:154:SER:HB2 | 1.91 | 0.53 |
| 1:AO:166:GLU:CG | 1:AO:171:MET:HG3 | 2.39 | 0.53 |
| 1:BG:50:ILE:HG23 | 1:BG:61:ASP:OD2 | 2.10 | 0.52 |
| 1:BO:166:GLU:CG | 1:BO:171:MET:HG3 | 2.39 | 0.52 |
| 2:CL:93:GLU:HA | 2:CL:119:TYR:HE2 | 1.74 | 0.52 |
| 1:CO:75:PHE:HB3 | 1:CO:126:TYR:HD1 | 1.74 | 0.52 |
| 2:CQ:75:MET:O | 2:CQ:79:TRP:HB2 | 2.08 | 0.52 |
| 2:DL:93:GLU:HA | 2:DL:119:TYR:HE2 | 1.74 | 0.52 |
| 1:BB:19:ILE:HD13 | 1:BB:43:SER:HB3 | 1.90 | 0.52 |
| 2:BD:151:ASP:HB3 | 2:BD:154:SER:HB2 | 1.91 | 0.52 |
| 2:BD:152:ASP:OD1 | 2:AW:152:ASP:OD2 | 2.27 | 0.52 |
| 1:BN:122:THR:HG22 | 1:BN:180:MET:HG2 | 1.90 | 0.52 |
| 1:BS:73:PRO:HB3 | 1:BS:128:ASP:HA | 1.90 | 0.52 |
| 2:CD:192:LEU:HB3 | 2:CD:231:GLN:HG3 | 1.92 | 0.52 |
| 1:AB:19:ILE:HD13 | 1:AB:43:SER:HB3 | 1.90 | 0.52 |
| 1:CI:167:THR:HG23 | 1:CI:169:ALA:H | 1.74 | 0.52 |
| 1:CO:166:GLU:CG | 1:CO:171:MET:HG3 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CW:73:SER:OG | 2:DD:110:ARG:NH2 | 2.42 | 0.52 |
| 2:CX:22:SER:HB3 | 2:CX:27:LEU:HD12 | 1.91 | 0.52 |
| 1:DB:20:THR:OG1 | 1:DB:21:ARG:N | 2.42 | 0.52 |
| 1:AN:122:THR:HG22 | 1:AN:180:MET:HG2 | 1.90 | 0.52 |
| 1:BI:19:ILE:CD1 | 1:BI:43:SER:HG | 2.18 | 0.52 |
| 2:BX:22:SER:HB3 | 2:BX:27:LEU:HD12 | 1.91 | 0.52 |
| 1:CB:20:THR:OG1 | 1:CB:21:ARG:N | 2.42 | 0.52 |
| 1:CI:73:PRO:HA | 1:CI:127:CYS:O | 2.10 | 0.52 |
| 2:AD:151:ASP:HB3 | 2:AD:154:SER:HB2 | 1.91 | 0.52 |
| 1:AG:50:ILE:HG23 | 1:AG:61:ASP:OD2 | 2.10 | 0.52 |
| 1:AG:171:MET:CG | 1:AG:174:ARG:HH21 | 2.21 | 0.52 |
| 1:AS:73:PRO:HB3 | 1:AS:128:ASP:HA | 1.90 | 0.52 |
| 1:AS:166:GLU:OE1 | 1:AS:166:GLU:N | 2.41 | 0.52 |
| 2:BE:158:ASP:OD1 | 2:BE:158:ASP:N | 2.41 | 0.52 |
| 1:BI:73:PRO:HA | 1:BI:127:CYS:O | 2.10 | 0.52 |
| 1:DB:19:ILE:HD13 | 1:DB:43:SER:HB3 | 1.90 | 0.52 |
| 2:DD:192:LEU:HB3 | 2:DD:231:GLN:HG3 | 1.92 | 0.52 |
| 1:DI:73:PRO:HA | 1:DI:127:CYS:O | 2.10 | 0.52 |
| 1:AI:73:PRO:HA | 1:AI:127:CYS:O | 2.10 | 0.52 |
| 2:AL:93:GLU:HA | 2:AL:119:TYR:HE2 | 1.74 | 0.52 |
| 2:BD:192:LEU:HB3 | 2:BD:231:GLN:HG3 | 1.92 | 0.52 |
| 1:CU:14:MET:HG3 | 1:CU:16:ILE:HD11 | 1.90 | 0.52 |
| 1:DI:167:THR:HG23 | 1:DI:169:ALA:H | 1.74 | 0.52 |
| 2:AD:170:THR:OG1 | 2:AD:173:ASP:OD1 | 2.25 | 0.52 |
| 2:AX:22:SER:HB3 | 2:AX:27:LEU:HD12 | 1.91 | 0.52 |
| 1:AB:20:THR:OG1 | 1:AB:21:ARG:N | 2.42 | 0.52 |
| 2:CQ:77:ARG:NH1 | 2:DL:110:ARG:HH21 | 2.08 | 0.52 |
| 2:AL:258:LEU:O | 2:AL:262:VAL:HG12 | 2.09 | 0.52 |
| 1:AN:19:ILE:HD11 | 1:AN:70:VAL:HG23 | 1.90 | 0.52 |
| 2:AQ:75:MET:O | 2:AQ:79:TRP:HB2 | 2.08 | 0.52 |
| 2:BD:252:GLU:OE1 | 2:BD:252:GLU:N | 2.43 | 0.52 |
| 1:BO:55:VAL:CG1 | 1:BO:123:ILE:CD1 | 2.84 | 0.52 |
| 1:CC:118:LEU:HG | 1:CC:143:ILE:HD11 | 1.90 | 0.52 |
| 1:CN:100:LYS:HD2 | 1:CO:87:ASN:O | 2.10 | 0.52 |
| 1:CS:73:PRO:HB3 | 1:CS:128:ASP:HA | 1.90 | 0.52 |
| 2:AD:192:LEU:HB3 | 2:AD:231:GLN:HG3 | 1.92 | 0.52 |
| 2:AD:252:GLU:OE1 | 2:AD:252:GLU:N | 2.43 | 0.52 |
| 1:AN:100:LYS:HD2 | 1:AO:87:ASN:O | 2.09 | 0.52 |
| 2:BL:258:LEU:O | 2:BL:262:VAL:HG12 | 2.09 | 0.52 |
| 1:DC:118:LEU:HG | 1:DC:143:ILE:HD11 | 1.90 | 0.52 |
| 2:AE:158:ASP:OD1 | 2:AE:158:ASP:N | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AO:55:VAL:CG1 | 1:AO:123:ILE:CD1 | 2.84 | 0.52 |
| 2:AX:116:LEU:CD1 | 2:AX:142:ILE:CD1 | 2.71 | 0.52 |
| 1:BO:75:PHE:HB3 | 1:BO:126:TYR:HD1 | 1.74 | 0.52 |
| 2:CD:252:GLU:OE1 | 2:CD:252:GLU:N | 2.43 | 0.52 |
| 1:CG:50:ILE:HG23 | 1:CG:61:ASP:OD2 | 2.10 | 0.52 |
| 1:CI:30:ASN:O | 1:CI:34:SER:OG | 2.27 | 0.52 |
| 2:CL:170:THR:OG1 | 2:CL:173:ASP:OD1 | 2.22 | 0.52 |
| 2:CL:258:LEU:O | 2:CL:262:VAL:HG12 | 2.09 | 0.52 |
| 2:BD:170:THR:OG1 | 2:BD:173:ASP:OD1 | 2.25 | 0.52 |
| 1:BI:167:THR:HG23 | 1:BI:169:ALA:H | 1.74 | 0.52 |
| 2:BL:93:GLU:HA | 2:BL:119:TYR:HE2 | 1.74 | 0.52 |
| 1:DC:102:GLN:OE1 | 1:DC:102:GLN:HA | 2.10 | 0.52 |
| 1:DG:50:ILE:HG23 | 1:DG:61:ASP:OD2 | 2.10 | 0.52 |
| 1:AG:25:LYS:NZ | 3:AG:201:Y43:OAO | 2.36 | 0.52 |
| 1:BB:20:THR:OG1 | 1:BB:21:ARG:N | 2.42 | 0.52 |
| 1:CC:102:GLN:OE1 | 1:CC:102:GLN:HA | 2.11 | 0.51 |
| 2:DD:252:GLU:OE1 | 2:DD:252:GLU:N | 2.43 | 0.51 |
| 2:DE:158:ASP:OD1 | 2:DE:158:ASP:N | 2.41 | 0.51 |
| 2:AE:3:GLN:OE1 | 2:AE:3:GLN:N | 2.37 | 0.51 |
| 2:AX:192:LEU:O | 2:AX:198:ARG:NH1 | 2.40 | 0.51 |
| 2:DL:66:GLY:O | 2:DL:67:LYS:HD3 | 2.10 | 0.51 |
| 2:DL:258:LEU:O | 2:DL:262:VAL:HG12 | 2.09 | 0.51 |
| 1:AO:64:LEU:O | 1:AO:68:LYS:HG2 | 2.10 | 0.51 |
| 1:BC:102:GLN:OE1 | 1:BC:102:GLN:HA | 2.10 | 0.51 |
| 2:BX:104:TYR:OH | 2:BX:179:ASP:OD2 | 2.29 | 0.51 |
| 1:CU:25:LYS:HG2 | 1:CU:181:ARG:HH12 | 1.75 | 0.51 |
| 1:BU:25:LYS:HG2 | 1:BU:181:ARG:HH12 | 1.75 | 0.51 |
| 1:AI:167:THR:HG23 | 1:AI:169:ALA:H | 1.74 | 0.51 |
| 2:BQ:129:VAL:HG22 | 2:BQ:171:PRO:CG | 2.34 | 0.51 |
| 2:BX:55:LEU:HD21 | 2:BX:162:TYR:CE2 | 2.46 | 0.51 |
| 2:CE:158:ASP:OD1 | 2:CE:158:ASP:N | 2.41 | 0.51 |
| 2:CD:191:SER:OG | 2:CD:197:ILE:CD1 | 2.52 | 0.51 |
| 1:CO:64:LEU:O | 1:CO:68:LYS:HG2 | 2.10 | 0.51 |
| 2:CW:192:LEU:HD11 | 2:CW:201:PHE:HD2 | 1.76 | 0.51 |
| 1:DG:93:LEU:HD11 | 1:DI:96:ILE:HD12 | 1.93 | 0.51 |
| 2:AK:55:LEU:CD2 | 2:AK:195:ILE:HG22 | 2.08 | 0.51 |
| 2:AX:55:LEU:HD21 | 2:AX:162:TYR:CE2 | 2.46 | 0.51 |
| 1:AC:102:GLN:OE1 | 1:AC:102:GLN:HA | 2.11 | 0.51 |
| 2:DK:2:GLU:H | 2:DK:2:GLU:CD | 2.18 | 0.51 |
| 1:BS:111:GLY:HA2 | 1:BS:143:ILE:HG13 | 1.92 | 0.51 |
| 2:CX:55:LEU:HD21 | 2:CX:162:TYR:CE2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AP:71:LEU:O | 2:AP:75:MET:HG3 | 2.11 | 0.51 |
| 2:BW:192:LEU:HD11 | 2:BW:201:PHE:HD2 | 1.76 | 0.51 |
| 1:CG:93:LEU:HD11 | 1:CI:96:ILE:HD12 | 1.93 | 0.51 |
| 2:DD:247:ASN:OD1 | 2:DD:249:ASN:N | 2.44 | 0.51 |
| 1:BN:100:LYS:HD2 | 1:BO:87:ASN:O | 2.10 | 0.51 |
| 2:CE:213:LEU:HB3 | 2:CE:217:GLN:HB2 | 1.93 | 0.51 |
| 1:CN:25:LYS:O | 1:CN:29:ILE:HG12 | 2.11 | 0.51 |
| 1:CS:111:GLY:HA2 | 1:CS:143:ILE:HG13 | 1.92 | 0.51 |
| 2:AK:146:HIS:HE1 | 2:AK:196:ASN:HB3 | 1.76 | 0.51 |
| 1:AN:25:LYS:O | 1:AN:29:ILE:HG12 | 2.11 | 0.51 |
| 1:AU:25:LYS:HG2 | 1:AU:181:ARG:HH12 | 1.75 | 0.51 |
| 2:CD:247:ASN:OD1 | 2:CD:249:ASN:N | 2.44 | 0.50 |
| 2:CK:146:HIS:HE1 | 2:CK:196:ASN:HB3 | 1.76 | 0.50 |
| 2:CX:190:TYR:OH | 2:CX:194:ASP:OD2 | 2.22 | 0.50 |
| 2:DD:158:ASP:OD1 | 2:DD:158:ASP:N | 2.43 | 0.50 |
| 2:DE:213:LEU:HB3 | 2:DE:217:GLN:HB2 | 1.93 | 0.50 |
| 2:AE:213:LEU:HB3 | 2:AE:217:GLN:HB2 | 1.93 | 0.50 |
| 1:AS:111:GLY:HA2 | 1:AS:143:ILE:HG13 | 1.92 | 0.50 |
| 1:BO:64:LEU:O | 1:BO:68:LYS:HG2 | 2.10 | 0.50 |
| 1:CO:17:ARG:NH2 | 2:CQ:248:ASP:OD1 | 2.44 | 0.50 |
| 2:CX:192:LEU:O | 2:CX:198:ARG:NH1 | 2.40 | 0.50 |
| 2:DK:146:HIS:HE1 | 2:DK:196:ASN:HB3 | 1.76 | 0.50 |
| 2:AD:158:ASP:OD1 | 2:AD:158:ASP:N | 2.43 | 0.50 |
| 2:AD:247:ASN:OD1 | 2:AD:249:ASN:N | 2.44 | 0.50 |
| 1:AG:93:LEU:HD11 | 1:AI:96:ILE:HD12 | 1.93 | 0.50 |
| 1:AO:17:ARG:NH2 | 2:AQ:248:ASP:OD1 | 2.44 | 0.50 |
| 1:BG:171:MET:CE | 1:BG:174:ARG:NH2 | 2.52 | 0.50 |
| 2:CP:71:LEU:O | 2:CP:75:MET:HG3 | 2.11 | 0.50 |
| 2:CW:231:GLN:NE2 | 2:CX:56:GLU:OE1 | 2.44 | 0.50 |
| 2:BE:213:LEU:HB3 | 2:BE:217:GLN:HB2 | 1.93 | 0.50 |
| 2:AW:192:LEU:HD11 | 2:AW:201:PHE:HD2 | 1.76 | 0.50 |
| 2:BD:110:ARG:NH2 | 2:AW:73:SER:OG | 2.44 | 0.50 |
| 2:BD:191:SER:OG | 2:BD:197:ILE:CD1 | 2.52 | 0.50 |
| 2:BK:146:HIS:HE1 | 2:BK:196:ASN:HB3 | 1.76 | 0.50 |
| 2:BD:158:ASP:OD1 | 2:BD:158:ASP:N | 2.43 | 0.50 |
| 2:BW:231:GLN:NE2 | 2:BX:56:GLU:OE1 | 2.44 | 0.50 |
| 2:BP:71:LEU:O | 2:BP:75:MET:HG3 | 2.11 | 0.50 |
| 1:BS:12:SER:OG | 1:BS:13:GLY:N | 2.44 | 0.50 |
| 1:CC:83:ILE:CD1 | 1:CC:110:LEU:HD11 | 2.42 | 0.50 |
| 2:DD:191:SER:OG | 2:DD:197:ILE:CD1 | 2.52 | 0.50 |
| 2:DL:170:THR:OG1 | 2:DL:173:ASP:OD1 | 2.22 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:191:SER:OG | 2:AD:197:ILE:CD1 | 2.52 | 0.50 |
| 2:BK:2:GLU:H | 2:BK:2:GLU:CD | 2.18 | 0.50 |
| 1:BN:22:ASN:HB2 | 1:BN:25:LYS:HD2 | 1.94 | 0.50 |
| 1:BN:25:LYS:O | 1:BN:29:ILE:HG12 | 2.11 | 0.50 |
| 2:CW:35:ASP:OD1 | 2:CW:49:ARG:NH2 | 2.45 | 0.50 |
| 2:AK:54:ALA:CB | 2:AK:195:ILE:CD1 | 2.85 | 0.50 |
| 1:AS:12:SER:OG | 1:AS:13:GLY:N | 2.44 | 0.50 |
| 2:AW:231:GLN:NE2 | 2:AX:56:GLU:OE1 | 2.44 | 0.50 |
| 1:CS:12:SER:OG | 1:CS:13:GLY:N | 2.44 | 0.50 |
| 2:AW:72:ARG:NE | 2:AW:152:ASP:OD1 | 2.40 | 0.50 |
| 1:BO:17:ARG:NH2 | 2:BQ:248:ASP:OD1 | 2.44 | 0.49 |
| 2:BW:35:ASP:OD1 | 2:BW:49:ARG:NH2 | 2.45 | 0.49 |
| 2:DK:94:TYR:HB3 | 2:DK:262:VAL:HG21 | 1.93 | 0.49 |
| 2:AK:3:GLN:OE1 | 2:AK:3:GLN:N | 2.38 | 0.49 |
| 2:CK:94:TYR:HB3 | 2:CK:262:VAL:HG21 | 1.93 | 0.49 |
| 2:CW:15:LEU:HD11 | 2:CW:188:ILE:HG12 | 1.94 | 0.49 |
| 1:DB:123:ILE:HG12 | 1:DB:136:GLU:HG3 | 1.93 | 0.49 |
| 2:AK:2:GLU:H | 2:AK:2:GLU:CD | 2.18 | 0.49 |
| 2:AQ:160:THR:O | 2:AQ:164:GLN:HG3 | 2.12 | 0.49 |
| 2:AW:5:LEU:O | 2:AW:9:LYS:HG2 | 2.12 | 0.49 |
| 1:BC:83:ILE:CD1 | 1:BC:110:LEU:HD11 | 2.42 | 0.49 |
| 2:BD:247:ASN:OD1 | 2:BD:249:ASN:N | 2.44 | 0.49 |
| 1:BG:93:LEU:HD11 | 1:BI:96:ILE:HD12 | 1.93 | 0.49 |
| 2:BK:94:TYR:HB3 | 2:BK:262:VAL:HG21 | 1.93 | 0.49 |
| 1:BO:104:ASP:O | 1:BO:108:GLN:HG2 | 2.12 | 0.49 |
| 1:BS:23:ARG:O | 1:BS:27:LYS:NZ | 2.45 | 0.49 |
| 2:CQ:160:THR:O | 2:CQ:164:GLN:HG3 | 2.12 | 0.49 |
| 2:DK:3:GLN:OE1 | 2:DK:3:GLN:N | 2.38 | 0.49 |
| 1:CO:82:TYR:HB2 | 1:CO:119:VAL:HG22 | 1.95 | 0.49 |
| 1:AG:12:SER:OG | 1:AG:13:GLY:N | 2.45 | 0.49 |
| 2:AW:35:ASP:OD1 | 2:AW:49:ARG:NH2 | 2.45 | 0.49 |
| 1:BO:82:TYR:HB2 | 1:BO:119:VAL:HG22 | 1.95 | 0.49 |
| 2:BQ:160:THR:O | 2:BQ:164:GLN:HG3 | 2.12 | 0.49 |
| 2:BW:5:LEU:O | 2:BW:9:LYS:HG2 | 2.12 | 0.49 |
| 1:CG:153:PHE:HE2 | 1:CG:181:ARG:HH12 | 1.61 | 0.49 |
| 2:CK:2:GLU:H | 2:CK:2:GLU:CD | 2.18 | 0.49 |
| 1:CN:22:ASN:HB2 | 1:CN:25:LYS:HD2 | 1.94 | 0.49 |
| 1:CN:51:GLN:N | 1:CO:49:GLU:O | 2.40 | 0.49 |
| 1:CO:104:ASP:O | 1:CO:108:GLN:HG2 | 2.12 | 0.49 |
| 2:DD:170:THR:OG1 | 2:DD:173:ASP:OD1 | 2.25 | 0.49 |
| 2:DD:204:LEU:HD13 | 2:DD:240:ILE:HD11 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AC:83:ILE:CD1 | 1:AC:110:LEU:HD11 | 2.42 | 0.49 |
| 2:AD:204:LEU:HD13 | 2:AD:240:ILE:HD11 | 1.94 | 0.49 |
| 1:AS:159:PHE:HD2 | 1:AS:168:PHE:HE2 | 1.60 | 0.49 |
| 2:BD:204:LEU:HD13 | 2:BD:240:ILE:HD11 | 1.94 | 0.49 |
| 1:BS:159:PHE:HD2 | 1:BS:168:PHE:HE2 | 1.60 | 0.49 |
| 2:BW:105:THR:HG21 | 2:BW:112:ILE:CD1 | 2.40 | 0.49 |
| 2:CP:170:THR:OG1 | 2:CP:173:ASP:OD1 | 2.31 | 0.49 |
| 1:CS:159:PHE:HD2 | 1:CS:168:PHE:HE2 | 1.60 | 0.49 |
| 2:DL:85:ASP:OD1 | 2:DL:85:ASP:N | 2.46 | 0.49 |
| 1:AO:104:ASP:O | 1:AO:108:GLN:HG2 | 2.12 | 0.49 |
| 2:AQ:116:LEU:HD22 | 2:AQ:142:ILE:HD11 | 1.95 | 0.49 |
| 1:AS:23:ARG:O | 1:AS:27:LYS:NZ | 2.45 | 0.49 |
| 2:AW:209:LYS:HD3 | 2:AW:237:GLN:O | 2.12 | 0.49 |
| 1:BC:25:LYS:O | 1:BC:29:ILE:HG12 | 2.13 | 0.49 |
| 1:BG:153:PHE:HE2 | 1:BG:181:ARG:HH12 | 1.61 | 0.49 |
| 2:BL:85:ASP:OD1 | 2:BL:85:ASP:N | 2.46 | 0.49 |
| 1:BS:19:ILE:HD11 | 1:BS:70:VAL:HB | 1.95 | 0.49 |
| 2:BW:217:GLN:HB2 | 2:BW:239:ARG:HD3 | 1.94 | 0.49 |
| 1:AB:123:ILE:HG12 | 1:AB:136:GLU:HG3 | 1.93 | 0.49 |
| 2:CL:85:ASP:OD1 | 2:CL:85:ASP:N | 2.46 | 0.49 |
| 2:CW:105:THR:HG21 | 2:CW:112:ILE:CD1 | 2.40 | 0.49 |
| 2:CW:209:LYS:HD3 | 2:CW:237:GLN:O | 2.12 | 0.49 |
| 2:AP:170:THR:OG1 | 2:AP:173:ASP:OD1 | 2.31 | 0.49 |
| 2:BK:149:PHE:O | 2:BX:72:ARG:NH2 | 2.46 | 0.49 |
| 1:BN:123:ILE:HD13 | 1:BN:136:GLU:HB3 | 1.94 | 0.49 |
| 2:BP:170:THR:OG1 | 2:BP:173:ASP:OD1 | 2.31 | 0.49 |
| 1:CC:25:LYS:O | 1:CC:29:ILE:HG12 | 2.13 | 0.49 |
| 2:CK:54:ALA:CB | 2:CK:195:ILE:CD1 | 2.85 | 0.49 |
| 1:CO:166:GLU:HG2 | 1:CO:171:MET:HG3 | 1.95 | 0.49 |
| 1:CS:23:ARG:O | 1:CS:27:LYS:NZ | 2.45 | 0.49 |
| 2:CW:5:LEU:O | 2:CW:9:LYS:HG2 | 2.12 | 0.49 |
| 1:AN:51:GLN:N | 1:AO:49:GLU:O | 2.40 | 0.49 |
| 2:CK:149:PHE:O | 2:CX:72:ARG:NH2 | 2.46 | 0.49 |
| 2:CQ:208:TRP:CH2 | 2:CQ:217:GLN:HB3 | 2.48 | 0.49 |
| 1:DB:119:VAL:CG2 | 1:DB:140:GLN:HE21 | 2.26 | 0.49 |
| 1:DG:153:PHE:HE2 | 1:DG:181:ARG:HH12 | 1.61 | 0.49 |
| 1:DI:30:ASN:O | 1:DI:34:SER:OG | 2.27 | 0.49 |
| 2:DK:192:LEU:C | 2:DK:197:ILE:HG12 | 2.32 | 0.49 |
| 2:AK:94:TYR:HB3 | 2:AK:262:VAL:HG21 | 1.93 | 0.49 |
| 2:AK:149:PHE:O | 2:AX:72:ARG:NH2 | 2.46 | 0.49 |
| 1:AO:82:TYR:HB2 | 1:AO:119:VAL:HG22 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AX:190:TYR:OH | 2:AX:194:ASP:OD2 | 2.22 | 0.49 |
| 1:BO:166:GLU:HG2 | 1:BO:171:MET:HG3 | 1.95 | 0.49 |
| 2:BQ:116:LEU:HD22 | 2:BQ:142:ILE:HD11 | 1.95 | 0.49 |
| 1:CB:123:ILE:HG12 | 1:CB:136:GLU:HG3 | 1.93 | 0.49 |
| 1:DG:12:SER:OG | 1:DG:13:GLY:N | 2.45 | 0.49 |
| 1:AO:166:GLU:HG2 | 1:AO:171:MET:HG3 | 1.95 | 0.49 |
| 2:AQ:208:TRP:CH2 | 2:AQ:217:GLN:HB3 | 2.48 | 0.49 |
| 1:BB:119:VAL:CG2 | 1:BB:140:GLN:HE21 | 2.26 | 0.49 |
| 1:BG:171:MET:CE | 1:BG:174:ARG:CZ | 2.85 | 0.48 |
| 2:BL:19:ALA:O | 2:BL:23:MET:HG2 | 2.14 | 0.48 |
| 2:BW:152:ASP:OD2 | 2:CD:152:ASP:CG | 2.55 | 0.48 |
| 2:BW:209:LYS:HD3 | 2:BW:237:GLN:O | 2.13 | 0.48 |
| 1:CS:51:GLN:CD | 1:CU:93:LEU:CD2 | 2.85 | 0.48 |
| 2:CW:217:GLN:HB2 | 2:CW:239:ARG:HD3 | 1.94 | 0.48 |
| 1:DC:83:ILE:CD1 | 1:DC:110:LEU:HD11 | 2.42 | 0.48 |
| 1:DC:98:TRP:NE1 | 1:DC:154:GLN:OE1 | 2.41 | 0.48 |
| 2:AD:203:LYS:O | 2:AD:207:LEU:HB2 | 2.13 | 0.48 |
| 1:AG:152:ASP:OD1 | 1:AG:152:ASP:N | 2.42 | 0.48 |
| 1:AG:153:PHE:HE2 | 1:AG:181:ARG:HH12 | 1.61 | 0.48 |
| 1:AN:22:ASN:HB2 | 1:AN:25:LYS:HD2 | 1.94 | 0.48 |
| 2:AW:217:GLN:HB2 | 2:AW:239:ARG:HD3 | 1.94 | 0.48 |
| 2:BD:203:LYS:O | 2:BD:207:LEU:HB2 | 2.13 | 0.48 |
| 1:BS:51:GLN:CD | 1:BU:93:LEU:CD2 | 2.85 | 0.48 |
| 1:CS:19:ILE:HD11 | 1:CS:70:VAL:HB | 1.95 | 0.48 |
| 2:BK:198:ARG:O | 2:BK:202:TYR:HB3 | 2.13 | 0.48 |
| 2:CL:19:ALA:O | 2:CL:23:MET:HG2 | 2.14 | 0.48 |
| 1:DC:25:LYS:O | 1:DC:29:ILE:HG12 | 2.13 | 0.48 |
| 2:DK:198:ARG:O | 2:DK:202:TYR:HB3 | 2.13 | 0.48 |
| 1:AS:19:ILE:HD11 | 1:AS:70:VAL:HB | 1.95 | 0.48 |
| 1:AS:51:GLN:CD | 1:AU:93:LEU:CD2 | 2.85 | 0.48 |
| 2:AW:105:THR:HG21 | 2:AW:112:ILE:CD1 | 2.40 | 0.48 |
| 2:BW:15:LEU:HD11 | 2:BW:188:ILE:HG12 | 1.94 | 0.48 |
| 1:CN:123:ILE:HD13 | 1:CN:136:GLU:HB3 | 1.94 | 0.48 |
| 2:AL:19:ALA:O | 2:AL:23:MET:HG2 | 2.14 | 0.48 |
| 2:BL:112:ILE:O | 2:BL:116:LEU:HD12 | 2.14 | 0.48 |
| 2:DK:54:ALA:CB | 2:DK:195:ILE:CD1 | 2.85 | 0.48 |
| 1:AN:123:ILE:HD13 | 1:AN:136:GLU:HB3 | 1.94 | 0.48 |
| 2:AW:56:GLU:OE1 | 2:AX:231:GLN:NE2 | 2.46 | 0.48 |
| 2:BK:54:ALA:CB | 2:BK:195:ILE:CD1 | 2.85 | 0.48 |
| 2:CP:169:GLU:HA | 2:CP:169:GLU:OE2 | 2.13 | 0.48 |
| 2:CW:209:LYS:CD | 2:CW:238:TRP:HD1 | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DI:19:ILE:CD1 | 1:DI:43:SER:HG | 2.19 | 0.48 |
| 2:DL:112:ILE:O | 2:DL:116:LEU:HD12 | 2.14 | 0.48 |
| 2:BQ:208:TRP:CH2 | 2:BQ:217:GLN:HB3 | 2.48 | 0.48 |
| 2:BW:56:GLU:OE1 | 2:BX:231:GLN:NE2 | 2.46 | 0.48 |
| 2:CW:56:GLU:OE1 | 2:CX:231:GLN:NE2 | 2.46 | 0.48 |
| 1:AS:61:ASP:OD2 | 1:AS:65:LYS:NZ | 2.46 | 0.48 |
| 1:BB:123:ILE:HG12 | 1:BB:136:GLU:HG3 | 1.93 | 0.48 |
| 2:CK:60:TYR:HB2 | 2:CL:230:ILE:HG23 | 1.96 | 0.48 |
| 2:CL:112:ILE:O | 2:CL:116:LEU:HD12 | 2.14 | 0.48 |
| 2:DL:19:ALA:O | 2:DL:23:MET:HG2 | 2.14 | 0.48 |
| 2:AK:198:ARG:O | 2:AK:202:TYR:HB3 | 2.13 | 0.48 |
| 1:AS:93:LEU:HB3 | 1:AU:93:LEU:HD13 | 1.96 | 0.48 |
| 2:AW:15:LEU:HD11 | 2:AW:188:ILE:HG12 | 1.94 | 0.48 |
| 2:AW:209:LYS:CD | 2:AW:238:TRP:HD1 | 2.26 | 0.48 |
| 2:BW:209:LYS:CD | 2:BW:238:TRP:HD1 | 2.26 | 0.48 |
| 2:CD:81:SER:OG | 2:CD:83:ASP:OD1 | 2.31 | 0.48 |
| 1:CG:12:SER:OG | 1:CG:13:GLY:N | 2.45 | 0.48 |
| 1:AG:89:PHE:CG | 1:AG:90:PRO:HA | 2.49 | 0.48 |
| 2:AL:112:ILE:O | 2:AL:116:LEU:HD12 | 2.14 | 0.48 |
| 1:BI:83:ILE:HD12 | 1:BI:86:LEU:HD12 | 1.95 | 0.48 |
| 1:CG:89:PHE:CG | 1:CG:90:PRO:HA | 2.49 | 0.48 |
| 1:DG:89:PHE:CG | 1:DG:90:PRO:HA | 2.49 | 0.48 |
| 1:AI:30:ASN:O | 1:AI:34:SER:OG | 2.27 | 0.48 |
| 1:CB:119:VAL:CG2 | 1:CB:140:GLN:HE21 | 2.26 | 0.47 |
| 2:CD:203:LYS:O | 2:CD:207:LEU:HB2 | 2.13 | 0.47 |
| 2:CK:198:ARG:O | 2:CK:202:TYR:HB3 | 2.13 | 0.47 |
| 2:DD:203:LYS:O | 2:DD:207:LEU:HB2 | 2.13 | 0.47 |
| 1:AC:25:LYS:O | 1:AC:29:ILE:HG12 | 2.13 | 0.47 |
| 1:BG:89:PHE:CG | 1:BG:90:PRO:HA | 2.49 | 0.47 |
| 2:BP:169:GLU:HA | 2:BP:169:GLU:OE2 | 2.13 | 0.47 |
| 1:CN:171:MET:HB2 | 1:CN:174:ARG:HB2 | 1.96 | 0.47 |
| 1:DI:86:LEU:HB3 | 1:DI:89:PHE:HB3 | 1.96 | 0.47 |
| 1:AN:171:MET:HB2 | 1:AN:174:ARG:HB2 | 1.97 | 0.47 |
| 2:BW:170:THR:OG1 | 2:BW:173:ASP:OD1 | 2.32 | 0.47 |
| 1:CI:86:LEU:HB3 | 1:CI:89:PHE:HB3 | 1.96 | 0.47 |
| 2:CQ:116:LEU:HD22 | 2:CQ:142:ILE:HD11 | 1.95 | 0.47 |
| 1:CS:61:ASP:OD2 | 1:CS:65:LYS:NZ | 2.46 | 0.47 |
| 2:DL:21:VAL:O | 2:DL:24:ASN:ND2 | 2.47 | 0.47 |
| 1:AG:98:TRP:NE1 | 1:AG:154:GLN:OE1 | 2.42 | 0.47 |
| 2:AP:169:GLU:OE2 | 2:AP:169:GLU:HA | 2.13 | 0.47 |
| 2:AW:170:THR:OG1 | 2:AW:173:ASP:OD1 | 2.32 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BK:60:TYR:HB2 | 2:BL:230:ILE:HG23 | 1.96 | 0.47 |
| 2:BK:201:PHE:CE2 | 2:BL:163:PHE:CE2 | 3.03 | 0.47 |
| 2:CD:204:LEU:HD13 | 2:CD:240:ILE:HD11 | 1.94 | 0.47 |
| 1:CI:154:GLN:HA | 1:CI:154:GLN:OE1 | 2.15 | 0.47 |
| 2:CQ:77:ARG:HH11 | 2:DL:110:ARG:HH21 | 1.63 | 0.47 |
| 1:CS:93:LEU:HB3 | 1:CU:93:LEU:HD13 | 1.96 | 0.47 |
| 2:CW:170:THR:OG1 | 2:CW:173:ASP:OD1 | 2.32 | 0.47 |
| 1:DG:171:MET:CE | 1:DG:174:ARG:CZ | 2.85 | 0.47 |
| 2:DK:124:ILE:HD11 | 2:DK:139:LYS:HD2 | 1.95 | 0.47 |
| 2:DK:201:PHE:CE2 | 2:DL:163:PHE:CE2 | 3.03 | 0.47 |
| 2:AK:60:TYR:HB2 | 2:AL:230:ILE:HG23 | 1.96 | 0.47 |
| 2:AK:201:PHE:CE2 | 2:AL:163:PHE:CE2 | 3.03 | 0.47 |
| 2:BK:124:ILE:HD11 | 2:BK:139:LYS:HD2 | 1.95 | 0.47 |
| 1:BS:61:ASP:OD2 | 1:BS:65:LYS:NZ | 2.46 | 0.47 |
| 1:CI:83:ILE:HD12 | 1:CI:86:LEU:HD12 | 1.95 | 0.47 |
| 2:CK:3:GLN:OE1 | 2:CK:3:GLN:N | 2.38 | 0.47 |
| 1:CO:130:MET:HE2 | 1:CO:130:MET:HB3 | 1.84 | 0.47 |
| 2:CP:51:PHE:HB3 | 2:CQ:230:ILE:HG13 | 1.96 | 0.47 |
| 2:CW:199:LEU:HA | 2:CW:202:TYR:CE1 | 2.50 | 0.47 |
| 2:AL:21:VAL:O | 2:AL:24:ASN:ND2 | 2.47 | 0.47 |
| 1:AS:93:LEU:HD22 | 1:AU:93:LEU:HD22 | 1.97 | 0.47 |
| 2:AX:170:THR:HB | 2:AX:173:ASP:OD1 | 2.15 | 0.47 |
| 2:BX:170:THR:HB | 2:BX:173:ASP:OD1 | 2.15 | 0.47 |
| 1:AB:119:VAL:CG2 | 1:AB:140:GLN:HE21 | 2.26 | 0.47 |
| 2:CX:170:THR:HB | 2:CX:173:ASP:OD1 | 2.15 | 0.47 |
| 1:AU:175:LYS:O | 1:AU:179:SER:OG | 2.21 | 0.47 |
| 1:BI:154:GLN:OE1 | 1:BI:154:GLN:HA | 2.14 | 0.47 |
| 2:BP:51:PHE:HB3 | 2:BQ:230:ILE:HG13 | 1.96 | 0.47 |
| 2:BP:116:LEU:HD12 | 2:BP:142:ILE:CD1 | 2.39 | 0.47 |
| 1:BS:93:LEU:HB3 | 1:BU:93:LEU:HD13 | 1.96 | 0.47 |
| 1:BU:168:PHE:HD2 | 1:BU:175:LYS:HG3 | 1.80 | 0.47 |
| 2:BX:129:VAL:HG22 | 2:BX:171:PRO:HG2 | 1.97 | 0.47 |
| 1:AB:189:LYS:HB3 | 1:AB:189:LYS:HE3 | 1.65 | 0.47 |
| 2:CK:124:ILE:HD11 | 2:CK:139:LYS:HD2 | 1.95 | 0.47 |
| 2:CK:201:PHE:CE2 | 2:CL:163:PHE:CE2 | 3.03 | 0.47 |
| 2:CL:21:VAL:O | 2:CL:24:ASN:ND2 | 2.47 | 0.47 |
| 1:CN:115:ASN:ND2 | 1:CN:117:ARG:HH21 | 2.12 | 0.47 |
| 2:CX:129:VAL:HG22 | 2:CX:171:PRO:HG2 | 1.97 | 0.47 |
| 1:DB:52:THR:HG21 | 1:DC:48:ASP:OD2 | 2.14 | 0.47 |
| 1:DI:154:GLN:OE1 | 1:DI:154:GLN:HA | 2.15 | 0.47 |
| 1:AI:154:GLN:OE1 | 1:AI:154:GLN:HA | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:124:ILE:HD11 | 2:AK:139:LYS:HD2 | 1.95 | 0.47 |
| 2:AP:51:PHE:HB3 | 2:AQ:230:ILE:HG13 | 1.96 | 0.47 |
| 1:AU:168:PHE:HD2 | 1:AU:175:LYS:HG3 | 1.80 | 0.47 |
| 2:BL:21:VAL:O | 2:BL:24:ASN:ND2 | 2.47 | 0.47 |
| 1:BS:20:THR:OG1 | 3:BS:201:Y43:OAR | 2.25 | 0.47 |
| 2:BW:203:LYS:HE3 | 2:BW:203:LYS:HB2 | 1.82 | 0.47 |
| 1:DI:83:ILE:HD12 | 1:DI:86:LEU:HD12 | 1.95 | 0.47 |
| 1:AI:83:ILE:HD12 | 1:AI:86:LEU:HD12 | 1.95 | 0.47 |
| 2:BW:199:LEU:HA | 2:BW:202:TYR:CE1 | 2.50 | 0.47 |
| 1:DC:130:MET:HE1 | 2:DD:43:TYR:CZ | 2.50 | 0.47 |
| 2:AQ:90:LYS:HD3 | 2:AQ:90:LYS:HA | 1.65 | 0.47 |
| 1:AS:89:PHE:CG | 1:AS:90:PRO:HA | 2.50 | 0.47 |
| 1:BU:122:THR:HG23 | 1:BU:180:MET:SD | 2.56 | 0.46 |
| 2:BW:209:LYS:HE2 | 2:BW:238:TRP:CD1 | 2.50 | 0.46 |
| 1:AB:52:THR:HG21 | 1:AC:48:ASP:OD2 | 2.14 | 0.46 |
| 1:CG:51:GLN:HB2 | 1:CI:51:GLN:HG2 | 1.98 | 0.46 |
| 2:CP:148:ASP:OD1 | 2:CP:149:PHE:N | 2.46 | 0.46 |
| 1:CU:168:PHE:HD2 | 1:CU:175:LYS:HG3 | 1.80 | 0.46 |
| 1:DI:23:ARG:NH1 | 1:DI:23:ARG:HB3 | 2.30 | 0.46 |
| 2:DK:60:TYR:HB2 | 2:DL:230:ILE:HG23 | 1.96 | 0.46 |
| 1:AI:19:ILE:CD1 | 1:AI:43:SER:HG | 2.18 | 0.46 |
| 1:AI:86:LEU:HB3 | 1:AI:89:PHE:HB3 | 1.96 | 0.46 |
| 1:AU:122:THR:HG23 | 1:AU:180:MET:SD | 2.56 | 0.46 |
| 2:AW:209:LYS:HE2 | 2:AW:238:TRP:CD1 | 2.50 | 0.46 |
| 1:BG:51:GLN:HB2 | 1:BI:51:GLN:HG2 | 1.98 | 0.46 |
| 1:CI:23:ARG:HB3 | 1:CI:23:ARG:NH1 | 2.30 | 0.46 |
| 2:CK:192:LEU:C | 2:CK:197:ILE:HG12 | 2.32 | 0.46 |
| 1:CU:122:THR:HG23 | 1:CU:180:MET:SD | 2.56 | 0.46 |
| 1:AC:130:MET:HE1 | 2:AD:43:TYR:CZ | 2.50 | 0.46 |
| 1:AI:23:ARG:NH1 | 1:AI:23:ARG:HB3 | 2.31 | 0.46 |
| 1:BS:93:LEU:HD22 | 1:BU:93:LEU:HD22 | 1.97 | 0.46 |
| 1:CG:98:TRP:NE1 | 1:CG:154:GLN:OE1 | 2.43 | 0.46 |
| 1:CI:144:SER:HB3 | 1:CI:160:ILE:HG23 | 1.98 | 0.46 |
| 1:CS:89:PHE:CG | 1:CS:90:PRO:HA | 2.50 | 0.46 |
| 2:CW:209:LYS:HE2 | 2:CW:238:TRP:CD1 | 2.50 | 0.46 |
| 2:DE:212:LYS:HE2 | 2:DE:212:LYS:HB2 | 1.67 | 0.46 |
| 1:BG:98:TRP:NE1 | 1:BG:154:GLN:OE1 | 2.43 | 0.46 |
| 1:BI:23:ARG:HB3 | 1:BI:23:ARG:NH1 | 2.31 | 0.46 |
| 1:BI:86:LEU:HB3 | 1:BI:89:PHE:HB3 | 1.96 | 0.46 |
| 2:BP:159:GLU:HA | 2:BP:162:TYR:CE1 | 2.51 | 0.46 |
| 1:BS:89:PHE:CG | 1:BS:90:PRO:HA | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CD:217:GLN:HB2 | 2:CD:239:ARG:HD3 | 1.97 | 0.46 |
| 1:CG:139:THR:HG23 | 1:CG:180:MET:HB3 | 1.97 | 0.46 |
| 1:DI:144:SER:HB3 | 1:DI:160:ILE:HG23 | 1.98 | 0.46 |
| 1:AG:51:GLN:HB2 | 1:AI:51:GLN:HG2 | 1.98 | 0.46 |
| 2:AK:2:GLU:HG2 | 2:AK:3:GLN:OE1 | 2.16 | 0.46 |
| 1:BN:171:MET:HB2 | 1:BN:174:ARG:HB2 | 1.96 | 0.46 |
| 1:BS:96:ILE:HD12 | 1:BU:93:LEU:HD11 | 1.97 | 0.46 |
| 2:BW:165:ARG:HB3 | 2:BW:200:LEU:HD13 | 1.98 | 0.46 |
| 1:CB:52:THR:HG21 | 1:CC:48:ASP:OD2 | 2.14 | 0.46 |
| 1:CS:93:LEU:HD22 | 1:CU:93:LEU:HD22 | 1.97 | 0.46 |
| 2:CW:165:ARG:HB3 | 2:CW:200:LEU:HD13 | 1.98 | 0.46 |
| 2:DD:217:GLN:HB2 | 2:DD:239:ARG:HD3 | 1.97 | 0.46 |
| 2:DE:3:GLN:OE1 | 2:DE:3:GLN:N | 2.37 | 0.46 |
| 1:DG:51:GLN:HB2 | 1:DI:51:GLN:HG2 | 1.98 | 0.46 |
| 2:DK:258:LEU:O | 2:DK:262:VAL:HG23 | 2.15 | 0.46 |
| 1:AN:180:MET:N | 1:AN:180:MET:SD | 2.89 | 0.46 |
| 2:AX:129:VAL:HG22 | 2:AX:171:PRO:HG2 | 1.97 | 0.46 |
| 1:BI:30:ASN:O | 1:BI:34:SER:OG | 2.27 | 0.46 |
| 1:BI:144:SER:HB3 | 1:BI:160:ILE:HG23 | 1.98 | 0.46 |
| 1:BN:180:MET:N | 1:BN:180:MET:SD | 2.89 | 0.46 |
| 2:BW:152:ASP:OD2 | 2:CD:152:ASP:OD2 | 2.33 | 0.46 |
| 2:BX:156:VAL:HA | 2:BX:161:SER:OG | 2.15 | 0.46 |
| 1:AB:171:MET:SD | 1:AB:171:MET:N | 2.88 | 0.46 |
| 1:CG:25:LYS:NZ | 3:CG:201:Y43:OAO | 2.36 | 0.46 |
| 2:CP:159:GLU:HA | 2:CP:162:TYR:CE1 | 2.51 | 0.46 |
| 2:AD:217:GLN:HB2 | 2:AD:239:ARG:HD3 | 1.97 | 0.46 |
| 2:AL:64:LYS:HD3 | 2:AL:64:LYS:HA | 1.85 | 0.46 |
| 3:AU:201:Y43:OAH | 3:AU:201:Y43:OAA | 2.34 | 0.46 |
| 2:AX:156:VAL:HA | 2:AX:161:SER:OG | 2.15 | 0.46 |
| 2:BK:2:GLU:HG2 | 2:BK:3:GLN:OE1 | 2.16 | 0.46 |
| 1:BO:166:GLU:CG | 1:BO:171:MET:CG | 2.94 | 0.46 |
| 1:AI:144:SER:HB3 | 1:AI:160:ILE:HG23 | 1.98 | 0.46 |
| 2:AL:190:TYR:OH | 2:AL:194:ASP:OD2 | 2.25 | 0.46 |
| 2:AQ:129:VAL:HG22 | 2:AQ:171:PRO:CG | 2.35 | 0.46 |
| 1:AS:96:ILE:HD12 | 1:AU:93:LEU:HD11 | 1.97 | 0.46 |
| 2:AW:199:LEU:HA | 2:AW:202:TYR:CE1 | 2.50 | 0.46 |
| 2:BD:217:GLN:HB2 | 2:BD:239:ARG:HD3 | 1.97 | 0.46 |
| 2:BK:212:LYS:HE2 | 2:BK:212:LYS:HB3 | 1.68 | 0.46 |
| 2:BP:148:ASP:OD1 | 2:BP:149:PHE:N | 2.46 | 0.46 |
| 2:CQ:129:VAL:HG22 | 2:CQ:171:PRO:CG | 2.34 | 0.46 |
| 1:CU:80:GLY:HA2 | 1:CU:94:THR:HG21 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CW:85:ASP:OD1 | 2:CW:87:ASN:N | 2.49 | 0.46 |
| 2:DD:212:LYS:HB2 | 2:DD:212:LYS:HE3 | 1.65 | 0.46 |
| 1:AG:139:THR:HG23 | 1:AG:180:MET:HB3 | 1.97 | 0.46 |
| 1:BI:24:HIS:HB3 | 1:BI:153:PHE:HE1 | 1.81 | 0.46 |
| 1:BU:80:GLY:HA2 | 1:BU:94:THR:HG21 | 1.97 | 0.46 |
| 2:CK:258:LEU:O | 2:CK:262:VAL:HG23 | 2.15 | 0.46 |
| 1:CO:166:GLU:CG | 1:CO:171:MET:CG | 2.94 | 0.46 |
| 2:AP:159:GLU:HA | 2:AP:162:TYR:CE1 | 2.51 | 0.46 |
| 2:AW:165:ARG:HB3 | 2:AW:200:LEU:HD13 | 1.98 | 0.46 |
| 3:BU:201:Y43:OAA | 3:BU:201:Y43:OAH | 2.34 | 0.46 |
| 1:CN:180:MET:N | 1:CN:180:MET:SD | 2.89 | 0.46 |
| 2:AD:81:SER:OG | 2:AD:83:ASP:OD1 | 2.31 | 0.46 |
| 2:AP:148:ASP:OD1 | 2:AP:149:PHE:N | 2.46 | 0.46 |
| 2:BD:90:LYS:HE3 | 2:BD:90:LYS:HB3 | 1.70 | 0.45 |
| 1:BI:124:ILE:HD11 | 1:BI:185:PHE:CE1 | 2.51 | 0.45 |
| 2:CL:129:VAL:HG22 | 2:CL:171:PRO:CG | 2.35 | 0.45 |
| 1:CN:131:LYS:HB2 | 1:CN:131:LYS:HE3 | 1.75 | 0.45 |
| 2:CP:116:LEU:HD12 | 2:CP:142:ILE:CD1 | 2.39 | 0.45 |
| 2:CP:196:ASN:OD1 | 2:CP:197:ILE:HG12 | 2.16 | 0.45 |
| 1:CS:96:ILE:HD12 | 1:CU:93:LEU:HD11 | 1.97 | 0.45 |
| 1:DG:139:THR:HG23 | 1:DG:180:MET:HB3 | 1.97 | 0.45 |
| 1:AO:166:GLU:CG | 1:AO:171:MET:CG | 2.94 | 0.45 |
| 2:AW:85:ASP:OD1 | 2:AW:87:ASN:N | 2.49 | 0.45 |
| 1:BC:48:ASP:OD2 | 1:BB:52:THR:HG21 | 2.14 | 0.45 |
| 2:BK:203:LYS:O | 2:BK:204:LEU:C | 2.58 | 0.45 |
| 2:BK:258:LEU:O | 2:BK:262:VAL:HG23 | 2.15 | 0.45 |
| 2:BW:85:ASP:OD1 | 2:BW:87:ASN:N | 2.49 | 0.45 |
| 1:CB:86:LEU:HB3 | 1:CB:89:PHE:HB3 | 1.99 | 0.45 |
| 1:CS:130:MET:HE2 | 1:CS:130:MET:HB3 | 1.76 | 0.45 |
| 2:DK:203:LYS:O | 2:DK:204:LEU:C | 2.58 | 0.45 |
| 2:AL:208:TRP:CG | 2:AL:217:GLN:HG3 | 2.52 | 0.45 |
| 2:BE:3:GLN:OE1 | 2:BE:3:GLN:N | 2.37 | 0.45 |
| 1:BG:12:SER:OG | 1:BG:13:GLY:N | 2.45 | 0.45 |
| 2:CE:3:GLN:OE1 | 2:CE:3:GLN:N | 2.37 | 0.45 |
| 1:CG:166:GLU:OE2 | 1:CG:171:MET:HG2 | 2.17 | 0.45 |
| 1:CI:24:HIS:HB3 | 1:CI:153:PHE:HE1 | 1.81 | 0.45 |
| 2:CK:2:GLU:HG2 | 2:CK:3:GLN:OE1 | 2.16 | 0.45 |
| 2:CK:203:LYS:HE3 | 2:CK:207:LEU:HD22 | 1.99 | 0.45 |
| 2:CL:208:TRP:CG | 2:CL:217:GLN:HG3 | 2.52 | 0.45 |
| 1:DB:86:LEU:HB3 | 1:DB:89:PHE:HB3 | 1.99 | 0.45 |
| 1:DI:124:ILE:HD11 | 1:DI:185:PHE:CE1 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DK:2:GLU:HG2 | 2:DK:3:GLN:OE1 | 2.16 | 0.45 |
| 2:DL:208:TRP:CG | 2:DL:217:GLN:HG3 | 2.52 | 0.45 |
| 2:AD:68:ILE:HD11 | 2:AD:157:LEU:HD23 | 1.99 | 0.45 |
| 1:AG:166:GLU:OE2 | 1:AG:171:MET:HG2 | 2.17 | 0.45 |
| 2:AK:203:LYS:HE3 | 2:AK:207:LEU:HD22 | 1.99 | 0.45 |
| 1:BG:166:GLU:OE2 | 1:BG:171:MET:HG2 | 2.17 | 0.45 |
| 2:CD:68:ILE:HD11 | 2:CD:157:LEU:HD23 | 1.99 | 0.45 |
| 1:CI:124:ILE:HD11 | 1:CI:185:PHE:CE1 | 2.51 | 0.45 |
| 2:CX:156:VAL:HA | 2:CX:161:SER:OG | 2.15 | 0.45 |
| 2:DL:129:VAL:HG22 | 2:DL:171:PRO:CG | 2.35 | 0.45 |
| 1:AG:136:GLU:OE1 | 1:AG:137:GLY:N | 2.50 | 0.45 |
| 1:AO:59:ILE:HD12 | 1:AO:59:ILE:HA | 1.84 | 0.45 |
| 1:BC:130:MET:HE1 | 2:BD:43:TYR:CZ | 2.50 | 0.45 |
| 2:BD:68:ILE:HD11 | 2:BD:157:LEU:HD23 | 1.99 | 0.45 |
| 2:BE:10:LYS:HA | 2:BE:10:LYS:HD3 | 1.80 | 0.45 |
| 2:BL:217:GLN:O | 2:BL:239:ARG:NH2 | 2.50 | 0.45 |
| 1:BO:20:THR:HG1 | 3:BO:201:Y43:PAQ | 2.39 | 0.45 |
| 1:CB:60:LYS:HE2 | 1:CB:60:LYS:HB2 | 1.74 | 0.45 |
| 1:AI:124:ILE:HD11 | 1:AI:185:PHE:CE1 | 2.51 | 0.45 |
| 1:AO:95:GLN:HG3 | 1:AO:96:ILE:N | 2.32 | 0.45 |
| 1:BC:106:PHE:CE1 | 1:BC:110:LEU:HD12 | 2.51 | 0.45 |
| 1:BG:136:GLU:OE1 | 1:BG:137:GLY:N | 2.50 | 0.45 |
| 1:BS:168:PHE:CE1 | 1:BS:175:LYS:HG3 | 2.52 | 0.45 |
| 1:BU:79:THR:HG23 | 1:BU:122:THR:HG22 | 1.99 | 0.45 |
| 2:BX:55:LEU:HD21 | 2:BX:162:TYR:HE2 | 1.82 | 0.45 |
| 1:CI:171:MET:HE2 | 1:CI:174:ARG:NE | 2.32 | 0.45 |
| 2:CK:5:LEU:O | 2:CK:9:LYS:HG2 | 2.17 | 0.45 |
| 2:CK:203:LYS:O | 2:CK:204:LEU:C | 2.58 | 0.45 |
| 2:DD:68:ILE:HD11 | 2:DD:157:LEU:HD23 | 1.99 | 0.45 |
| 1:AC:73:PRO:HA | 1:AC:127:CYS:O | 2.16 | 0.45 |
| 1:AC:106:PHE:CE1 | 1:AC:110:LEU:HD12 | 2.51 | 0.45 |
| 2:AK:5:LEU:O | 2:AK:9:LYS:HG2 | 2.17 | 0.45 |
| 2:AK:258:LEU:O | 2:AK:262:VAL:HG23 | 2.15 | 0.45 |
| 1:AU:80:GLY:HA2 | 1:AU:94:THR:HG21 | 1.97 | 0.45 |
| 1:BG:139:THR:HG23 | 1:BG:180:MET:HB3 | 1.97 | 0.45 |
| 2:BK:5:LEU:O | 2:BK:9:LYS:HG2 | 2.17 | 0.45 |
| 2:BL:208:TRP:CG | 2:BL:217:GLN:HG3 | 2.52 | 0.45 |
| 1:BN:51:GLN:N | 1:BO:49:GLU:O | 2.40 | 0.45 |
| 1:BO:95:GLN:HG3 | 1:BO:96:ILE:N | 2.32 | 0.45 |
| 1:CG:136:GLU:OE1 | 1:CG:137:GLY:N | 2.50 | 0.45 |
| 1:DC:73:PRO:HA | 1:DC:127:CYS:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DG:98:TRP:NE1 | 1:DG:154:GLN:OE1 | 2.43 | 0.45 |
| 1:DG:166:GLU:OE2 | 1:DG:171:MET:HG2 | 2.17 | 0.45 |
| 2:DL:217:GLN:O | 2:DL:239:ARG:NH2 | 2.50 | 0.45 |
| 2:AX:86:ILE:HD12 | 2:AX:86:ILE:HA | 1.85 | 0.45 |
| 1:BB:70:VAL:HG12 | 1:BB:72:ARG:N | 2.31 | 0.45 |
| 1:BB:171:MET:SD | 1:BB:171:MET:N | 2.88 | 0.45 |
| 1:BU:116:PRO:C | 1:BU:117:ARG:HD2 | 2.42 | 0.45 |
| 1:CS:168:PHE:CE1 | 1:CS:175:LYS:HG3 | 2.52 | 0.45 |
| 3:CU:201:Y43:OAH | 3:CU:201:Y43:OAA | 2.34 | 0.45 |
| 1:DB:189:LYS:HB3 | 1:DB:189:LYS:HE3 | 1.65 | 0.45 |
| 1:DG:136:GLU:OE1 | 1:DG:137:GLY:N | 2.50 | 0.45 |
| 1:AS:81:LEU:HD11 | 1:AS:118:LEU:HD12 | 1.99 | 0.45 |
| 1:AU:79:THR:HG23 | 1:AU:122:THR:HG22 | 1.99 | 0.45 |
| 1:BB:86:LEU:HB3 | 1:BB:89:PHE:HB3 | 1.99 | 0.45 |
| 2:BD:152:ASP:CG | 2:AW:152:ASP:OD2 | 2.60 | 0.45 |
| 1:CO:20:THR:HG1 | 3:CO:201:Y43:PAQ | 2.39 | 0.45 |
| 1:CU:79:THR:HG23 | 1:CU:122:THR:HG22 | 1.99 | 0.45 |
| 1:CU:116:PRO:C | 1:CU:117:ARG:HD2 | 2.42 | 0.45 |
| 2:CW:239:ARG:HE | 2:CW:239:ARG:HB3 | 1.67 | 0.45 |
| 1:DC:182:LYS:HA | 1:DC:182:LYS:HD2 | 1.88 | 0.45 |
| 1:DI:24:HIS:HB3 | 1:DI:153:PHE:HE1 | 1.81 | 0.45 |
| 2:DK:5:LEU:O | 2:DK:9:LYS:HG2 | 2.17 | 0.45 |
| 2:DK:203:LYS:HE3 | 2:DK:207:LEU:HD22 | 1.99 | 0.45 |
| 2:AE:242:MET:HE3 | 2:AE:242:MET:HB3 | 1.92 | 0.45 |
| 1:AI:14:MET:HE2 | 1:AI:14:MET:HB2 | 1.83 | 0.45 |
| 1:AI:171:MET:HE2 | 1:AI:174:ARG:NE | 2.32 | 0.45 |
| 2:AQ:18:GLY:HA3 | 2:AQ:190:TYR:HB2 | 1.99 | 0.45 |
| 1:BC:73:PRO:HA | 1:BC:127:CYS:O | 2.16 | 0.45 |
| 1:AB:164:GLU:HG3 | 1:AB:166:GLU:H | 1.82 | 0.45 |
| 2:CW:226:ARG:HE | 2:CW:226:ARG:HB2 | 1.62 | 0.45 |
| 2:CX:55:LEU:HD21 | 2:CX:162:TYR:HE2 | 1.82 | 0.45 |
| 1:DB:164:GLU:HG3 | 1:DB:166:GLU:H | 1.82 | 0.45 |
| 2:AD:23:MET:SD | 2:AD:24:ASN:N | 2.90 | 0.45 |
| 1:AI:24:HIS:HB3 | 1:AI:153:PHE:HE1 | 1.81 | 0.45 |
| 2:AL:217:GLN:O | 2:AL:239:ARG:NH2 | 2.50 | 0.45 |
| 2:AP:196:ASN:OD1 | 2:AP:197:ILE:HG12 | 2.17 | 0.45 |
| 1:AU:116:PRO:C | 1:AU:117:ARG:HD2 | 2.42 | 0.45 |
| 1:BS:51:GLN:HG2 | 1:BU:93:LEU:CD2 | 2.47 | 0.44 |
| 1:CO:59:ILE:HD12 | 1:CO:59:ILE:HA | 1.84 | 0.44 |
| 1:DC:106:PHE:CE1 | 1:DC:110:LEU:HD12 | 2.51 | 0.44 |
| 2:AK:203:LYS:O | 2:AK:204:LEU:C | 2.58 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AX:65:LYS:HA | 2:AX:65:LYS:HD3 | 1.77 | 0.44 |
| 1:BI:171:MET:HE2 | 1:BI:174:ARG:NE | 2.32 | 0.44 |
| 1:BO:59:ILE:HD12 | 1:BO:59:ILE:HA | 1.84 | 0.44 |
| 2:BP:196:ASN:OD1 | 2:BP:197:ILE:HG12 | 2.17 | 0.44 |
| 1:CC:100:LYS:HD2 | 1:CC:100:LYS:HA | 1.71 | 0.44 |
| 2:CL:217:GLN:O | 2:CL:239:ARG:NH2 | 2.50 | 0.44 |
| 1:CS:84:GLU:H | 1:CS:84:GLU:CD | 2.24 | 0.44 |
| 2:DE:10:LYS:HA | 2:DE:10:LYS:HD3 | 1.81 | 0.44 |
| 2:AK:201:PHE:CE1 | 2:AK:238:TRP:CH2 | 3.06 | 0.44 |
| 1:AS:168:PHE:CE1 | 1:AS:175:LYS:HG3 | 2.52 | 0.44 |
| 1:BC:100:LYS:HD2 | 1:BC:100:LYS:HA | 1.71 | 0.44 |
| 2:BD:23:MET:SD | 2:BD:24:ASN:N | 2.90 | 0.44 |
| 2:BK:201:PHE:CE1 | 2:BK:238:TRP:CH2 | 3.06 | 0.44 |
| 2:CK:201:PHE:CE1 | 2:CK:238:TRP:CH2 | 3.06 | 0.44 |
| 1:CO:95:GLN:HG3 | 1:CO:96:ILE:N | 2.32 | 0.44 |
| 1:CS:81:LEU:HD11 | 1:CS:118:LEU:HD12 | 1.99 | 0.44 |
| 2:DK:201:PHE:CE1 | 2:DK:238:TRP:CH2 | 3.06 | 0.44 |
| 2:AW:226:ARG:HE | 2:AW:226:ARG:HB2 | 1.62 | 0.44 |
| 2:BD:67:LYS:HE2 | 2:BD:67:LYS:HB2 | 1.81 | 0.44 |
| 1:BU:152:ASP:OD1 | 1:BU:152:ASP:N | 2.51 | 0.44 |
| 1:CC:106:PHE:CE1 | 1:CC:110:LEU:HD12 | 2.51 | 0.44 |
| 1:AB:161:PRO:HD3 | 1:AB:168:PHE:HD1 | 1.83 | 0.44 |
| 1:CS:20:THR:OG1 | 3:CS:201:Y43:OAR | 2.25 | 0.44 |
| 1:CU:152:ASP:N | 1:CU:152:ASP:OD1 | 2.51 | 0.44 |
| 2:CX:64:LYS:HA | 2:CX:64:LYS:HD3 | 1.82 | 0.44 |
| 1:DC:106:PHE:C | 1:DC:106:PHE:CD1 | 2.96 | 0.44 |
| 1:BB:165:SER:O | 1:BB:165:SER:OG | 2.33 | 0.44 |
| 2:AE:212:LYS:HB2 | 2:AE:212:LYS:HE2 | 1.67 | 0.44 |
| 1:AS:51:GLN:HG2 | 1:AU:93:LEU:CD2 | 2.47 | 0.44 |
| 1:BB:121:LYS:HB3 | 1:BB:121:LYS:HE3 | 1.79 | 0.44 |
| 1:BB:161:PRO:HD3 | 1:BB:168:PHE:HD1 | 1.83 | 0.44 |
| 1:BB:189:LYS:O | 1:BB:193:LEU:HD13 | 2.18 | 0.44 |
| 1:CB:171:MET:SD | 1:CB:171:MET:N | 2.88 | 0.44 |
| 1:CC:73:PRO:HA | 1:CC:127:CYS:O | 2.16 | 0.44 |
| 1:CC:106:PHE:CD1 | 1:CC:106:PHE:C | 2.96 | 0.44 |
| 1:CC:130:MET:HE1 | 2:CD:43:TYR:CZ | 2.50 | 0.44 |
| 1:AB:165:SER:O | 1:AB:165:SER:OG | 2.33 | 0.44 |
| 1:AB:183:LYS:H | 1:AB:183:LYS:HG3 | 1.60 | 0.44 |
| 1:CN:86:LEU:HD11 | 1:CN:110:LEU:CD1 | 2.48 | 0.44 |
| 2:CQ:252:GLU:H | 2:CQ:252:GLU:HG2 | 1.62 | 0.44 |
| 1:CS:51:GLN:HG2 | 1:CU:93:LEU:CD2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DD:23:MET:SD | 2:DD:24:ASN:N | 2.90 | 0.44 |
| 2:AL:170:THR:OG1 | 2:AL:173:ASP:OD1 | 2.22 | 0.44 |
| 2:AQ:190:TYR:OH | 2:AQ:194:ASP:OD2 | 2.25 | 0.44 |
| 2:BK:197:ILE:HD12 | 2:BK:197:ILE:HA | 1.76 | 0.44 |
| 1:BN:59:ILE:HD12 | 1:BN:59:ILE:HA | 1.83 | 0.44 |
| 1:BN:115:ASN:ND2 | 1:BN:117:ARG:HH21 | 2.12 | 0.44 |
| 2:BQ:18:GLY:HA3 | 2:BQ:190:TYR:HB2 | 1.99 | 0.44 |
| 1:DB:70:VAL:HG12 | 1:DB:72:ARG:N | 2.31 | 0.44 |
| 2:DE:165:ARG:HA | 2:DE:165:ARG:HD2 | 1.87 | 0.44 |
| 2:BK:203:LYS:HE3 | 2:BK:207:LEU:HD22 | 1.99 | 0.44 |
| 1:BS:81:LEU:HD11 | 1:BS:118:LEU:HD12 | 1.99 | 0.44 |
| 1:BS:156:ASP:OD2 | 1:BS:175:LYS:NZ | 2.47 | 0.44 |
| 1:CC:64:LEU:O | 1:CC:68:LYS:HG2 | 2.18 | 0.44 |
| 1:AB:86:LEU:HB3 | 1:AB:89:PHE:HB3 | 1.99 | 0.44 |
| 1:DC:100:LYS:HD2 | 1:DC:100:LYS:HA | 1.71 | 0.44 |
| 2:DD:67:LYS:HE2 | 2:DD:67:LYS:HB2 | 1.81 | 0.44 |
| 2:AP:22:SER:HB3 | 2:AP:27:LEU:HD12 | 2.00 | 0.44 |
| 2:BP:22:SER:HB3 | 2:BP:27:LEU:HD12 | 2.00 | 0.44 |
| 1:CB:189:LYS:O | 1:CB:193:LEU:HD13 | 2.18 | 0.44 |
| 1:AB:64:LEU:HD23 | 1:AB:64:LEU:HA | 1.87 | 0.44 |
| 1:AB:189:LYS:O | 1:AB:193:LEU:HD13 | 2.17 | 0.44 |
| 1:DB:161:PRO:HD3 | 1:DB:168:PHE:HD1 | 1.83 | 0.44 |
| 1:AC:106:PHE:C | 1:AC:106:PHE:CD1 | 2.96 | 0.44 |
| 1:AN:115:ASN:ND2 | 1:AN:117:ARG:HH21 | 2.12 | 0.44 |
| 1:BB:164:GLU:HG3 | 1:BB:166:GLU:H | 1.82 | 0.44 |
| 1:BC:98:TRP:CZ3 | 1:BC:155:TRP:HB3 | 2.53 | 0.43 |
| 1:BN:131:LYS:HB2 | 1:BN:131:LYS:HE3 | 1.75 | 0.43 |
| 1:BO:160:ILE:HG22 | 1:BO:167:THR:HA | 2.01 | 0.43 |
| 1:CB:119:VAL:HG23 | 1:CB:140:GLN:HE21 | 1.83 | 0.43 |
| 2:CD:23:MET:SD | 2:CD:24:ASN:N | 2.90 | 0.43 |
| 2:CD:129:VAL:HB | 2:CD:171:PRO:HG3 | 1.99 | 0.43 |
| 2:CP:22:SER:HB3 | 2:CP:27:LEU:HD12 | 2.00 | 0.43 |
| 2:CQ:18:GLY:HA3 | 2:CQ:190:TYR:HB2 | 1.99 | 0.43 |
| 1:CU:89:PHE:CD2 | 1:CU:90:PRO:HA | 2.53 | 0.43 |
| 1:AC:98:TRP:CZ3 | 1:AC:155:TRP:HB3 | 2.53 | 0.43 |
| 1:DI:171:MET:HE2 | 1:DI:174:ARG:NE | 2.32 | 0.43 |
| 1:AO:29:ILE:HD13 | 1:AO:29:ILE:HA | 1.83 | 0.43 |
| 2:AQ:85:ASP:HB3 | 2:AQ:88:LYS:HG3 | 2.00 | 0.43 |
| 1:BC:64:LEU:O | 1:BC:68:LYS:HG2 | 2.18 | 0.43 |
| 1:CB:93:LEU:HG | 1:CC:51:GLN:HE21 | 1.83 | 0.43 |
| 2:CQ:59:GLU:OE2 | 2:CQ:160:THR:OG1 | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DD:167:GLU:HG3 | 2:DD:169:GLU:HB2 | 2.00 | 0.43 |
| 1:AN:86:LEU:HD11 | 1:AN:110:LEU:CD1 | 2.48 | 0.43 |
| 2:AQ:72:ARG:HE | 2:AQ:72:ARG:HB3 | 1.63 | 0.43 |
| 1:AU:152:ASP:OD1 | 1:AU:152:ASP:N | 2.51 | 0.43 |
| 2:BK:3:GLN:OE1 | 2:BK:3:GLN:N | 2.38 | 0.43 |
| 2:BL:129:VAL:HG22 | 2:BL:171:PRO:CG | 2.35 | 0.43 |
| 1:CB:164:GLU:HG3 | 1:CB:166:GLU:H | 1.82 | 0.43 |
| 2:CD:202:TYR:CE1 | 2:CE:163:PHE:CD1 | 3.06 | 0.43 |
| 1:BB:130:MET:HE2 | 1:BB:130:MET:HB3 | 1.89 | 0.43 |
| 1:BC:106:PHE:CD1 | 1:BC:106:PHE:C | 2.96 | 0.43 |
| 2:BD:64:LYS:HA | 2:BD:64:LYS:HD2 | 1.85 | 0.43 |
| 1:BG:112:THR:O | 1:BG:112:THR:OG1 | 2.31 | 0.43 |
| 1:BN:86:LEU:HD11 | 1:BN:110:LEU:CD1 | 2.48 | 0.43 |
| 2:CK:197:ILE:HA | 2:CK:197:ILE:HD12 | 1.76 | 0.43 |
| 2:CK:212:LYS:HE2 | 2:CK:212:LYS:HB3 | 1.68 | 0.43 |
| 2:CL:64:LYS:HD3 | 2:CL:64:LYS:HA | 1.85 | 0.43 |
| 2:CQ:85:ASP:HB3 | 2:CQ:88:LYS:HG3 | 2.00 | 0.43 |
| 2:DD:90:LYS:HE3 | 2:DD:90:LYS:HB3 | 1.70 | 0.43 |
| 2:AD:53:SER:O | 2:AD:57:LEU:HG | 2.18 | 0.43 |
| 1:AO:160:ILE:HG22 | 1:AO:167:THR:HA | 2.01 | 0.43 |
| 2:AP:18:GLY:HA3 | 2:AP:190:TYR:HB2 | 2.01 | 0.43 |
| 1:AU:89:PHE:CD2 | 1:AU:90:PRO:HA | 2.53 | 0.43 |
| 2:BD:167:GLU:HG3 | 2:BD:169:GLU:HB2 | 2.00 | 0.43 |
| 2:BK:200:LEU:HA | 2:BK:204:LEU:HD12 | 2.01 | 0.43 |
| 1:BN:89:PHE:CG | 1:BN:90:PRO:HA | 2.53 | 0.43 |
| 1:BS:130:MET:HE2 | 1:BS:130:MET:HB3 | 1.76 | 0.43 |
| 2:CD:53:SER:O | 2:CD:57:LEU:HG | 2.18 | 0.43 |
| 1:AB:119:VAL:HG23 | 1:AB:140:GLN:HE21 | 1.84 | 0.43 |
| 2:CK:200:LEU:HA | 2:CK:204:LEU:HD12 | 2.01 | 0.43 |
| 1:CO:160:ILE:HG22 | 1:CO:167:THR:HA | 2.01 | 0.43 |
| 1:CS:144:SER:OG | 1:CS:146:VAL:O | 2.36 | 0.43 |
| 2:DD:81:SER:OG | 2:DD:83:ASP:OD1 | 2.31 | 0.43 |
| 2:DD:129:VAL:HB | 2:DD:171:PRO:HG3 | 2.00 | 0.43 |
| 2:DE:207:LEU:O | 2:DE:211:GLN:HB2 | 2.19 | 0.43 |
| 1:DG:174:ARG:O | 1:DG:178:ILE:HG22 | 2.19 | 0.43 |
| 1:DI:14:MET:HE2 | 1:DI:14:MET:HB2 | 1.83 | 0.43 |
| 2:AD:129:VAL:HB | 2:AD:171:PRO:HG3 | 2.00 | 0.43 |
| 2:AD:167:GLU:HG3 | 2:AD:169:GLU:HB2 | 2.00 | 0.43 |
| 2:AD:202:TYR:CE1 | 2:AE:163:PHE:CD1 | 3.06 | 0.43 |
| 2:BD:81:SER:OG | 2:BD:83:ASP:OD1 | 2.31 | 0.43 |
| 2:BD:129:VAL:HB | 2:BD:171:PRO:HG3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:CB:165:SER:O | 1:CB:165:SER:OG | 2.33 | 0.43 |
| 1:AB:93:LEU:HG | 1:AC:51:GLN:HE21 | 1.84 | 0.43 |
| 1:CG:174:ARG:O | 1:CG:178:ILE:HG22 | 2.19 | 0.43 |
| 2:CQ:72:ARG:HE | 2:CQ:72:ARG:HB3 | 1.63 | 0.43 |
| 2:CW:109:ASP:OD1 | 2:CW:109:ASP:N | 2.51 | 0.43 |
| 1:DB:93:LEU:HG | 1:DC:51:GLN:HE21 | 1.84 | 0.43 |
| 1:DC:98:TRP:CZ3 | 1:DC:155:TRP:HB3 | 2.53 | 0.43 |
| 2:DK:200:LEU:HA | 2:DK:204:LEU:HD12 | 2.01 | 0.43 |
| 2:AK:162:TYR:HD2 | 2:AK:199:LEU:HD13 | 1.83 | 0.43 |
| 2:AL:129:VAL:HG22 | 2:AL:171:PRO:CG | 2.35 | 0.43 |
| 1:AN:28:GLU:OE1 | 1:AN:181:ARG:NH1 | 2.52 | 0.43 |
| 1:AN:89:PHE:CG | 1:AN:90:PRO:HA | 2.53 | 0.43 |
| 2:BP:88:LYS:HE3 | 2:BP:88:LYS:HB2 | 1.80 | 0.43 |
| 2:BQ:252:GLU:H | 2:BQ:252:GLU:HG2 | 1.62 | 0.43 |
| 1:CB:161:PRO:HD3 | 1:CB:168:PHE:HD1 | 1.83 | 0.43 |
| 2:CD:167:GLU:HG3 | 2:CD:169:GLU:HB2 | 2.00 | 0.43 |
| 1:DB:189:LYS:O | 1:DB:193:LEU:HD13 | 2.18 | 0.43 |
| 2:AE:207:LEU:O | 2:AE:211:GLN:HB2 | 2.19 | 0.43 |
| 1:AO:178:ILE:O | 1:AO:183:LYS:NZ | 2.52 | 0.43 |
| 2:BE:207:LEU:O | 2:BE:211:GLN:HB2 | 2.19 | 0.43 |
| 1:BS:93:LEU:HD23 | 1:BU:51:GLN:NE2 | 2.33 | 0.43 |
| 1:BU:128:ASP:O | 1:BU:129:SER:OG | 2.34 | 0.43 |
| 1:CO:29:ILE:HD13 | 1:CO:29:ILE:HA | 1.83 | 0.43 |
| 2:CP:18:GLY:HA3 | 2:CP:190:TYR:HB2 | 2.01 | 0.43 |
| 1:CS:93:LEU:HD23 | 1:CU:51:GLN:NE2 | 2.33 | 0.43 |
| 1:CS:156:ASP:OD2 | 1:CS:175:LYS:NZ | 2.47 | 0.43 |
| 2:AP:88:LYS:HB2 | 2:AP:88:LYS:HE3 | 1.80 | 0.43 |
| 1:AS:156:ASP:OD2 | 1:AS:175:LYS:NZ | 2.47 | 0.43 |
| 1:AS:183:LYS:HE3 | 1:AS:183:LYS:HB3 | 1.79 | 0.43 |
| 2:AW:109:ASP:OD1 | 2:AW:109:ASP:N | 2.51 | 0.43 |
| 1:BC:51:GLN:HE21 | 1:BB:93:LEU:HG | 1.84 | 0.43 |
| 2:BK:192:LEU:C | 2:BK:197:ILE:HG12 | 2.32 | 0.43 |
| 1:BN:25:LYS:NZ | 1:BN:77:GLU:OE2 | 2.36 | 0.43 |
| 1:BO:178:ILE:O | 1:BO:183:LYS:NZ | 2.52 | 0.43 |
| 1:BS:84:GLU:OE2 | 1:BS:84:GLU:N | 2.36 | 0.43 |
| 2:BW:60:TYR:HB2 | 2:BX:230:ILE:HG23 | 2.01 | 0.43 |
| 1:CC:98:TRP:CZ3 | 1:CC:155:TRP:HB3 | 2.53 | 0.43 |
| 1:AB:119:VAL:HG22 | 1:AB:140:GLN:CD | 2.44 | 0.43 |
| 2:CK:162:TYR:HD2 | 2:CK:199:LEU:HD13 | 1.83 | 0.43 |
| 1:CU:98:TRP:CZ3 | 1:CU:155:TRP:HB3 | 2.54 | 0.43 |
| 1:DG:72:ARG:NH2 | 2:DL:245:SER:O | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DK:212:LYS:HB3 | 2:DK:212:LYS:HE2 | 1.67 | 0.43 |
| 2:AD:110:ARG:NH1 | 2:AD:150:ASP:OD1 | 2.50 | 0.43 |
| 2:AK:200:LEU:HA | 2:AK:204:LEU:HD12 | 2.01 | 0.43 |
| 1:AU:98:TRP:CZ3 | 1:AU:155:TRP:HB3 | 2.54 | 0.43 |
| 1:BC:183:LYS:H | 1:BC:183:LYS:HG2 | 1.55 | 0.43 |
| 2:BQ:59:GLU:OE2 | 2:BQ:160:THR:OG1 | 2.36 | 0.43 |
| 1:BU:89:PHE:CD2 | 1:BU:90:PRO:HA | 2.53 | 0.43 |
| 1:CB:189:LYS:HE3 | 1:CB:189:LYS:HB3 | 1.65 | 0.43 |
| 1:AB:121:LYS:HE3 | 1:AB:121:LYS:HB3 | 1.78 | 0.43 |
| 2:CE:212:LYS:HB2 | 2:CE:212:LYS:HE2 | 1.67 | 0.43 |
| 1:DC:144:SER:OG | 1:DC:146:VAL:O | 2.37 | 0.43 |
| 1:AC:64:LEU:O | 1:AC:68:LYS:HG2 | 2.18 | 0.43 |
| 2:DL:72:ARG:HE | 2:DL:155:ILE:HD13 | 1.84 | 0.43 |
| 1:AG:72:ARG:NH2 | 2:AL:245:SER:O | 2.52 | 0.43 |
| 2:AK:55:LEU:HD11 | 2:AK:195:ILE:HG23 | 2.01 | 0.43 |
| 2:AQ:1:MET:SD | 2:AQ:1:MET:N | 2.92 | 0.43 |
| 1:AS:111:GLY:HA3 | 1:AS:145:PRO:HA | 2.01 | 0.43 |
| 1:AU:31:LYS:HE3 | 1:AU:31:LYS:HB2 | 1.84 | 0.43 |
| 1:BB:189:LYS:HE3 | 1:BB:189:LYS:HB3 | 1.65 | 0.43 |
| 2:BD:110:ARG:NH1 | 2:BD:150:ASP:OD1 | 2.50 | 0.42 |
| 2:BL:72:ARG:HE | 2:BL:155:ILE:HD13 | 1.84 | 0.42 |
| 2:BQ:85:ASP:HB3 | 2:BQ:88:LYS:HG3 | 2.00 | 0.42 |
| 1:BS:89:PHE:CD2 | 1:BS:90:PRO:HA | 2.54 | 0.42 |
| 1:BS:144:SER:OG | 1:BS:146:VAL:O | 2.36 | 0.42 |
| 2:BX:64:LYS:HA | 2:BX:64:LYS:HD3 | 1.82 | 0.42 |
| 1:AB:60:LYS:HB2 | 1:AB:60:LYS:HE2 | 1.74 | 0.42 |
| 2:CE:170:THR:OG1 | 2:CE:173:ASP:OD1 | 2.31 | 0.42 |
| 1:CO:178:ILE:O | 1:CO:183:LYS:NZ | 2.52 | 0.42 |
| 1:DC:64:LEU:O | 1:DC:68:LYS:HG2 | 2.18 | 0.42 |
| 2:DD:110:ARG:NH1 | 2:DD:150:ASP:OD1 | 2.50 | 0.42 |
| 2:DD:202:TYR:CE1 | 2:DE:163:PHE:CD1 | 3.06 | 0.42 |
| 1:DG:64:LEU:HD23 | 1:DG:64:LEU:HA | 1.91 | 0.42 |
| 2:DK:162:TYR:HD2 | 2:DK:199:LEU:HD13 | 1.83 | 0.42 |
| 2:AL:85:ASP:OD1 | 2:AL:85:ASP:N | 2.46 | 0.42 |
| 1:AS:93:LEU:HD23 | 1:AU:51:GLN:NE2 | 2.33 | 0.42 |
| 1:BG:174:ARG:O | 1:BG:178:ILE:HG22 | 2.19 | 0.42 |
| 1:BI:98:TRP:CZ3 | 1:BI:155:TRP:HB3 | 2.55 | 0.42 |
| 1:BN:28:GLU:OE1 | 1:BN:181:ARG:NH1 | 2.52 | 0.42 |
| 2:CQ:131:ASP:OD1 | 2:CQ:131:ASP:N | 2.53 | 0.42 |
| 2:DL:192:LEU:HD23 | 2:DL:192:LEU:HA | 1.87 | 0.42 |
| 1:AS:89:PHE:CD2 | 1:AS:90:PRO:HA | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BB:119:VAL:HG22 | 1:BB:140:GLN:CD | 2.44 | 0.42 |
| 1:BG:174:ARG:HA | 1:BG:177:GLU:OE1 | 2.20 | 0.42 |
| 2:BX:144:LYS:H | 2:BX:144:LYS:HG2 | 1.66 | 0.42 |
| 2:CD:110:ARG:NH1 | 2:CD:150:ASP:OD1 | 2.50 | 0.42 |
| 1:CG:72:ARG:NH2 | 2:CL:245:SER:O | 2.52 | 0.42 |
| 1:CG:174:ARG:HA | 1:CG:177:GLU:OE1 | 2.20 | 0.42 |
| 1:CI:98:TRP:CZ3 | 1:CI:155:TRP:HB3 | 2.54 | 0.42 |
| 1:CN:89:PHE:CG | 1:CN:90:PRO:HA | 2.53 | 0.42 |
| 1:DG:174:ARG:HA | 1:DG:177:GLU:OE1 | 2.20 | 0.42 |
| 1:AG:53:GLU:H | 1:AG:53:GLU:HG3 | 1.70 | 0.42 |
| 2:AK:192:LEU:O | 2:AK:197:ILE:HG21 | 2.20 | 0.42 |
| 2:AX:35:ASP:OD1 | 2:AX:36:HIS:N | 2.52 | 0.42 |
| 1:BB:23:ARG:O | 1:BB:27:LYS:HG3 | 2.20 | 0.42 |
| 2:BD:202:TYR:CE1 | 2:BE:163:PHE:CD1 | 3.06 | 0.42 |
| 2:BE:170:THR:OG1 | 2:BE:173:ASP:OD1 | 2.31 | 0.42 |
| 2:BK:54:ALA:HB3 | 2:BK:195:ILE:HD12 | 1.97 | 0.42 |
| 2:BK:162:TYR:HD2 | 2:BK:199:LEU:HD13 | 1.83 | 0.42 |
| 2:BK:192:LEU:O | 2:BK:197:ILE:HG21 | 2.20 | 0.42 |
| 2:BP:18:GLY:HA3 | 2:BP:190:TYR:HB2 | 2.01 | 0.42 |
| 1:BS:84:GLU:H | 1:BS:84:GLU:CD | 2.24 | 0.42 |
| 1:BS:111:GLY:HA3 | 1:BS:145:PRO:HA | 2.01 | 0.42 |
| 1:BU:98:TRP:CZ3 | 1:BU:155:TRP:HB3 | 2.54 | 0.42 |
| 1:BU:175:LYS:O | 1:BU:179:SER:OG | 2.21 | 0.42 |
| 2:BX:15:LEU:HD11 | 2:BX:188:ILE:HG12 | 2.01 | 0.42 |
| 1:CC:144:SER:OG | 1:CC:146:VAL:O | 2.37 | 0.42 |
| 2:CE:207:LEU:O | 2:CE:211:GLN:HB2 | 2.19 | 0.42 |
| 1:CI:100:LYS:HA | 1:CI:100:LYS:HD2 | 1.85 | 0.42 |
| 2:CL:72:ARG:HE | 2:CL:155:ILE:HD13 | 1.84 | 0.42 |
| 1:CS:89:PHE:CD2 | 1:CS:90:PRO:HA | 2.54 | 0.42 |
| 2:CX:15:LEU:HD11 | 2:CX:188:ILE:HG12 | 2.01 | 0.42 |
| 2:DL:206:LYS:HB3 | 2:DL:206:LYS:HE2 | 1.82 | 0.42 |
| 1:AG:174:ARG:HA | 1:AG:177:GLU:OE1 | 2.20 | 0.42 |
| 2:AQ:59:GLU:OE2 | 2:AQ:160:THR:OG1 | 2.36 | 0.42 |
| 1:AU:59:ILE:HD12 | 1:AU:59:ILE:HA | 1.89 | 0.42 |
| 2:AW:60:TYR:HB2 | 2:AX:230:ILE:HG23 | 2.01 | 0.42 |
| 2:AX:15:LEU:HD11 | 2:AX:188:ILE:HG12 | 2.01 | 0.42 |
| 2:AX:55:LEU:HD21 | 2:AX:162:TYR:HE2 | 1.82 | 0.42 |
| 2:BK:55:LEU:HD11 | 2:BK:195:ILE:HG23 | 2.01 | 0.42 |
| 1:BO:32:ILE:HD11 | 1:BO:176:ASN:OD1 | 2.20 | 0.42 |
| 1:BU:59:ILE:HG12 | 1:BU:123:ILE:HG22 | 2.02 | 0.42 |
| 1:BU:150:PRO:HD2 | 1:BU:169:ALA:HB1 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:BX:35:ASP:OD1 | 2:BX:36:HIS:N | 2.52 | 0.42 |
| 1:CU:59:ILE:HG12 | 1:CU:123:ILE:HG22 | 2.02 | 0.42 |
| 1:DB:119:VAL:HG22 | 1:DB:140:GLN:CD | 2.44 | 0.42 |
| 1:DB:183:LYS:H | 1:DB:183:LYS:HG3 | 1.60 | 0.42 |
| 1:DI:98:TRP:CZ3 | 1:DI:155:TRP:HB3 | 2.55 | 0.42 |
| 1:AI:98:TRP:CZ3 | 1:AI:155:TRP:HB3 | 2.55 | 0.42 |
| 1:AS:114:GLU:CD | 1:AS:114:GLU:H | 2.28 | 0.42 |
| 1:AU:59:ILE:HG12 | 1:AU:123:ILE:HG22 | 2.02 | 0.42 |
| 2:AW:212:LYS:HB2 | 2:AW:212:LYS:HE2 | 1.80 | 0.42 |
| 2:BD:53:SER:O | 2:BD:57:LEU:HG | 2.18 | 0.42 |
| 1:BG:59:ILE:HD12 | 1:BG:59:ILE:HA | 1.90 | 0.42 |
| 1:BI:14:MET:HE2 | 1:BI:14:MET:HB2 | 1.83 | 0.42 |
| 2:BK:212:LYS:HB2 | 2:BK:214:GLU:H | 1.85 | 0.42 |
| 2:BX:224:LEU:HD23 | 2:BX:224:LEU:HA | 1.82 | 0.42 |
| 2:CD:90:LYS:HB3 | 2:CD:90:LYS:HE3 | 1.70 | 0.42 |
| 2:CE:10:LYS:HD3 | 2:CE:10:LYS:HA | 1.80 | 0.42 |
| 1:CO:32:ILE:HD11 | 1:CO:176:ASN:OD1 | 2.20 | 0.42 |
| 1:CS:114:GLU:CD | 1:CS:114:GLU:H | 2.27 | 0.42 |
| 2:CX:35:ASP:OD1 | 2:CX:36:HIS:N | 2.52 | 0.42 |
| 1:DB:119:VAL:HG23 | 1:DB:140:GLN:HE21 | 1.83 | 0.42 |
| 1:DC:183:LYS:H | 1:DC:183:LYS:HG2 | 1.55 | 0.42 |
| 1:AC:79:THR:OG1 | 3:AC:201:Y43:OAK | 2.34 | 0.42 |
| 2:DK:55:LEU:HD11 | 2:DK:195:ILE:HG23 | 2.01 | 0.42 |
| 1:AU:150:PRO:HD2 | 1:AU:169:ALA:HB1 | 2.02 | 0.42 |
| 1:BG:72:ARG:NH2 | 2:BL:245:SER:O | 2.52 | 0.42 |
| 2:BL:64:LYS:HD3 | 2:BL:64:LYS:HA | 1.85 | 0.42 |
| 2:BQ:131:ASP:N | 2:BQ:131:ASP:OD1 | 2.53 | 0.42 |
| 1:AB:29:ILE:HD13 | 1:AB:29:ILE:HA | 1.93 | 0.42 |
| 1:CN:28:GLU:OE1 | 1:CN:181:ARG:NH1 | 2.52 | 0.42 |
| 1:CO:105:LYS:HE3 | 1:CO:105:LYS:HB2 | 1.94 | 0.42 |
| 1:DB:23:ARG:O | 1:DB:27:LYS:HG3 | 2.19 | 0.42 |
| 1:DB:171:MET:SD | 1:DB:171:MET:N | 2.88 | 0.42 |
| 1:AN:25:LYS:NZ | 1:AN:77:GLU:OE2 | 2.36 | 0.42 |
| 1:AO:32:ILE:HD11 | 1:AO:176:ASN:OD1 | 2.20 | 0.42 |
| 1:AS:73:PRO:HA | 1:AS:127:CYS:O | 2.20 | 0.42 |
| 1:BC:144:SER:OG | 1:BC:146:VAL:O | 2.37 | 0.42 |
| 2:BE:224:LEU:HD12 | 2:BE:242:MET:SD | 2.60 | 0.42 |
| 2:BQ:53:SER:O | 2:BQ:57:LEU:HG | 2.20 | 0.42 |
| 1:CB:23:ARG:O | 1:CB:27:LYS:HG3 | 2.20 | 0.42 |
| 2:CD:196:ASN:N | 2:CD:196:ASN:OD1 | 2.53 | 0.42 |
| 2:CK:201:PHE:CE2 | 2:CL:159:GLU:HG2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:CK:212:LYS:HB2 | 2:CK:214:GLU:H | 1.85 | 0.42 |
| 2:CQ:213:LEU:O | 2:CQ:217:GLN:HG2 | 2.20 | 0.42 |
| 1:CS:62:LYS:NZ | 3:CS:201:Y43:OAS | 2.46 | 0.42 |
| 1:CS:73:PRO:HA | 1:CS:127:CYS:O | 2.20 | 0.42 |
| 2:DD:53:SER:O | 2:DD:57:LEU:HG | 2.18 | 0.42 |
| 1:AO:122:THR:HG21 | 1:AO:181:ARG:HD2 | 2.01 | 0.42 |
| 1:AU:139:THR:OG1 | 1:AU:180:MET:HB2 | 2.20 | 0.42 |
| 2:AW:224:LEU:HD23 | 2:AW:224:LEU:HA | 1.85 | 0.42 |
| 2:BK:201:PHE:CE2 | 2:BL:159:GLU:HG2 | 2.55 | 0.42 |
| 1:BO:122:THR:HG21 | 1:BO:181:ARG:HD2 | 2.01 | 0.42 |
| 2:BW:212:LYS:HE2 | 2:BW:212:LYS:HB2 | 1.79 | 0.42 |
| 1:CB:119:VAL:HG22 | 1:CB:140:GLN:CD | 2.44 | 0.42 |
| 2:CD:212:LYS:HB2 | 2:CD:212:LYS:HE3 | 1.65 | 0.42 |
| 2:CD:247:ASN:OD1 | 2:CD:247:ASN:C | 2.63 | 0.42 |
| 2:CK:192:LEU:O | 2:CK:197:ILE:HG21 | 2.20 | 0.42 |
| 2:CL:67:LYS:HB3 | 2:CL:67:LYS:HE3 | 1.83 | 0.42 |
| 2:CW:203:LYS:HE3 | 2:CW:203:LYS:HB2 | 1.82 | 0.42 |
| 2:DD:247:ASN:OD1 | 2:DD:247:ASN:C | 2.63 | 0.42 |
| 1:DI:100:LYS:HD2 | 1:DI:100:LYS:HA | 1.84 | 0.42 |
| 2:DK:64:LYS:HA | 2:DK:64:LYS:HD2 | 1.91 | 0.42 |
| 2:AD:212:LYS:HB2 | 2:AD:212:LYS:HE3 | 1.66 | 0.42 |
| 2:AD:247:ASN:OD1 | 2:AD:247:ASN:C | 2.63 | 0.42 |
| 1:AG:174:ARG:O | 1:AG:178:ILE:HG22 | 2.19 | 0.42 |
| 2:AK:201:PHE:CE2 | 2:AL:159:GLU:HG2 | 2.55 | 0.42 |
| 1:AS:144:SER:OG | 1:AS:146:VAL:O | 2.36 | 0.42 |
| 1:BB:29:ILE:HD13 | 1:BB:29:ILE:HA | 1.93 | 0.42 |
| 2:BD:247:ASN:OD1 | 2:BD:247:ASN:C | 2.63 | 0.42 |
| 2:BE:165:ARG:HD2 | 2:BE:165:ARG:HA | 1.87 | 0.42 |
| 1:BI:115:ASN:HD21 | 1:BI:117:ARG:HH11 | 1.68 | 0.42 |
| 2:BQ:217:GLN:HA | 2:BQ:218:PRO:HD3 | 1.95 | 0.42 |
| 1:BS:114:GLU:H | 1:BS:114:GLU:CD | 2.27 | 0.42 |
| 1:CI:115:ASN:HD21 | 1:CI:117:ARG:HH11 | 1.68 | 0.42 |
| 1:CO:122:THR:HG21 | 1:CO:181:ARG:HD2 | 2.01 | 0.42 |
| 1:CS:111:GLY:HA3 | 1:CS:145:PRO:HA | 2.01 | 0.42 |
| 1:CS:167:THR:HG23 | 1:CS:169:ALA:H | 1.85 | 0.42 |
| 1:AC:100:LYS:HD2 | 1:AC:100:LYS:HA | 1.71 | 0.42 |
| 1:DG:59:ILE:HD12 | 1:DG:59:ILE:HA | 1.90 | 0.42 |
| 1:DI:98:TRP:CH2 | 1:DI:155:TRP:HB3 | 2.55 | 0.42 |
| 1:DI:160:ILE:HG22 | 1:DI:167:THR:HA | 2.02 | 0.42 |
| 2:DK:54:ALA:HB3 | 2:DK:195:ILE:HD12 | 1.97 | 0.42 |
| 2:DK:201:PHE:CE2 | 2:DL:159:GLU:HG2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AD:64:LYS:HA | 2:AD:64:LYS:HD2 | 1.85 | 0.42 |
| 2:AK:212:LYS:HB2 | 2:AK:214:GLU:H | 1.85 | 0.42 |
| 2:BD:212:LYS:HB2 | 2:BD:212:LYS:HE3 | 1.66 | 0.41 |
| 2:BK:55:LEU:CD1 | 2:BK:195:ILE:HG23 | 2.50 | 0.41 |
| 2:BW:109:ASP:N | 2:BW:109:ASP:OD1 | 2.51 | 0.41 |
| 1:AB:70:VAL:HG12 | 1:AB:72:ARG:N | 2.31 | 0.41 |
| 2:CE:199:LEU:HD23 | 2:CE:199:LEU:HA | 1.92 | 0.41 |
| 2:CE:224:LEU:HD12 | 2:CE:242:MET:SD | 2.60 | 0.41 |
| 1:CI:14:MET:HE2 | 1:CI:14:MET:HB2 | 1.83 | 0.41 |
| 1:CI:89:PHE:CG | 1:CI:90:PRO:HA | 2.55 | 0.41 |
| 1:CU:73:PRO:HA | 1:CU:127:CYS:O | 2.20 | 0.41 |
| 1:CU:150:PRO:HD2 | 1:CU:169:ALA:HB1 | 2.02 | 0.41 |
| 2:DE:86:ILE:HD12 | 2:DE:86:ILE:HA | 1.88 | 0.41 |
| 2:AD:2:GLU:H | 2:AD:2:GLU:HG2 | 1.69 | 0.41 |
| 2:AE:224:LEU:HD12 | 2:AE:242:MET:SD | 2.60 | 0.41 |
| 2:AL:72:ARG:HE | 2:AL:155:ILE:HD13 | 1.84 | 0.41 |
| 2:BL:18:GLY:HA3 | 2:BL:190:TYR:HB2 | 2.03 | 0.41 |
| 2:BW:166:LEU:HD21 | 2:BW:199:LEU:HG | 2.03 | 0.41 |
| 1:CC:150:PRO:HD2 | 1:CC:168:PHE:CE1 | 2.56 | 0.41 |
| 1:AB:23:ARG:O | 1:AB:27:LYS:HG3 | 2.19 | 0.41 |
| 2:CE:86:ILE:HD12 | 2:CE:86:ILE:HA | 1.88 | 0.41 |
| 2:CE:165:ARG:HA | 2:CE:165:ARG:HD2 | 1.87 | 0.41 |
| 1:CI:98:TRP:CH2 | 1:CI:155:TRP:HB3 | 2.55 | 0.41 |
| 1:CI:112:THR:O | 1:CI:112:THR:OG1 | 2.34 | 0.41 |
| 2:CK:55:LEU:CD1 | 2:CK:195:ILE:HG23 | 2.50 | 0.41 |
| 1:DC:89:PHE:CG | 1:DC:90:PRO:HA | 2.55 | 0.41 |
| 1:DC:150:PRO:HD2 | 1:DC:168:PHE:CE1 | 2.56 | 0.41 |
| 1:AC:89:PHE:CG | 1:AC:90:PRO:HA | 2.56 | 0.41 |
| 2:DK:192:LEU:O | 2:DK:197:ILE:HG21 | 2.20 | 0.41 |
| 2:DL:65:LYS:HA | 2:DL:65:LYS:HD3 | 1.82 | 0.41 |
| 2:AP:87:ASN:OD1 | 2:AP:118:ASN:ND2 | 2.49 | 0.41 |
| 2:AQ:252:GLU:H | 2:AQ:252:GLU:HG2 | 1.62 | 0.41 |
| 2:BQ:213:LEU:O | 2:BQ:217:GLN:HG2 | 2.20 | 0.41 |
| 2:CD:60:TYR:CG | 2:CE:230:ILE:HG12 | 2.55 | 0.41 |
| 1:CG:53:GLU:H | 1:CG:53:GLU:HG3 | 1.70 | 0.41 |
| 1:CS:25:LYS:HE3 | 1:CS:77:GLU:OE1 | 2.21 | 0.41 |
| 1:CU:139:THR:OG1 | 1:CU:180:MET:HB2 | 2.20 | 0.41 |
| 2:DE:224:LEU:HD12 | 2:DE:242:MET:SD | 2.60 | 0.41 |
| 1:AC:144:SER:OG | 1:AC:146:VAL:O | 2.37 | 0.41 |
| 2:DK:212:LYS:HB2 | 2:DK:214:GLU:H | 1.85 | 0.41 |
| 2:AD:196:ASN:OD1 | 2:AD:196:ASN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AI:98:TRP:CH2 | 1:AI:155:TRP:HB3 | 2.55 | 0.41 |
| 2:AQ:213:LEU:O | 2:AQ:217:GLN:HG2 | 2.20 | 0.41 |
| 1:AU:73:PRO:HB3 | 1:AU:128:ASP:HA | 2.02 | 0.41 |
| 1:BB:183:LYS:H | 1:BB:183:LYS:HG3 | 1.60 | 0.41 |
| 1:BC:150:PRO:HD2 | 1:BC:168:PHE:CE1 | 2.56 | 0.41 |
| 2:BD:60:TYR:CG | 2:BE:230:ILE:HG12 | 2.55 | 0.41 |
| 1:BS:25:LYS:HE3 | 1:BS:77:GLU:OE1 | 2.21 | 0.41 |
| 1:BU:139:THR:OG1 | 1:BU:180:MET:HB2 | 2.20 | 0.41 |
| 2:BW:144:LYS:HE3 | 2:BW:144:LYS:HB3 | 1.90 | 0.41 |
| 1:CC:89:PHE:CG | 1:CC:90:PRO:HA | 2.56 | 0.41 |
| 1:CI:31:LYS:HB2 | 1:CI:31:LYS:HE3 | 1.85 | 0.41 |
| 1:CN:128:ASP:O | 1:CN:129:SER:OG | 2.36 | 0.41 |
| 1:CN:154:GLN:HB2 | 1:CN:155:TRP:H | 1.67 | 0.41 |
| 2:CP:96:ALA:HA | 2:CP:116:LEU:CD2 | 2.51 | 0.41 |
| 1:DI:63:LEU:HD23 | 1:DI:132:ILE:HG23 | 2.02 | 0.41 |
| 1:DI:115:ASN:HD21 | 1:DI:117:ARG:HH11 | 1.68 | 0.41 |
| 1:AI:160:ILE:HG22 | 1:AI:167:THR:HA | 2.02 | 0.41 |
| 2:AK:55:LEU:CD1 | 2:AK:195:ILE:HG23 | 2.50 | 0.41 |
| 1:AO:20:THR:HG1 | 3:AO:201:Y43:PAQ | 2.42 | 0.41 |
| 2:AQ:53:SER:O | 2:AQ:57:LEU:HG | 2.20 | 0.41 |
| 1:AS:25:LYS:HE3 | 1:AS:77:GLU:OE1 | 2.21 | 0.41 |
| 1:AS:167:THR:HG23 | 1:AS:169:ALA:H | 1.85 | 0.41 |
| 1:BC:128:ASP:O | 1:BC:129:SER:OG | 2.35 | 0.41 |
| 2:BD:196:ASN:N | 2:BD:196:ASN:OD1 | 2.53 | 0.41 |
| 2:BE:3:GLN:NE2 | 2:BE:221:TYR:OH | 2.54 | 0.41 |
| 2:BK:55:LEU:HD23 | 2:BK:195:ILE:HG21 | 1.94 | 0.41 |
| 2:CE:3:GLN:NE2 | 2:CE:221:TYR:OH | 2.54 | 0.41 |
| 1:CI:160:ILE:HG22 | 1:CI:167:THR:HA | 2.02 | 0.41 |
| 2:CL:18:GLY:HA3 | 2:CL:190:TYR:HB2 | 2.02 | 0.41 |
| 2:CP:88:LYS:HE3 | 2:CP:88:LYS:HB2 | 1.80 | 0.41 |
| 2:CW:166:LEU:HD21 | 2:CW:199:LEU:HG | 2.02 | 0.41 |
| 2:DE:242:MET:HE3 | 2:DE:242:MET:HB3 | 1.92 | 0.41 |
| 1:AC:150:PRO:HD2 | 1:AC:168:PHE:CE1 | 2.55 | 0.41 |
| 2:AK:54:ALA:HB3 | 2:AK:195:ILE:HD12 | 1.97 | 0.41 |
| 2:AL:90:LYS:HA | 2:AL:90:LYS:HD3 | 1.89 | 0.41 |
| 1:AN:131:LYS:HE3 | 1:AN:131:LYS:HB2 | 1.75 | 0.41 |
| 1:AO:64:LEU:HD23 | 1:AO:64:LEU:HA | 1.88 | 0.41 |
| 2:AP:96:ALA:HA | 2:AP:116:LEU:CD2 | 2.50 | 0.41 |
| 1:AS:191:TYR:CD1 | 1:AS:191:TYR:C | 2.99 | 0.41 |
| 1:BG:192:LEU:HD12 | 1:BG:192:LEU:HA | 1.85 | 0.41 |
| 1:BS:62:LYS:NZ | 3:BS:201:Y43:OAS | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BU:73:PRO:HB3 | 1:BU:128:ASP:HA | 2.02 | 0.41 |
| 1:BU:73:PRO:HA | 1:BU:127:CYS:O | 2.20 | 0.41 |
| 1:CU:49:GLU:N | 1:CU:49:GLU:OE1 | 2.54 | 0.41 |
| 2:CW:60:TYR:HB2 | 2:CX:230:ILE:HG23 | 2.01 | 0.41 |
| 2:DE:3:GLN:NE2 | 2:DE:221:TYR:OH | 2.54 | 0.41 |
| 1:AC:182:LYS:HA | 1:AC:182:LYS:HD2 | 1.88 | 0.41 |
| 2:DK:53:SER:O | 2:DK:57:LEU:HG | 2.21 | 0.41 |
| 1:AI:89:PHE:CG | 1:AI:90:PRO:HA | 2.56 | 0.41 |
| 1:AI:115:ASN:HD21 | 1:AI:117:ARG:HH11 | 1.68 | 0.41 |
| 2:AK:197:ILE:HA | 2:AK:197:ILE:HD12 | 1.76 | 0.41 |
| 1:AN:100:LYS:HD3 | 1:AN:100:LYS:HA | 1.88 | 0.41 |
| 1:AU:73:PRO:HA | 1:AU:127:CYS:O | 2.20 | 0.41 |
| 1:BC:89:PHE:CG | 1:BC:90:PRO:HA | 2.56 | 0.41 |
| 1:BI:63:LEU:HD23 | 1:BI:132:ILE:HG23 | 2.02 | 0.41 |
| 1:BI:89:PHE:CG | 1:BI:90:PRO:HA | 2.56 | 0.41 |
| 2:BK:53:SER:O | 2:BK:57:LEU:HG | 2.21 | 0.41 |
| 1:BS:167:THR:HG23 | 1:BS:169:ALA:H | 1.85 | 0.41 |
| 1:BS:191:TYR:CD1 | 1:BS:191:TYR:C | 2.99 | 0.41 |
| 1:BU:49:GLU:OE1 | 1:BU:49:GLU:N | 2.54 | 0.41 |
| 1:CS:191:TYR:CD1 | 1:CS:191:TYR:C | 2.99 | 0.41 |
| 2:DD:215:GLU:H | 2:DD:215:GLU:HG3 | 1.69 | 0.41 |
| 1:AC:70:VAL:HG12 | 1:AC:72:ARG:N | 2.32 | 0.41 |
| 1:DI:89:PHE:CG | 1:DI:90:PRO:HA | 2.56 | 0.41 |
| 1:AI:63:LEU:HD23 | 1:AI:132:ILE:HG23 | 2.02 | 0.41 |
| 2:AK:53:SER:O | 2:AK:57:LEU:HG | 2.21 | 0.41 |
| 2:AK:55:LEU:HD23 | 2:AK:195:ILE:HG21 | 1.95 | 0.41 |
| 2:AW:166:LEU:HD21 | 2:AW:199:LEU:HG | 2.02 | 0.41 |
| 2:BD:76:ASP:OD2 | 2:AW:73:SER:OG | 2.24 | 0.41 |
| 2:BQ:150:ASP:O | 2:CL:67:LYS:NZ | 2.53 | 0.41 |
| 2:CP:196:ASN:OD1 | 2:CP:197:ILE:N | 2.54 | 0.41 |
| 1:DB:64:LEU:HD23 | 1:DB:64:LEU:HA | 1.87 | 0.41 |
| 2:DD:196:ASN:OD1 | 2:DD:196:ASN:N | 2.53 | 0.41 |
| 2:DD:214:GLU:HA | 2:DD:217:GLN:HG3 | 2.02 | 0.41 |
| 2:DK:55:LEU:HD23 | 2:DK:195:ILE:HG21 | 1.94 | 0.41 |
| 2:DK:55:LEU:CD1 | 2:DK:195:ILE:HG23 | 2.50 | 0.41 |
| 2:DL:18:GLY:HA3 | 2:DL:190:TYR:HB2 | 2.02 | 0.41 |
| 2:AD:60:TYR:CG | 2:AE:230:ILE:HG12 | 2.55 | 0.41 |
| 2:AE:3:GLN:NE2 | 2:AE:221:TYR:OH | 2.54 | 0.41 |
| 1:AI:183:LYS:H | 1:AI:183:LYS:HG3 | 1.65 | 0.41 |
| 1:AS:90:PRO:HB2 | 1:AS:94:THR:CG2 | 2.44 | 0.41 |
| 1:AU:49:GLU:OE1 | 1:AU:49:GLU:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:BC:167:THR:HG23 | 1:BC:169:ALA:H | 1.85 | 0.41 |
| 1:BI:59:ILE:HD12 | 1:BI:59:ILE:HA | 1.89 | 0.41 |
| 2:BP:167:GLU:H | 2:BP:167:GLU:HG2 | 1.70 | 0.41 |
| 2:BQ:194:ASP:O | 2:BQ:198:ARG:HG3 | 2.21 | 0.41 |
| 1:BS:73:PRO:HA | 1:BS:127:CYS:O | 2.20 | 0.41 |
| 1:BS:82:TYR:CD1 | 1:BS:91:GLY:HA2 | 2.56 | 0.41 |
| 2:BW:53:SER:O | 2:BW:57:LEU:HG | 2.20 | 0.41 |
| 2:BW:213:LEU:C | 2:BW:217:GLN:HG3 | 2.46 | 0.41 |
| 1:CI:63:LEU:HD23 | 1:CI:132:ILE:HG23 | 2.02 | 0.41 |
| 2:CK:55:LEU:HD11 | 2:CK:195:ILE:HG23 | 2.01 | 0.41 |
| 2:CL:190:TYR:OH | 2:CL:194:ASP:OD2 | 2.25 | 0.41 |
| 2:CQ:53:SER:O | 2:CQ:57:LEU:HG | 2.20 | 0.41 |
| 2:CQ:194:ASP:O | 2:CQ:198:ARG:HG3 | 2.21 | 0.41 |
| 2:CW:53:SER:O | 2:CW:57:LEU:HG | 2.20 | 0.41 |
| 1:DI:59:ILE:HD12 | 1:DI:59:ILE:HA | 1.89 | 0.41 |
| 2:AD:148:ASP:OD1 | 2:AD:149:PHE:N | 2.50 | 0.41 |
| 1:AI:79:THR:HG21 | 3:AI:201:Y43:C8 | 2.51 | 0.41 |
| 2:AQ:194:ASP:O | 2:AQ:198:ARG:HG3 | 2.21 | 0.41 |
| 2:BD:88:LYS:HA | 2:BD:88:LYS:HD3 | 1.97 | 0.41 |
| 2:BP:98:ALA:O | 2:BP:121:LYS:NZ | 2.54 | 0.41 |
| 1:CG:81:LEU:HD21 | 1:CG:155:TRP:CH2 | 2.56 | 0.41 |
| 2:CP:87:ASN:OD1 | 2:CP:118:ASN:ND2 | 2.49 | 0.41 |
| 1:CS:106:PHE:CE1 | 1:CS:110:LEU:HD12 | 2.56 | 0.41 |
| 1:DC:128:ASP:O | 1:DC:129:SER:OG | 2.35 | 0.41 |
| 2:DD:60:TYR:CG | 2:DE:230:ILE:HG12 | 2.55 | 0.41 |
| 2:DD:148:ASP:OD1 | 2:DD:149:PHE:N | 2.50 | 0.41 |
| 1:AC:167:THR:HG23 | 1:AC:169:ALA:H | 1.85 | 0.41 |
| 2:DK:55:LEU:CD1 | 2:DK:195:ILE:CG2 | 2.99 | 0.41 |
| 2:DL:66:GLY:O | 2:DL:67:LYS:CD | 2.68 | 0.41 |
| 2:DL:66:GLY:O | 2:DL:67:LYS:HG2 | 2.21 | 0.41 |
| 2:AW:53:SER:O | 2:AW:57:LEU:HG | 2.20 | 0.41 |
| 2:BK:55:LEU:CD1 | 2:BK:195:ILE:CG2 | 2.99 | 0.40 |
| 2:BP:196:ASN:OD1 | 2:BP:197:ILE:N | 2.54 | 0.40 |
| 2:CE:198:ARG:NH1 | 2:CE:234:ILE:HG21 | 2.37 | 0.40 |
| 1:CN:100:LYS:HD3 | 1:CN:100:LYS:HA | 1.88 | 0.40 |
| 1:CO:25:LYS:O | 1:CO:29:ILE:HG12 | 2.22 | 0.40 |
| 1:CO:131:LYS:HB2 | 1:CO:131:LYS:HE3 | 1.86 | 0.40 |
| 2:CQ:55:LEU:HD23 | 2:CQ:159:GLU:HA | 2.04 | 0.40 |
| 2:CQ:166:LEU:HD23 | 2:CQ:166:LEU:HA | 1.92 | 0.40 |
| 2:CW:213:LEU:C | 2:CW:217:GLN:HG3 | 2.46 | 0.40 |
| 2:DK:86:ILE:HD12 | 2:DK:86:ILE:HA | 1.92 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:AO:25:LYS:O | 1:AO:29:ILE:HG12 | 2.22 | 0.40 |
| 2:AQ:55:LEU:HD23 | 2:AQ:159:GLU:HA | 2.03 | 0.40 |
| 2:AQ:131:ASP:OD1 | 2:AQ:131:ASP:N | 2.53 | 0.40 |
| 1:AU:116:PRO:O | 1:AU:117:ARG:HD2 | 2.21 | 0.40 |
| 1:BG:81:LEU:HD21 | 1:BG:155:TRP:CH2 | 2.56 | 0.40 |
| 2:CD:158:ASP:OD1 | 2:CD:158:ASP:N | 2.43 | 0.40 |
| 1:CG:59:ILE:HD12 | 1:CG:59:ILE:HA | 1.90 | 0.40 |
| 1:CS:82:TYR:CD1 | 1:CS:91:GLY:HA2 | 2.56 | 0.40 |
| 1:DI:79:THR:HG21 | 3:DI:201:Y43:C8 | 2.51 | 0.40 |
| 1:AG:81:LEU:HD21 | 1:AG:155:TRP:CH2 | 2.56 | 0.40 |
| 1:AI:95:GLN:HG3 | 1:AI:96:ILE:N | 2.36 | 0.40 |
| 2:AP:98:ALA:O | 2:AP:121:LYS:NZ | 2.54 | 0.40 |
| 1:AS:49:GLU:O | 1:AU:51:GLN:N | 2.53 | 0.40 |
| 1:BG:64:LEU:HD23 | 1:BG:64:LEU:HA | 1.91 | 0.40 |
| 1:BI:95:GLN:HG3 | 1:BI:96:ILE:N | 2.36 | 0.40 |
| 2:BQ:55:LEU:HD23 | 2:BQ:159:GLU:HA | 2.04 | 0.40 |
| 2:BW:224:LEU:HD23 | 2:BW:224:LEU:HA | 1.85 | 0.40 |
| 2:CD:148:ASP:OD1 | 2:CD:149:PHE:N | 2.49 | 0.40 |
| 2:CK:201:PHE:CD2 | 2:CL:163:PHE:CE2 | 3.09 | 0.40 |
| 2:CP:98:ALA:O | 2:CP:121:LYS:NZ | 2.54 | 0.40 |
| 1:CS:183:LYS:HE3 | 1:CS:183:LYS:HB3 | 1.79 | 0.40 |
| 1:CU:31:LYS:HE3 | 1:CU:31:LYS:HB2 | 1.84 | 0.40 |
| 1:DB:31:LYS:HB2 | 1:DB:31:LYS:HE3 | 1.78 | 0.40 |
| 2:DL:242:MET:HE2 | 2:DL:242:MET:HB3 | 2.00 | 0.40 |
| 2:AD:67:LYS:HE2 | 2:AD:67:LYS:HB2 | 1.81 | 0.40 |
| 2:AP:196:ASN:OD1 | 2:AP:197:ILE:N | 2.54 | 0.40 |
| 2:AW:144:LYS:HE3 | 2:AW:144:LYS:HB3 | 1.90 | 0.40 |
| 2:BE:53:SER:O | 2:BE:57:LEU:HG | 2.22 | 0.40 |
| 2:BE:198:ARG:NH1 | 2:BE:234:ILE:HG21 | 2.37 | 0.40 |
| 1:BI:160:ILE:HG22 | 1:BI:167:THR:HA | 2.02 | 0.40 |
| 1:BO:29:ILE:HD13 | 1:BO:29:ILE:HA | 1.83 | 0.40 |
| 2:BP:96:ALA:HA | 2:BP:116:LEU:CD2 | 2.51 | 0.40 |
| 1:AB:191:TYR:O | 1:AB:194:GLU:HG3 | 2.22 | 0.40 |
| 1:CI:79:THR:HG21 | 3:CI:201:Y43:C8 | 2.51 | 0.40 |
| 2:CK:53:SER:O | 2:CK:57:LEU:HG | 2.21 | 0.40 |
| 2:CW:194:ASP:OD1 | 2:CW:194:ASP:N | 2.55 | 0.40 |
| 2:CW:224:LEU:HD23 | 2:CW:224:LEU:HA | 1.85 | 0.40 |
| 2:CX:224:LEU:HA | 2:CX:224:LEU:HD23 | 1.82 | 0.40 |
| 1:DC:48:ASP:N | 1:DC:48:ASP:OD1 | 2.55 | 0.40 |
| 1:DC:70:VAL:HG12 | 1:DC:72:ARG:N | 2.31 | 0.40 |
| 2:DE:53:SER:O | 2:DE:57:LEU:HG | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:AK:60:TYR:O | 2:AK:64:LYS:HG2 | 2.22 | 0.40 |
| 2:AQ:192:LEU:HD11 | 2:AQ:231:GLN:OE1 | 2.22 | 0.40 |
| 1:BB:119:VAL:HG23 | 1:BB:140:GLN:HE21 | 1.84 | 0.40 |
| 1:BB:191:TYR:O | 1:BB:194:GLU:HG3 | 2.22 | 0.40 |
| 1:BG:144:SER:OG | 1:BG:146:VAL:O | 2.40 | 0.40 |
| 1:BI:98:TRP:CH2 | 1:BI:155:TRP:HB3 | 2.55 | 0.40 |
| 1:BN:101:LEU:HD11 | 1:BO:86:LEU:HD22 | 2.04 | 0.40 |
| 2:BP:87:ASN:OD1 | 2:BP:118:ASN:ND2 | 2.49 | 0.40 |
| 1:BU:116:PRO:O | 1:BU:117:ARG:HD2 | 2.21 | 0.40 |
| 1:CC:167:THR:HG23 | 1:CC:169:ALA:H | 1.86 | 0.40 |
| 2:CD:67:LYS:HE2 | 2:CD:67:LYS:HB2 | 1.81 | 0.40 |
| 2:CD:214:GLU:HA | 2:CD:217:GLN:HG3 | 2.02 | 0.40 |
| 2:CE:53:SER:O | 2:CE:57:LEU:HG | 2.22 | 0.40 |
| 2:CK:54:ALA:HB3 | 2:CK:195:ILE:HD12 | 1.97 | 0.40 |
| 2:CL:4:LEU:HD13 | 2:CL:221:TYR:HD2 | 1.87 | 0.40 |
| 1:CN:101:LEU:HD11 | 1:CO:86:LEU:HD22 | 2.04 | 0.40 |
| 2:CQ:73:SER:OG | 2:DL:110:ARG:NH2 | 2.54 | 0.40 |
| 1:CU:73:PRO:HB3 | 1:CU:128:ASP:HA | 2.02 | 0.40 |
| 2:DE:198:ARG:NH1 | 2:DE:234:ILE:HG21 | 2.36 | 0.40 |
| 1:DG:81:LEU:HD21 | 1:DG:155:TRP:CH2 | 2.56 | 0.40 |
| 1:DG:144:SER:OG | 1:DG:146:VAL:O | 2.40 | 0.40 |
| 2:DL:64:LYS:HD3 | 2:DL:64:LYS:HA | 1.85 | 0.40 |
| 2:AE:53:SER:O | 2:AE:57:LEU:HG | 2.22 | 0.40 |
| 2:AK:201:PHE:CD2 | 2:AL:163:PHE:CE2 | 3.09 | 0.40 |
| 2:AL:206:LYS:HE2 | 2:AL:206:LYS:HB3 | 1.82 | 0.40 |
| 2:AQ:255:GLU:HG3 | 2:AQ:255:GLU:H | 1.74 | 0.40 |
| 1:AU:16:ILE:H | 1:AU:16:ILE:HG12 | 1.75 | 0.40 |
| 1:BB:118:LEU:HD23 | 1:BB:143:ILE:HD11 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | AB | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | AC | 184/197 (93%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | AG | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | AI | 184/197 (93%) | 181 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | AN | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | AO | 184/197 (93%) | 175 (95%) | 9 (5%) | 0 | 100 | 100 |
| 1 | AS | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | AU | 184/197 (93%) | 176 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | BB | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | BC | 184/197 (93%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | BG | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | BI | 184/197 (93%) | 181 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | BN | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | BO | 184/197 (93%) | 175 (95%) | 9 (5%) | 0 | 100 | 100 |
| 1 | BS | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | BU | 184/197 (93%) | 175 (95%) | 9 (5%) | 0 | 100 | 100 |
| 1 | CB | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | CC | 184/197 (93%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | CG | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | CI | 184/197 (93%) | 181 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | CN | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | CO | 184/197 (93%) | 175 (95%) | 9 (5%) | 0 | 100 | 100 |
| 1 | CS | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | CU | 184/197 (93%) | 176 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | DB | 184/197 (93%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | DC | 184/197 (93%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | DG | 184/197 (93%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | DI | 184/197 (93%) | 181 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | AD | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | AE | 262/264 (99%) | 262 (100%) | 0 | 0 | 100 | 100 |
| 2 | AK | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | AL | 262/264 (99%) | 255 (97%) | 7 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | AP | 262/264 (99%) | 259 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | AQ | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | AW | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | AX | 262/264 (99%) | 258 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | BD | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | BE | 262/264 (99%) | 262 (100%) | 0 | 0 | 100 | 100 |
| 2 | BK | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | BL | 262/264 (99%) | 256 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | BP | 262/264 (99%) | 259 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | BQ | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | BW | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | BX | 262/264 (99%) | 258 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | CD | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | CE | 262/264 (99%) | 262 (100%) | 0 | 0 | 100 | 100 |
| 2 | CK | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | CL | 262/264 (99%) | 256 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | CP | 262/264 (99%) | 259 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | CQ | 262/264 (99%) | 259 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | CW | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | CX | 262/264 (99%) | 258 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | DD | 262/264 (99%) | 257 (98%) | 5 (2%) | 0 | 100 | 100 |
| 2 | DE | 262/264 (99%) | 262 (100%) | 0 | 0 | 100 | 100 |
| 2 | DK | 262/264 (99%) | 260 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | DL | 262/264 (99%) | 256 (98%) | 6 (2%) | 0 | 100 | 100 |
| All | All | 12488/12908 (97%) | 12217 (98%) | 271 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 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 EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | AB | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | AC | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | AG | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | AI | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | AN | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | AO | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | AS | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | AU | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BB | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BC | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BG | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BI | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BN | 162/172 (94%) | 160 (99%) | 2 (1%) | 63 | 77 |
| 1 | BO | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | BS | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | BU | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CB | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CC | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CG | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CI | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CN | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | CO | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | CS | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | CU | 162/172 (94%) | 161 (99%) | 1 (1%) | 78 | 83 |
| 1 | DB | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | DC | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | DG | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 1 | DI | 162/172 (94%) | 162 (100%) | 0 | 100 | 100 |
| 2 | AD | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 | 85 |
| 2 | AE | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | AK | 240/240 (100%) | 237 (99%) | 3 (1%) | 61 75 |
| 2 | AL | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | AP | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | AQ | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | AW | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | AX | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | BD | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | BE | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | BK | 240/240 (100%) | 237 (99%) | 3 (1%) | 61 75 |
| 2 | BL | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | BP | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | BQ | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | BW | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | BX | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | CD | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | CE | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | CK | 240/240 (100%) | 237 (99%) | 3 (1%) | 61 75 |
| 2 | CL | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | CP | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | CQ | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | CW | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | CX | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | DD | 240/240 (100%) | 240 (100%) | 0 | 100 100 |
| 2 | DE | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| 2 | DK | 240/240 (100%) | 237 (99%) | 3 (1%) | 61 75 |
| 2 | DL | 240/240 (100%) | 239 (100%) | 1 (0%) | 84 85 |
| All | All | 11256/11536 (98%) | 11222 (100%) | 34 (0%) | 84 87 |

All (34) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | BD | 5 | LEU |
| 2 | BE | 203 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | BK | 192 | LEU |
| 2 | BK | 197 | ILE |
| 2 | BK | 242 | MET |
| 1 | BN | 138 | GLU |
| 1 | BN | 142 | THR |
| 1 | BO | 29 | ILE |
| 2 | BW | 202 | TYR |
| 2 | CD | 5 | LEU |
| 2 | CE | 203 | LYS |
| 2 | CK | 192 | LEU |
| 2 | CK | 197 | ILE |
| 2 | CK | 242 | MET |
| 1 | CO | 29 | ILE |
| 2 | CP | 105 | THR |
| 2 | CQ | 116 | LEU |
| 1 | CS | 76 | VAL |
| 1 | CU | 158 | ILE |
| 2 | CW | 202 | TYR |
| 2 | DE | 203 | LYS |
| 2 | DK | 192 | LEU |
| 2 | DK | 197 | ILE |
| 2 | DK | 242 | MET |
| 2 | DL | 53 | SER |
| 2 | AD | 5 | LEU |
| 2 | AE | 203 | LYS |
| 2 | AK | 192 | LEU |
| 2 | AK | 197 | ILE |
| 2 | AK | 242 | MET |
| 1 | AN | 138 | GLU |
| 1 | AO | 29 | ILE |
| 1 | AS | 76 | VAL |
| 2 | AW | 202 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | BC | 51 | GLN |
| 1 | BC | 56 | HIS |
| 1 | BC | 115 | ASN |
| 2 | BD | 36 | HIS |
| 2 | BD | 87 | ASN |
| 2 | BD | 211 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | BE | 146 | HIS |
| 2 | BE | 196 | ASN |
| 2 | BK | 146 | HIS |
| 2 | BK | 231 | GLN |
| 2 | BL | 217 | GLN |
| 2 | BL | 247 | ASN |
| 2 | BL | 249 | ASN |
| 1 | BN | 102 | GLN |
| 1 | BO | 22 | ASN |
| 1 | BO | 78 | HIS |
| 1 | BO | 87 | ASN |
| 2 | BP | 247 | ASN |
| 2 | BQ | 36 | HIS |
| 1 | BU | 22 | ASN |
| 1 | BU | 30 | ASN |
| 1 | BU | 51 | GLN |
| 1 | BU | 95 | GLN |
| 2 | BX | 92 | HIS |
| 2 | BX | 228 | ASN |
| 1 | CB | 176 | ASN |
| 1 | CC | 51 | GLN |
| 1 | CC | 56 | HIS |
| 1 | CC | 115 | ASN |
| 1 | CC | 140 | GLN |
| 2 | CD | 36 | HIS |
| 2 | CD | 87 | ASN |
| 2 | CD | 211 | GLN |
| 1 | AB | 176 | ASN |
| 2 | CE | 146 | HIS |
| 2 | CE | 196 | ASN |
| 2 | CK | 146 | HIS |
| 2 | CK | 231 | GLN |
| 2 | CL | 217 | GLN |
| 2 | CL | 247 | ASN |
| 2 | CL | 249 | ASN |
| 1 | CN | 102 | GLN |
| 1 | CN | 115 | ASN |
| 1 | CO | 22 | ASN |
| 1 | CO | 78 | HIS |
| 1 | CO | 87 | ASN |
| 2 | CP | 24 | ASN |
| 2 | CP | 92 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | CP | 247 | ASN |
| 2 | CQ | 228 | ASN |
| 1 | CS | 78 | HIS |
| 1 | CU | 22 | ASN |
| 1 | CU | 30 | ASN |
| 1 | CU | 51 | GLN |
| 1 | CU | 95 | GLN |
| 2 | CX | 92 | HIS |
| 1 | DB | 95 | GLN |
| 1 | DB | 176 | ASN |
| 1 | DC | 51 | GLN |
| 1 | DC | 56 | HIS |
| 1 | DC | 115 | ASN |
| 1 | DC | 140 | GLN |
| 2 | DD | 36 | HIS |
| 2 | DD | 87 | ASN |
| 2 | DD | 211 | GLN |
| 2 | DE | 146 | HIS |
| 2 | DE | 196 | ASN |
| 1 | AC | 51 | GLN |
| 1 | AC | 56 | HIS |
| 1 | AC | 115 | ASN |
| 1 | AC | 140 | GLN |
| 2 | DK | 146 | HIS |
| 2 | DK | 231 | GLN |
| 2 | DL | 217 | GLN |
| 2 | DL | 247 | ASN |
| 2 | DL | 249 | ASN |
| 2 | AD | 36 | HIS |
| 2 | AD | 87 | ASN |
| 2 | AD | 211 | GLN |
| 2 | AE | 146 | HIS |
| 2 | AE | 196 | ASN |
| 1 | AI | 24 | HIS |
| 2 | AK | 146 | HIS |
| 2 | AK | 231 | GLN |
| 2 | AL | 217 | GLN |
| 2 | AL | 247 | ASN |
| 2 | AL | 249 | ASN |
| 1 | AN | 56 | HIS |
| 1 | AN | 102 | GLN |
| 1 | AN | 115 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AO | 22 | ASN |
| 1 | AO | 78 | HIS |
| 1 | AO | 87 | ASN |
| 2 | AP | 24 | ASN |
| 2 | AP | 92 | HIS |
| 2 | AP | 247 | ASN |
| 2 | AQ | 217 | GLN |
| 2 | AQ | 228 | ASN |
| 1 | AU | 22 | ASN |
| 1 | AU | 30 | ASN |
| 1 | AU | 51 | GLN |
| 1 | AU | 95 | GLN |
| 2 | AX | 92 | HIS |
| 2 | AX | 228 | ASN |
| 1 | BB | 176 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry

28 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | Y43 | BS | 201 | - | 28,32,32 | 2.51 | 9 (32%) | 35,50,50 | 1.67 | 6 (17%) |
| 3 | Y43 | CC | 201 | - | 28,32,32 | 2.54 | 9 (32%) | 35,50,50 | 1.75 | 6 (17%) |
| 3 | Y43 | AU | 201 | - | 28,32,32 | 2.48 | 9 (32%) | 35,50,50 | 1.69 | 6 (17%) |
| 3 | Y43 | AB | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.74 | 6 (17%) |
| 3 | Y43 | DC | 201 | - | 28,32,32 | 2.54 | 9 (32%) | 35,50,50 | 1.75 | 6 (17%) |
| 3 | Y43 | DI | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.69 | 7 (20%) |
| 3 | Y43 | BN | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.72 | 6 (17%) |
| 3 | Y43 | CI | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.69 | 7 (20%) |
| 3 | Y43 | AS | 201 | - | 28,32,32 | 2.50 | 9 (32%) | 35,50,50 | 1.67 | 6 (17%) |
| 3 | Y43 | DB | 201 | - | 28,32,32 | 2.57 | 9 (32%) | 35,50,50 | 1.73 | 6 (17%) |
| 3 | Y43 | CU | 201 | - | 28,32,32 | 2.48 | 8 (28%) | 35,50,50 | 1.69 | 6 (17%) |
| 3 | Y43 | BB | 201 | - | 28,32,32 | 2.57 | 9 (32%) | 35,50,50 | 1.74 | 6 (17%) |
| 3 | Y43 | BG | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.76 | 6 (17%) |
| 3 | Y43 | AG | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.75 | 6 (17%) |
| 3 | Y43 | BU | 201 | - | 28,32,32 | 2.48 | 8 (28%) | 35,50,50 | 1.69 | 6 (17%) |
| 3 | Y43 | CN | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.71 | 6 (17%) |
| 3 | Y43 | BC | 201 | - | 28,32,32 | 2.54 | 9 (32%) | 35,50,50 | 1.74 | 6 (17%) |
| 3 | Y43 | AN | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.72 | 6 (17%) |
| 3 | Y43 | CS | 201 | - | 28,32,32 | 2.51 | 9 (32%) | 35,50,50 | 1.67 | 6 (17%) |
| 3 | Y43 | AO | 201 | - | 28,32,32 | 2.49 | 9 (32%) | 35,50,50 | 1.69 | 6 (17%) |
| 3 | Y43 | AC | 201 | - | 28,32,32 | 2.54 | 9 (32%) | 35,50,50 | 1.74 | 6 (17%) |
| 3 | Y43 | CB | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.74 | 6 (17%) |
| 3 | Y43 | CG | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.76 | 6 (17%) |
| 3 | Y43 | BI | 201 | - | 28,32,32 | 2.56 | 9 (32%) | 35,50,50 | 1.69 | 7 (20%) |
| 3 | Y43 | CO | 201 | - | 28,32,32 | 2.49 | 9 (32%) | 35,50,50 | 1.68 | 6 (17%) |
| 3 | Y43 | DG | 201 | - | 28,32,32 | 2.55 | 9 (32%) | 35,50,50 | 1.76 | 6 (17%) |
| 3 | Y43 | BO | 201 | - | 28,32,32 | 2.49 | 9 (32%) | 35,50,50 | 1.68 | 6 (17%) |
| 3 | Y43 | AI | 201 | - | 28,32,32 | 2.57 | 9 (32%) | 35,50,50 | 1.69 | 7 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | Y43 | BS | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | Y43 | CC | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AU | 201 | - | 2/2/6/6 | 2/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AB | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | DC | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | DI | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BN | 201 | - | 2/2/6/6 | 9/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CI | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AS | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | DB | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CU | 201 | - | 2/2/6/6 | 2/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BB | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BG | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AG | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BU | 201 | - | 2/2/6/6 | 2/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CN | 201 | - | 2/2/6/6 | 9/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BC | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AN | 201 | - | 2/2/6/6 | 9/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CS | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AO | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AC | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CB | 201 | - | 2/2/6/6 | 5/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CG | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BI | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | CO | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | DG | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | BO | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |
| 3 | Y43 | AI | 201 | - | 2/2/6/6 | 6/22/34/34 | 0/3/3/3 |

All (250) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | CB | 201 | Y43 | PAI-OAH | 7.77 | 1.90 | 1.59 |
| 3 | BB | 201 | Y43 | PAI-OAH | 7.77 | 1.90 | 1.59 |
| 3 | AB | 201 | Y43 | PAI-OAH | 7.77 | 1.90 | 1.59 |
| 3 | DB | 201 | Y43 | PAI-OAH | 7.75 | 1.90 | 1.59 |
| 3 | BS | 201 | Y43 | PAI-OAH | 7.59 | 1.90 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | AS | 201 | Y43 | PAI-OAH | 7.57 | 1.90 | 1.59 |
| 3 | CS | 201 | Y43 | PAI-OAH | 7.57 | 1.89 | 1.59 |
| 3 | CC | 201 | Y43 | PAI-OAH | 7.54 | 1.89 | 1.59 |
| 3 | DC | 201 | Y43 | PAI-OAH | 7.53 | 1.89 | 1.59 |
| 3 | BC | 201 | Y43 | PAI-OAH | 7.53 | 1.89 | 1.59 |
| 3 | AC | 201 | Y43 | PAI-OAH | 7.52 | 1.89 | 1.59 |
| 3 | CG | 201 | Y43 | PAI-OAH | 7.47 | 1.89 | 1.59 |
| 3 | BG | 201 | Y43 | PAI-OAH | 7.45 | 1.89 | 1.59 |
| 3 | AG | 201 | Y43 | PAI-OAH | 7.45 | 1.89 | 1.59 |
| 3 | DG | 201 | Y43 | PAI-OAH | 7.45 | 1.89 | 1.59 |
| 3 | AI | 201 | Y43 | PAI-OAH | 7.42 | 1.89 | 1.59 |
| 3 | CI | 201 | Y43 | PAI-OAH | 7.41 | 1.89 | 1.59 |
| 3 | BI | 201 | Y43 | PAI-OAH | 7.41 | 1.89 | 1.59 |
| 3 | DI | 201 | Y43 | PAI-OAH | 7.40 | 1.89 | 1.59 |
| 3 | BN | 201 | Y43 | PAI-OAH | 7.30 | 1.88 | 1.59 |
| 3 | CN | 201 | Y43 | PAI-OAH | 7.30 | 1.88 | 1.59 |
| 3 | AN | 201 | Y43 | PAI-OAH | 7.30 | 1.88 | 1.59 |
| 3 | CU | 201 | Y43 | PAI-OAH | 7.22 | 1.88 | 1.59 |
| 3 | BU | 201 | Y43 | PAI-OAH | 7.21 | 1.88 | 1.59 |
| 3 | AU | 201 | Y43 | PAI-OAH | 7.20 | 1.88 | 1.59 |
| 3 | AO | 201 | Y43 | PAI-OAH | 7.17 | 1.88 | 1.59 |
| 3 | BO | 201 | Y43 | PAI-OAH | 7.16 | 1.88 | 1.59 |
| 3 | CO | 201 | Y43 | PAI-OAH | 7.14 | 1.88 | 1.59 |
| 3 | CN | 201 | Y43 | C2-N1 | 5.85 | 1.40 | 1.30 |
| 3 | AN | 201 | Y43 | C2-N1 | 5.84 | 1.40 | 1.30 |
| 3 | BN | 201 | Y43 | C2-N1 | 5.83 | 1.40 | 1.30 |
| 3 | CS | 201 | Y43 | C2-N1 | 5.79 | 1.40 | 1.30 |
| 3 | AG | 201 | Y43 | C2-N1 | 5.79 | 1.40 | 1.30 |
| 3 | CG | 201 | Y43 | C2-N1 | 5.78 | 1.40 | 1.30 |
| 3 | BS | 201 | Y43 | C2-N1 | 5.77 | 1.40 | 1.30 |
| 3 | BG | 201 | Y43 | C2-N1 | 5.75 | 1.40 | 1.30 |
| 3 | AS | 201 | Y43 | C2-N1 | 5.75 | 1.40 | 1.30 |
| 3 | DG | 201 | Y43 | C2-N1 | 5.75 | 1.40 | 1.30 |
| 3 | CC | 201 | Y43 | C2-N1 | 5.73 | 1.40 | 1.30 |
| 3 | CU | 201 | Y43 | C2-N1 | 5.72 | 1.40 | 1.30 |
| 3 | DC | 201 | Y43 | C2-N1 | 5.72 | 1.40 | 1.30 |
| 3 | BB | 201 | Y43 | C2-N1 | 5.71 | 1.40 | 1.30 |
| 3 | DB | 201 | Y43 | C2-N1 | 5.71 | 1.40 | 1.30 |
| 3 | AO | 201 | Y43 | C2-N1 | 5.71 | 1.40 | 1.30 |
| 3 | BO | 201 | Y43 | C2-N1 | 5.71 | 1.40 | 1.30 |
| 3 | AC | 201 | Y43 | C2-N1 | 5.70 | 1.40 | 1.30 |
| 3 | BC | 201 | Y43 | C2-N1 | 5.70 | 1.40 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BU | 201 | Y43 | C2-N1 | 5.70 | 1.40 | 1.30 |
| 3 | CB | 201 | Y43 | C2-N1 | 5.68 | 1.40 | 1.30 |
| 3 | CO | 201 | Y43 | C2-N1 | 5.68 | 1.40 | 1.30 |
| 3 | AB | 201 | Y43 | C2-N1 | 5.67 | 1.40 | 1.30 |
| 3 | AU | 201 | Y43 | C2-N1 | 5.66 | 1.40 | 1.30 |
| 3 | BI | 201 | Y43 | C2-N1 | 5.65 | 1.40 | 1.30 |
| 3 | CI | 201 | Y43 | C2-N1 | 5.65 | 1.40 | 1.30 |
| 3 | AI | 201 | Y43 | C2-N1 | 5.65 | 1.40 | 1.30 |
| 3 | DI | 201 | Y43 | C2-N1 | 5.64 | 1.40 | 1.30 |
| 3 | AI | 201 | Y43 | C4-N9 | 5.08 | 1.42 | 1.37 |
| 3 | BI | 201 | Y43 | C4-N9 | 5.00 | 1.42 | 1.37 |
| 3 | CI | 201 | Y43 | C4-N9 | 4.95 | 1.42 | 1.37 |
| 3 | DI | 201 | Y43 | C4-N9 | 4.92 | 1.42 | 1.37 |
| 3 | AU | 201 | Y43 | CAG-CAF | 4.61 | 1.66 | 1.51 |
| 3 | CU | 201 | Y43 | CAG-CAF | 4.59 | 1.65 | 1.51 |
| 3 | BU | 201 | Y43 | CAG-CAF | 4.59 | 1.65 | 1.51 |
| 3 | CN | 201 | Y43 | CAG-CAF | 4.57 | 1.65 | 1.51 |
| 3 | AI | 201 | Y43 | CAG-CAF | 4.56 | 1.65 | 1.51 |
| 3 | CO | 201 | Y43 | C4-N9 | 4.56 | 1.42 | 1.37 |
| 3 | CI | 201 | Y43 | CAG-CAF | 4.55 | 1.65 | 1.51 |
| 3 | AN | 201 | Y43 | C4-N9 | 4.55 | 1.42 | 1.37 |
| 3 | BI | 201 | Y43 | CAG-CAF | 4.55 | 1.65 | 1.51 |
| 3 | BN | 201 | Y43 | CAG-CAF | 4.55 | 1.65 | 1.51 |
| 3 | AN | 201 | Y43 | CAG-CAF | 4.55 | 1.65 | 1.51 |
| 3 | DG | 201 | Y43 | CAG-CAF | 4.54 | 1.65 | 1.51 |
| 3 | BO | 201 | Y43 | C4-N9 | 4.54 | 1.42 | 1.37 |
| 3 | CN | 201 | Y43 | C4-N9 | 4.53 | 1.42 | 1.37 |
| 3 | BG | 201 | Y43 | CAG-CAF | 4.52 | 1.65 | 1.51 |
| 3 | BB | 201 | Y43 | CAG-CAF | 4.52 | 1.65 | 1.51 |
| 3 | AB | 201 | Y43 | CAG-CAF | 4.52 | 1.65 | 1.51 |
| 3 | DI | 201 | Y43 | CAG-CAF | 4.52 | 1.65 | 1.51 |
| 3 | BN | 201 | Y43 | C4-N9 | 4.51 | 1.42 | 1.37 |
| 3 | CG | 201 | Y43 | CAG-CAF | 4.51 | 1.65 | 1.51 |
| 3 | CB | 201 | Y43 | CAG-CAF | 4.50 | 1.65 | 1.51 |
| 3 | AO | 201 | Y43 | C4-N9 | 4.50 | 1.41 | 1.37 |
| 3 | AG | 201 | Y43 | CAG-CAF | 4.50 | 1.65 | 1.51 |
| 3 | DB | 201 | Y43 | CAG-CAF | 4.50 | 1.65 | 1.51 |
| 3 | CS | 201 | Y43 | CAG-CAF | 4.49 | 1.65 | 1.51 |
| 3 | DC | 201 | Y43 | CAG-CAF | 4.49 | 1.65 | 1.51 |
| 3 | BC | 201 | Y43 | CAG-CAF | 4.48 | 1.65 | 1.51 |
| 3 | BS | 201 | Y43 | CAG-CAF | 4.48 | 1.65 | 1.51 |
| 3 | DG | 201 | Y43 | C4-N9 | 4.48 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BG | 201 | Y43 | C4-N9 | 4.47 | 1.41 | 1.37 |
| 3 | AS | 201 | Y43 | CAG-CAF | 4.47 | 1.65 | 1.51 |
| 3 | CC | 201 | Y43 | CAG-CAF | 4.47 | 1.65 | 1.51 |
| 3 | AC | 201 | Y43 | CAG-CAF | 4.47 | 1.65 | 1.51 |
| 3 | DB | 201 | Y43 | C4-N9 | 4.45 | 1.41 | 1.37 |
| 3 | DC | 201 | Y43 | C4-N9 | 4.44 | 1.41 | 1.37 |
| 3 | CG | 201 | Y43 | C4-N9 | 4.44 | 1.41 | 1.37 |
| 3 | AG | 201 | Y43 | C4-N9 | 4.43 | 1.41 | 1.37 |
| 3 | CO | 201 | Y43 | CAG-CAF | 4.42 | 1.65 | 1.51 |
| 3 | AC | 201 | Y43 | C4-N9 | 4.41 | 1.41 | 1.37 |
| 3 | BO | 201 | Y43 | CAG-CAF | 4.41 | 1.65 | 1.51 |
| 3 | AO | 201 | Y43 | CAG-CAF | 4.41 | 1.65 | 1.51 |
| 3 | BC | 201 | Y43 | C4-N9 | 4.41 | 1.41 | 1.37 |
| 3 | BB | 201 | Y43 | C4-N9 | 4.40 | 1.41 | 1.37 |
| 3 | CC | 201 | Y43 | C4-N9 | 4.37 | 1.41 | 1.37 |
| 3 | CB | 201 | Y43 | C4-N9 | 4.37 | 1.41 | 1.37 |
| 3 | AB | 201 | Y43 | C4-N9 | 4.33 | 1.41 | 1.37 |
| 3 | AU | 201 | Y43 | C4-N9 | 4.21 | 1.41 | 1.37 |
| 3 | BU | 201 | Y43 | C4-N9 | 4.18 | 1.41 | 1.37 |
| 3 | CU | 201 | Y43 | C4-N9 | 4.11 | 1.41 | 1.37 |
| 3 | AS | 201 | Y43 | C4-N9 | 4.07 | 1.41 | 1.37 |
| 3 | CS | 201 | Y43 | C4-N9 | 4.01 | 1.41 | 1.37 |
| 3 | BS | 201 | Y43 | C4-N9 | 3.99 | 1.41 | 1.37 |
| 3 | DI | 201 | Y43 | CAD-N9 | 3.64 | 1.57 | 1.48 |
| 3 | CI | 201 | Y43 | CAD-N9 | 3.63 | 1.57 | 1.48 |
| 3 | BI | 201 | Y43 | CAD-N9 | 3.63 | 1.57 | 1.48 |
| 3 | AI | 201 | Y43 | CAD-N9 | 3.63 | 1.57 | 1.48 |
| 3 | DB | 201 | Y43 | CAD-N9 | 3.49 | 1.57 | 1.48 |
| 3 | AB | 201 | Y43 | CAD-N9 | 3.49 | 1.57 | 1.48 |
| 3 | CB | 201 | Y43 | CAD-N9 | 3.48 | 1.57 | 1.48 |
| 3 | BB | 201 | Y43 | CAD-N9 | 3.48 | 1.57 | 1.48 |
| 3 | BC | 201 | Y43 | CAD-N9 | 3.42 | 1.57 | 1.48 |
| 3 | DC | 201 | Y43 | CAD-N9 | 3.42 | 1.57 | 1.48 |
| 3 | AC | 201 | Y43 | CAD-N9 | 3.42 | 1.57 | 1.48 |
| 3 | DG | 201 | Y43 | CAD-N9 | 3.41 | 1.56 | 1.48 |
| 3 | AG | 201 | Y43 | CAD-N9 | 3.41 | 1.56 | 1.48 |
| 3 | CC | 201 | Y43 | CAD-N9 | 3.40 | 1.56 | 1.48 |
| 3 | CG | 201 | Y43 | CAD-N9 | 3.40 | 1.56 | 1.48 |
| 3 | BG | 201 | Y43 | CAD-N9 | 3.39 | 1.56 | 1.48 |
| 3 | CN | 201 | Y43 | CAD-N9 | 3.38 | 1.56 | 1.48 |
| 3 | BN | 201 | Y43 | CAD-N9 | 3.36 | 1.56 | 1.48 |
| 3 | AN | 201 | Y43 | CAD-N9 | 3.36 | 1.56 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BO | 201 | Y43 | CAD-N9 | 3.31 | 1.56 | 1.48 |
| 3 | AO | 201 | Y43 | CAD-N9 | 3.30 | 1.56 | 1.48 |
| 3 | CO | 201 | Y43 | CAD-N9 | 3.29 | 1.56 | 1.48 |
| 3 | CS | 201 | Y43 | CAD-N9 | 3.20 | 1.56 | 1.48 |
| 3 | AS | 201 | Y43 | CAD-N9 | 3.20 | 1.56 | 1.48 |
| 3 | BS | 201 | Y43 | CAD-N9 | 3.19 | 1.56 | 1.48 |
| 3 | CU | 201 | Y43 | CAD-N9 | 3.06 | 1.56 | 1.48 |
| 3 | BU | 201 | Y43 | CAD-N9 | 3.06 | 1.56 | 1.48 |
| 3 | AU | 201 | Y43 | CAD-N9 | 3.05 | 1.56 | 1.48 |
| 3 | DC | 201 | Y43 | OAH-CAG | -3.03 | 1.33 | 1.44 |
| 3 | AO | 201 | Y43 | OAH-CAG | -3.02 | 1.33 | 1.44 |
| 3 | BO | 201 | Y43 | OAH-CAG | -3.01 | 1.33 | 1.44 |
| 3 | CC | 201 | Y43 | OAH-CAG | -3.01 | 1.33 | 1.44 |
| 3 | CO | 201 | Y43 | OAH-CAG | -3.00 | 1.33 | 1.44 |
| 3 | AC | 201 | Y43 | OAH-CAG | -3.00 | 1.33 | 1.44 |
| 3 | BC | 201 | Y43 | OAH-CAG | -2.99 | 1.33 | 1.44 |
| 3 | BI | 201 | Y43 | OAH-CAG | -2.99 | 1.33 | 1.44 |
| 3 | AI | 201 | Y43 | OAH-CAG | -2.99 | 1.33 | 1.44 |
| 3 | CG | 201 | Y43 | OAH-CAG | -2.98 | 1.33 | 1.44 |
| 3 | CI | 201 | Y43 | OAH-CAG | -2.98 | 1.33 | 1.44 |
| 3 | DG | 201 | Y43 | OAH-CAG | -2.98 | 1.33 | 1.44 |
| 3 | BG | 201 | Y43 | OAH-CAG | -2.98 | 1.33 | 1.44 |
| 3 | DI | 201 | Y43 | OAH-CAG | -2.97 | 1.33 | 1.44 |
| 3 | AU | 201 | Y43 | OAH-CAG | -2.97 | 1.33 | 1.44 |
| 3 | CN | 201 | Y43 | OAH-CAG | -2.97 | 1.33 | 1.44 |
| 3 | AN | 201 | Y43 | OAH-CAG | -2.97 | 1.33 | 1.44 |
| 3 | CU | 201 | Y43 | OAH-CAG | -2.96 | 1.33 | 1.44 |
| 3 | AG | 201 | Y43 | OAH-CAG | -2.96 | 1.33 | 1.44 |
| 3 | BU | 201 | Y43 | OAH-CAG | -2.96 | 1.33 | 1.44 |
| 3 | BN | 201 | Y43 | OAH-CAG | -2.95 | 1.33 | 1.44 |
| 3 | BB | 201 | Y43 | OAH-CAG | -2.94 | 1.33 | 1.44 |
| 3 | BS | 201 | Y43 | OAH-CAG | -2.94 | 1.33 | 1.44 |
| 3 | CB | 201 | Y43 | OAH-CAG | -2.94 | 1.33 | 1.44 |
| 3 | AS | 201 | Y43 | OAH-CAG | -2.93 | 1.33 | 1.44 |
| 3 | CS | 201 | Y43 | OAH-CAG | -2.93 | 1.33 | 1.44 |
| 3 | DB | 201 | Y43 | OAH-CAG | -2.92 | 1.33 | 1.44 |
| 3 | AB | 201 | Y43 | OAH-CAG | -2.92 | 1.33 | 1.44 |
| 3 | AB | 201 | Y43 | C4-N3 | 2.69 | 1.42 | 1.37 |
| 3 | AO | 201 | Y43 | C4-N3 | 2.69 | 1.42 | 1.37 |
| 3 | BN | 201 | Y43 | C4-N3 | 2.69 | 1.42 | 1.37 |
| 3 | BG | 201 | Y43 | C4-N3 | 2.68 | 1.42 | 1.37 |
| 3 | CO | 201 | Y43 | C4-N3 | 2.68 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | CG | 201 | Y43 | C4-N3 | 2.67 | 1.42 | 1.37 |
| 3 | AG | 201 | Y43 | C4-N3 | 2.67 | 1.42 | 1.37 |
| 3 | BB | 201 | Y43 | C4-N3 | 2.67 | 1.42 | 1.37 |
| 3 | AN | 201 | Y43 | C4-N3 | 2.66 | 1.42 | 1.37 |
| 3 | DG | 201 | Y43 | C4-N3 | 2.66 | 1.42 | 1.37 |
| 3 | BO | 201 | Y43 | C4-N3 | 2.65 | 1.42 | 1.37 |
| 3 | CC | 201 | Y43 | C4-N3 | 2.65 | 1.42 | 1.37 |
| 3 | CB | 201 | Y43 | C4-N3 | 2.65 | 1.42 | 1.37 |
| 3 | AU | 201 | Y43 | C4-N3 | 2.65 | 1.42 | 1.37 |
| 3 | CN | 201 | Y43 | C4-N3 | 2.65 | 1.42 | 1.37 |
| 3 | BC | 201 | Y43 | C4-N3 | 2.63 | 1.42 | 1.37 |
| 3 | DB | 201 | Y43 | C4-N3 | 2.63 | 1.42 | 1.37 |
| 3 | AC | 201 | Y43 | C4-N3 | 2.62 | 1.42 | 1.37 |
| 3 | CU | 201 | Y43 | C4-N3 | 2.62 | 1.42 | 1.37 |
| 3 | BU | 201 | Y43 | C4-N3 | 2.61 | 1.42 | 1.37 |
| 3 | DC | 201 | Y43 | C4-N3 | 2.60 | 1.41 | 1.37 |
| 3 | CI | 201 | Y43 | C4-N3 | 2.60 | 1.41 | 1.37 |
| 3 | DI | 201 | Y43 | C4-N3 | 2.59 | 1.41 | 1.37 |
| 3 | BI | 201 | Y43 | C4-N3 | 2.54 | 1.41 | 1.37 |
| 3 | AI | 201 | Y43 | C4-N3 | 2.54 | 1.41 | 1.37 |
| 3 | BS | 201 | Y43 | C4-N3 | 2.53 | 1.41 | 1.37 |
| 3 | DB | 201 | Y43 | C5-C4 | 2.52 | 1.42 | 1.38 |
| 3 | CS | 201 | Y43 | C4-N3 | 2.51 | 1.41 | 1.37 |
| 3 | AS | 201 | Y43 | C4-N3 | 2.51 | 1.41 | 1.37 |
| 3 | BN | 201 | Y43 | C5-C4 | 2.51 | 1.42 | 1.38 |
| 3 | AN | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | CN | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | AB | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | CI | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | DI | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | BI | 201 | Y43 | C5-C4 | 2.50 | 1.42 | 1.38 |
| 3 | CC | 201 | Y43 | C5-C4 | 2.49 | 1.42 | 1.38 |
| 3 | BB | 201 | Y43 | C5-C4 | 2.48 | 1.42 | 1.38 |
| 3 | CB | 201 | Y43 | C5-C4 | 2.48 | 1.42 | 1.38 |
| 3 | BC | 201 | Y43 | C5-C4 | 2.47 | 1.42 | 1.38 |
| 3 | CG | 201 | Y43 | C5-C4 | 2.46 | 1.42 | 1.38 |
| 3 | AI | 201 | Y43 | C5-C4 | 2.45 | 1.42 | 1.38 |
| 3 | AC | 201 | Y43 | C5-C4 | 2.45 | 1.42 | 1.38 |
| 3 | DC | 201 | Y43 | C5-C4 | 2.45 | 1.42 | 1.38 |
| 3 | DG | 201 | Y43 | C5-C4 | 2.44 | 1.42 | 1.38 |
| 3 | AG | 201 | Y43 | C5-C4 | 2.43 | 1.42 | 1.38 |
| 3 | AU | 201 | Y43 | C5-C4 | 2.41 | 1.42 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | BG | 201 | Y43 | C5-C4 | 2.41 | 1.42 | 1.38 |
| 3 | BU | 201 | Y43 | C5-C4 | 2.41 | 1.42 | 1.38 |
| 3 | CO | 201 | Y43 | C5-C4 | 2.40 | 1.42 | 1.38 |
| 3 | BS | 201 | Y43 | C5-C4 | 2.39 | 1.42 | 1.38 |
| 3 | BO | 201 | Y43 | C5-C4 | 2.39 | 1.42 | 1.38 |
| 3 | CS | 201 | Y43 | C5-C4 | 2.37 | 1.42 | 1.38 |
| 3 | CU | 201 | Y43 | C5-C4 | 2.37 | 1.42 | 1.38 |
| 3 | AS | 201 | Y43 | C5-C4 | 2.37 | 1.42 | 1.38 |
| 3 | AO | 201 | Y43 | C5-C4 | 2.36 | 1.42 | 1.38 |
| 3 | BN | 201 | Y43 | C6-N1 | 2.19 | 1.43 | 1.39 |
| 3 | AN | 201 | Y43 | C6-N1 | 2.17 | 1.43 | 1.39 |
| 3 | CN | 201 | Y43 | C6-N1 | 2.16 | 1.43 | 1.39 |
| 3 | AG | 201 | Y43 | C6-N1 | 2.11 | 1.43 | 1.39 |
| 3 | BG | 201 | Y43 | C6-N1 | 2.10 | 1.43 | 1.39 |
| 3 | BO | 201 | Y43 | C6-N1 | 2.09 | 1.43 | 1.39 |
| 3 | CO | 201 | Y43 | C6-N1 | 2.09 | 1.43 | 1.39 |
| 3 | BS | 201 | Y43 | C6-N1 | 2.08 | 1.43 | 1.39 |
| 3 | AO | 201 | Y43 | C6-N1 | 2.08 | 1.43 | 1.39 |
| 3 | DG | 201 | Y43 | C6-N1 | 2.08 | 1.43 | 1.39 |
| 3 | AS | 201 | Y43 | C6-N1 | 2.07 | 1.43 | 1.39 |
| 3 | CG | 201 | Y43 | C6-N1 | 2.07 | 1.43 | 1.39 |
| 3 | CC | 201 | Y43 | C6-N1 | 2.07 | 1.43 | 1.39 |
| 3 | BC | 201 | Y43 | C6-N1 | 2.06 | 1.43 | 1.39 |
| 3 | CS | 201 | Y43 | C6-N1 | 2.05 | 1.43 | 1.39 |
| 3 | DI | 201 | Y43 | C6-N1 | 2.05 | 1.43 | 1.39 |
| 3 | DB | 201 | Y43 | C6-N1 | 2.04 | 1.43 | 1.39 |
| 3 | AC | 201 | Y43 | C6-N1 | 2.04 | 1.43 | 1.39 |
| 3 | AB | 201 | Y43 | C6-N1 | 2.04 | 1.43 | 1.39 |
| 3 | BB | 201 | Y43 | C6-N1 | 2.03 | 1.43 | 1.39 |
| 3 | CB | 201 | Y43 | C6-N1 | 2.03 | 1.43 | 1.39 |
| 3 | DC | 201 | Y43 | C6-N1 | 2.03 | 1.43 | 1.39 |
| 3 | AI | 201 | Y43 | C6-N1 | 2.02 | 1.43 | 1.39 |
| 3 | CI | 201 | Y43 | C6-N1 | 2.01 | 1.43 | 1.39 |
| 3 | BI | 201 | Y43 | C6-N1 | 2.01 | 1.43 | 1.39 |
| 3 | AU | 201 | Y43 | C6-N1 | 2.01 | 1.43 | 1.39 |

All (172) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | BB | 201 | Y43 | O6-C6-N1 | -4.61 | 114.58 | 120.52 |
| 3 | DB | 201 | Y43 | O6-C6-N1 | -4.61 | 114.59 | 120.52 |
| 3 | AB | 201 | Y43 | O6-C6-N1 | -4.59 | 114.61 | 120.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | CB | 201 | Y43 | O6-C6-N1 | -4.58 | 114.62 | 120.52 |
| 3 | DC | 201 | Y43 | O6-C6-N1 | -4.55 | 114.66 | 120.52 |
| 3 | CC | 201 | Y43 | O6-C6-N1 | -4.54 | 114.67 | 120.52 |
| 3 | BC | 201 | Y43 | O6-C6-N1 | -4.54 | 114.68 | 120.52 |
| 3 | BN | 201 | Y43 | O6-C6-N1 | -4.54 | 114.68 | 120.52 |
| 3 | AN | 201 | Y43 | O6-C6-N1 | -4.53 | 114.69 | 120.52 |
| 3 | AC | 201 | Y43 | O6-C6-N1 | -4.53 | 114.69 | 120.52 |
| 3 | CN | 201 | Y43 | O6-C6-N1 | -4.52 | 114.69 | 120.52 |
| 3 | DI | 201 | Y43 | O6-C6-N1 | -4.51 | 114.72 | 120.52 |
| 3 | CG | 201 | Y43 | O6-C6-N1 | -4.50 | 114.73 | 120.52 |
| 3 | BI | 201 | Y43 | O6-C6-N1 | -4.49 | 114.73 | 120.52 |
| 3 | AO | 201 | Y43 | O6-C6-N1 | -4.49 | 114.74 | 120.52 |
| 3 | AU | 201 | Y43 | O6-C6-N1 | -4.49 | 114.74 | 120.52 |
| 3 | CU | 201 | Y43 | O6-C6-N1 | -4.49 | 114.75 | 120.52 |
| 3 | AI | 201 | Y43 | O6-C6-N1 | -4.48 | 114.75 | 120.52 |
| 3 | BG | 201 | Y43 | O6-C6-N1 | -4.48 | 114.75 | 120.52 |
| 3 | AG | 201 | Y43 | O6-C6-N1 | -4.48 | 114.76 | 120.52 |
| 3 | BO | 201 | Y43 | O6-C6-N1 | -4.47 | 114.76 | 120.52 |
| 3 | BS | 201 | Y43 | O6-C6-N1 | -4.47 | 114.77 | 120.52 |
| 3 | AS | 201 | Y43 | O6-C6-N1 | -4.47 | 114.77 | 120.52 |
| 3 | BU | 201 | Y43 | O6-C6-N1 | -4.47 | 114.77 | 120.52 |
| 3 | CS | 201 | Y43 | O6-C6-N1 | -4.47 | 114.77 | 120.52 |
| 3 | CI | 201 | Y43 | O6-C6-N1 | -4.45 | 114.78 | 120.52 |
| 3 | DG | 201 | Y43 | O6-C6-N1 | -4.45 | 114.80 | 120.52 |
| 3 | CO | 201 | Y43 | O6-C6-N1 | -4.44 | 114.80 | 120.52 |
| 3 | AI | 201 | Y43 | C8-N9-C4 | -4.20 | 103.21 | 106.71 |
| 3 | CI | 201 | Y43 | C8-N9-C4 | -4.18 | 103.23 | 106.71 |
| 3 | BI | 201 | Y43 | C8-N9-C4 | -4.17 | 103.24 | 106.71 |
| 3 | DI | 201 | Y43 | C8-N9-C4 | -4.16 | 103.25 | 106.71 |
| 3 | CN | 201 | Y43 | OAH-PAI-OAK | -4.07 | 93.15 | 109.07 |
| 3 | BN | 201 | Y43 | OAH-PAI-OAK | -4.07 | 93.16 | 109.07 |
| 3 | AN | 201 | Y43 | OAH-PAI-OAK | -4.07 | 93.18 | 109.07 |
| 3 | CU | 201 | Y43 | OAH-PAI-OAK | -4.05 | 93.24 | 109.07 |
| 3 | CI | 201 | Y43 | OAH-PAI-OAK | -4.05 | 93.25 | 109.07 |
| 3 | BI | 201 | Y43 | OAH-PAI-OAK | -4.05 | 93.25 | 109.07 |
| 3 | DI | 201 | Y43 | OAH-PAI-OAK | -4.05 | 93.26 | 109.07 |
| 3 | BU | 201 | Y43 | OAH-PAI-OAK | -4.05 | 93.26 | 109.07 |
| 3 | AI | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.26 | 109.07 |
| 3 | DC | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.27 | 109.07 |
| 3 | AU | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.27 | 109.07 |
| 3 | BC | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.29 | 109.07 |
| 3 | CC | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.29 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | AC | 201 | Y43 | OAH-PAI-OAK | -4.04 | 93.29 | 109.07 |
| 3 | CS | 201 | Y43 | OAH-PAI-OAK | -3.97 | 93.57 | 109.07 |
| 3 | BS | 201 | Y43 | OAH-PAI-OAK | -3.97 | 93.57 | 109.07 |
| 3 | AS | 201 | Y43 | OAH-PAI-OAK | -3.96 | 93.61 | 109.07 |
| 3 | CO | 201 | Y43 | OAH-PAI-OAK | -3.94 | 93.68 | 109.07 |
| 3 | BO | 201 | Y43 | OAH-PAI-OAK | -3.94 | 93.68 | 109.07 |
| 3 | AO | 201 | Y43 | OAH-PAI-OAK | -3.93 | 93.69 | 109.07 |
| 3 | AB | 201 | Y43 | OAH-PAI-OAK | -3.91 | 93.79 | 109.07 |
| 3 | BB | 201 | Y43 | OAH-PAI-OAK | -3.91 | 93.80 | 109.07 |
| 3 | CB | 201 | Y43 | OAH-PAI-OAK | -3.91 | 93.80 | 109.07 |
| 3 | DB | 201 | Y43 | OAH-PAI-OAK | -3.90 | 93.83 | 109.07 |
| 3 | CG | 201 | Y43 | OAH-PAI-OAK | -3.87 | 93.93 | 109.07 |
| 3 | BG | 201 | Y43 | C8-N9-C4 | -3.87 | 103.48 | 106.71 |
| 3 | AG | 201 | Y43 | OAH-PAI-OAK | -3.87 | 93.95 | 109.07 |
| 3 | DG | 201 | Y43 | OAH-PAI-OAK | -3.87 | 93.95 | 109.07 |
| 3 | BG | 201 | Y43 | OAH-PAI-OAK | -3.87 | 93.95 | 109.07 |
| 3 | CG | 201 | Y43 | C8-N9-C4 | -3.86 | 103.49 | 106.71 |
| 3 | DC | 201 | Y43 | C8-N9-C4 | -3.84 | 103.51 | 106.71 |
| 3 | DG | 201 | Y43 | C8-N9-C4 | -3.83 | 103.52 | 106.71 |
| 3 | CB | 201 | Y43 | C8-N9-C4 | -3.83 | 103.52 | 106.71 |
| 3 | BB | 201 | Y43 | C8-N9-C4 | -3.83 | 103.52 | 106.71 |
| 3 | CC | 201 | Y43 | C8-N9-C4 | -3.83 | 103.52 | 106.71 |
| 3 | DB | 201 | Y43 | C8-N9-C4 | -3.82 | 103.53 | 106.71 |
| 3 | BC | 201 | Y43 | C8-N9-C4 | -3.82 | 103.53 | 106.71 |
| 3 | AB | 201 | Y43 | C8-N9-C4 | -3.80 | 103.55 | 106.71 |
| 3 | AG | 201 | Y43 | C8-N9-C4 | -3.80 | 103.55 | 106.71 |
| 3 | AC | 201 | Y43 | C8-N9-C4 | -3.78 | 103.56 | 106.71 |
| 3 | BN | 201 | Y43 | C8-N9-C4 | -3.76 | 103.57 | 106.71 |
| 3 | AS | 201 | Y43 | C8-N9-C4 | -3.76 | 103.58 | 106.71 |
| 3 | AN | 201 | Y43 | C8-N9-C4 | -3.74 | 103.59 | 106.71 |
| 3 | BS | 201 | Y43 | C8-N9-C4 | -3.71 | 103.61 | 106.71 |
| 3 | CS | 201 | Y43 | C8-N9-C4 | -3.71 | 103.62 | 106.71 |
| 3 | CN | 201 | Y43 | C8-N9-C4 | -3.71 | 103.62 | 106.71 |
| 3 | AO | 201 | Y43 | C8-N9-C4 | -3.70 | 103.63 | 106.71 |
| 3 | AU | 201 | Y43 | C8-N9-C4 | -3.70 | 103.63 | 106.71 |
| 3 | CO | 201 | Y43 | C8-N9-C4 | -3.69 | 103.63 | 106.71 |
| 3 | BO | 201 | Y43 | C8-N9-C4 | -3.66 | 103.66 | 106.71 |
| 3 | CU | 201 | Y43 | C8-N9-C4 | -3.64 | 103.67 | 106.71 |
| 3 | BU | 201 | Y43 | C8-N9-C4 | -3.63 | 103.68 | 106.71 |
| 3 | AG | 201 | Y43 | OAE-CAD-N9 | 3.50 | 114.12 | 107.86 |
| 3 | CG | 201 | Y43 | OAE-CAD-N9 | 3.50 | 114.12 | 107.86 |
| 3 | DG | 201 | Y43 | OAE-CAD-N9 | 3.50 | 114.12 | 107.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | BG | 201 | Y43 | OAE-CAD-N9 | 3.50 | 114.11 | 107.86 |
| 3 | CG | 201 | Y43 | OAJ-PAI-OAH | -3.39 | 91.99 | 107.75 |
| 3 | AG | 201 | Y43 | OAJ-PAI-OAH | -3.39 | 92.00 | 107.75 |
| 3 | BG | 201 | Y43 | OAJ-PAI-OAH | -3.39 | 92.01 | 107.75 |
| 3 | AS | 201 | Y43 | C5-C4-N9 | 3.39 | 107.82 | 106.23 |
| 3 | DG | 201 | Y43 | OAJ-PAI-OAH | -3.39 | 92.02 | 107.75 |
| 3 | CS | 201 | Y43 | C5-C4-N9 | 3.38 | 107.81 | 106.23 |
| 3 | BS | 201 | Y43 | C5-C4-N9 | 3.37 | 107.81 | 106.23 |
| 3 | DC | 201 | Y43 | OAE-CAD-N9 | 3.28 | 113.73 | 107.86 |
| 3 | AC | 201 | Y43 | OAE-CAD-N9 | 3.28 | 113.72 | 107.86 |
| 3 | BC | 201 | Y43 | OAE-CAD-N9 | 3.27 | 113.72 | 107.86 |
| 3 | CC | 201 | Y43 | OAE-CAD-N9 | 3.27 | 113.71 | 107.86 |
| 3 | CB | 201 | Y43 | C5-C4-N9 | 3.23 | 107.75 | 106.23 |
| 3 | AB | 201 | Y43 | C5-C4-N9 | 3.23 | 107.75 | 106.23 |
| 3 | BB | 201 | Y43 | C5-C4-N9 | 3.22 | 107.74 | 106.23 |
| 3 | CB | 201 | Y43 | OAE-CAD-N9 | 3.22 | 113.61 | 107.86 |
| 3 | CC | 201 | Y43 | C5-C4-N9 | 3.22 | 107.74 | 106.23 |
| 3 | DB | 201 | Y43 | OAE-CAD-N9 | 3.22 | 113.61 | 107.86 |
| 3 | BB | 201 | Y43 | OAE-CAD-N9 | 3.21 | 113.60 | 107.86 |
| 3 | AB | 201 | Y43 | OAE-CAD-N9 | 3.21 | 113.60 | 107.86 |
| 3 | CU | 201 | Y43 | OAJ-PAI-OAH | -3.20 | 92.90 | 107.75 |
| 3 | BU | 201 | Y43 | OAJ-PAI-OAH | -3.19 | 92.92 | 107.75 |
| 3 | DC | 201 | Y43 | C5-C4-N9 | 3.19 | 107.72 | 106.23 |
| 3 | AU | 201 | Y43 | OAJ-PAI-OAH | -3.18 | 92.97 | 107.75 |
| 3 | CN | 201 | Y43 | OAE-CAD-N9 | 3.18 | 113.54 | 107.86 |
| 3 | BN | 201 | Y43 | OAE-CAD-N9 | 3.17 | 113.53 | 107.86 |
| 3 | BC | 201 | Y43 | C5-C4-N9 | 3.17 | 107.72 | 106.23 |
| 3 | AN | 201 | Y43 | OAE-CAD-N9 | 3.16 | 113.50 | 107.86 |
| 3 | DB | 201 | Y43 | C5-C4-N9 | 3.16 | 107.71 | 106.23 |
| 3 | AO | 201 | Y43 | OAE-CAD-N9 | 3.15 | 113.49 | 107.86 |
| 3 | AO | 201 | Y43 | OAJ-PAI-OAH | -3.15 | 93.12 | 107.75 |
| 3 | CO | 201 | Y43 | OAE-CAD-N9 | 3.14 | 113.48 | 107.86 |
| 3 | BO | 201 | Y43 | OAJ-PAI-OAH | -3.14 | 93.15 | 107.75 |
| 3 | CO | 201 | Y43 | OAJ-PAI-OAH | -3.14 | 93.16 | 107.75 |
| 3 | AU | 201 | Y43 | C5-C4-N9 | 3.14 | 107.70 | 106.23 |
| 3 | BO | 201 | Y43 | OAE-CAD-N9 | 3.13 | 113.46 | 107.86 |
| 3 | CN | 201 | Y43 | OAJ-PAI-OAH | -3.12 | 93.23 | 107.75 |
| 3 | BG | 201 | Y43 | C5-C4-N9 | 3.12 | 107.70 | 106.23 |
| 3 | AN | 201 | Y43 | OAJ-PAI-OAH | -3.12 | 93.25 | 107.75 |
| 3 | BN | 201 | Y43 | OAJ-PAI-OAH | -3.12 | 93.25 | 107.75 |
| 3 | CU | 201 | Y43 | C5-C4-N9 | 3.11 | 107.69 | 106.23 |
| 3 | DG | 201 | Y43 | C5-C4-N9 | 3.11 | 107.69 | 106.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | AC | 201 | Y43 | C5-C4-N9 | 3.10 | 107.69 | 106.23 |
| 3 | CG | 201 | Y43 | C5-C4-N9 | 3.09 | 107.68 | 106.23 |
| 3 | AB | 201 | Y43 | OAJ-PAI-OAH | -3.08 | 93.42 | 107.75 |
| 3 | CB | 201 | Y43 | OAJ-PAI-OAH | -3.08 | 93.45 | 107.75 |
| 3 | BB | 201 | Y43 | OAJ-PAI-OAH | -3.08 | 93.46 | 107.75 |
| 3 | DB | 201 | Y43 | OAJ-PAI-OAH | -3.07 | 93.46 | 107.75 |
| 3 | AO | 201 | Y43 | C5-C4-N9 | 3.06 | 107.67 | 106.23 |
| 3 | BU | 201 | Y43 | C5-C4-N9 | 3.06 | 107.67 | 106.23 |
| 3 | CI | 201 | Y43 | C5-C4-N9 | 3.05 | 107.66 | 106.23 |
| 3 | CC | 201 | Y43 | OAJ-PAI-OAH | -3.05 | 93.56 | 107.75 |
| 3 | BC | 201 | Y43 | OAJ-PAI-OAH | -3.05 | 93.57 | 107.75 |
| 3 | AG | 201 | Y43 | C5-C4-N9 | 3.05 | 107.66 | 106.23 |
| 3 | AC | 201 | Y43 | OAJ-PAI-OAH | -3.05 | 93.59 | 107.75 |
| 3 | DC | 201 | Y43 | OAJ-PAI-OAH | -3.05 | 93.59 | 107.75 |
| 3 | DI | 201 | Y43 | C5-C4-N9 | 3.04 | 107.66 | 106.23 |
| 3 | CO | 201 | Y43 | C5-C4-N9 | 3.03 | 107.65 | 106.23 |
| 3 | BI | 201 | Y43 | C5-C4-N9 | 3.00 | 107.64 | 106.23 |
| 3 | AI | 201 | Y43 | OAJ-PAI-OAH | -2.99 | 93.84 | 107.75 |
| 3 | CI | 201 | Y43 | OAJ-PAI-OAH | -2.99 | 93.85 | 107.75 |
| 3 | BO | 201 | Y43 | C5-C4-N9 | 2.99 | 107.63 | 106.23 |
| 3 | BI | 201 | Y43 | OAJ-PAI-OAH | -2.99 | 93.86 | 107.75 |
| 3 | DI | 201 | Y43 | OAJ-PAI-OAH | -2.99 | 93.87 | 107.75 |
| 3 | AI | 201 | Y43 | C5-C4-N9 | 2.98 | 107.63 | 106.23 |
| 3 | BS | 201 | Y43 | OAE-CAD-N9 | 2.95 | 113.14 | 107.86 |
| 3 | AS | 201 | Y43 | OAE-CAD-N9 | 2.94 | 113.12 | 107.86 |
| 3 | CS | 201 | Y43 | OAE-CAD-N9 | 2.94 | 113.11 | 107.86 |
| 3 | BN | 201 | Y43 | C5-C4-N9 | 2.93 | 107.61 | 106.23 |
| 3 | BS | 201 | Y43 | OAJ-PAI-OAH | -2.90 | 94.28 | 107.75 |
| 3 | CS | 201 | Y43 | OAJ-PAI-OAH | -2.89 | 94.31 | 107.75 |
| 3 | AS | 201 | Y43 | OAJ-PAI-OAH | -2.89 | 94.31 | 107.75 |
| 3 | AN | 201 | Y43 | C5-C4-N9 | 2.84 | 107.56 | 106.23 |
| 3 | CN | 201 | Y43 | C5-C4-N9 | 2.82 | 107.56 | 106.23 |
| 3 | CU | 201 | Y43 | OAE-CAD-N9 | 2.62 | 112.55 | 107.86 |
| 3 | BU | 201 | Y43 | OAE-CAD-N9 | 2.62 | 112.54 | 107.86 |
| 3 | AU | 201 | Y43 | OAE-CAD-N9 | 2.61 | 112.53 | 107.86 |
| 3 | AI | 201 | Y43 | OAE-CAD-N9 | 2.57 | 112.45 | 107.86 |
| 3 | BI | 201 | Y43 | OAE-CAD-N9 | 2.56 | 112.43 | 107.86 |
| 3 | CI | 201 | Y43 | OAE-CAD-N9 | 2.54 | 112.41 | 107.86 |
| 3 | DI | 201 | Y43 | OAE-CAD-N9 | 2.54 | 112.40 | 107.86 |
| 3 | BI | 201 | Y43 | CAD-N9-C8 | -2.06 | 123.23 | 127.85 |
| 3 | DI | 201 | Y43 | CAD-N9-C8 | -2.06 | 123.24 | 127.85 |
| 3 | CI | 201 | Y43 | CAD-N9-C8 | -2.06 | 123.24 | 127.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | AI | 201 | Y43 | CAD-N9-C8 | -2.05 | 123.26 | 127.85 |

All (56) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 3 | BC | 201 | Y43 | CAF |
| 3 | BC | 201 | Y43 | CAD |
| 3 | BG | 201 | Y43 | CAF |
| 3 | BG | 201 | Y43 | CAD |
| 3 | BI | 201 | Y43 | CAF |
| 3 | BI | 201 | Y43 | CAD |
| 3 | BN | 201 | Y43 | CAF |
| 3 | BN | 201 | Y43 | CAD |
| 3 | BO | 201 | Y43 | CAF |
| 3 | BO | 201 | Y43 | CAD |
| 3 | BS | 201 | Y43 | CAF |
| 3 | BS | 201 | Y43 | CAD |
| 3 | BU | 201 | Y43 | CAF |
| 3 | BU | 201 | Y43 | CAD |
| 3 | CB | 201 | Y43 | CAF |
| 3 | CB | 201 | Y43 | CAD |
| 3 | CC | 201 | Y43 | CAF |
| 3 | CC | 201 | Y43 | CAD |
| 3 | AB | 201 | Y43 | CAF |
| 3 | AB | 201 | Y43 | CAD |
| 3 | CG | 201 | Y43 | CAF |
| 3 | CG | 201 | Y43 | CAD |
| 3 | CI | 201 | Y43 | CAF |
| 3 | CI | 201 | Y43 | CAD |
| 3 | CN | 201 | Y43 | CAF |
| 3 | CN | 201 | Y43 | CAD |
| 3 | CO | 201 | Y43 | CAF |
| 3 | CO | 201 | Y43 | CAD |
| 3 | CS | 201 | Y43 | CAF |
| 3 | CS | 201 | Y43 | CAD |
| 3 | CU | 201 | Y43 | CAF |
| 3 | CU | 201 | Y43 | CAD |
| 3 | DB | 201 | Y43 | CAF |
| 3 | DB | 201 | Y43 | CAD |
| 3 | DC | 201 | Y43 | CAF |
| 3 | DC | 201 | Y43 | CAD |
| 3 | AC | 201 | Y43 | CAF |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 3 | AC | 201 | Y43 | CAD |
| 3 | DG | 201 | Y43 | CAF |
| 3 | DG | 201 | Y43 | CAD |
| 3 | DI | 201 | Y43 | CAF |
| 3 | DI | 201 | Y43 | CAD |
| 3 | AG | 201 | Y43 | CAF |
| 3 | AG | 201 | Y43 | CAD |
| 3 | AI | 201 | Y43 | CAF |
| 3 | AI | 201 | Y43 | CAD |
| 3 | AN | 201 | Y43 | CAF |
| 3 | AN | 201 | Y43 | CAD |
| 3 | AO | 201 | Y43 | CAF |
| 3 | AO | 201 | Y43 | CAD |
| 3 | AS | 201 | Y43 | CAF |
| 3 | AS | 201 | Y43 | CAD |
| 3 | AU | 201 | Y43 | CAF |
| 3 | AU | 201 | Y43 | CAD |
| 3 | BB | 201 | Y43 | CAF |
| 3 | BB | 201 | Y43 | CAD |

All (156) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | BC | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BG | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BG | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | BI | 201 | Y43 | CAC-CAD-N9-C4 |
| 3 | BI | 201 | Y43 | CAC-CAD-N9-C8 |
| 3 | BI | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BI | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BN | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BN | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | BO | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BO | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | BO | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | BS | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BS | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CB | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CB | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | CC | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AB | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AB | 201 | Y43 | CAG-OAH-PAI-OAL |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | CG | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CG | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | CI | 201 | Y43 | CAC-CAD-N9-C4 |
| 3 | CI | 201 | Y43 | CAC-CAD-N9-C8 |
| 3 | CI | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CI | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CN | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CN | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | CO | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CO | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | CO | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | CS | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CS | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | DB | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | DB | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | DC | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AC | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | DG | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | DG | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | DI | 201 | Y43 | CAC-CAD-N9-C4 |
| 3 | DI | 201 | Y43 | CAC-CAD-N9-C8 |
| 3 | DI | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | DI | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AG | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AG | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | AI | 201 | Y43 | CAC-CAD-N9-C4 |
| 3 | AI | 201 | Y43 | CAC-CAD-N9-C8 |
| 3 | AI | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AI | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AN | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AN | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | AO | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AO | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | AO | 201 | Y43 | PAM-OAL-PAI-OAH |
| 3 | AS | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AS | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BB | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BB | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | BC | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BG | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CC | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CG | 201 | Y43 | OAE-CAF-CAG-OAH |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | DC | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AC | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | DG | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AG | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BG | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BI | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BN | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CG | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CI | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CN | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | DG | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | DI | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AG | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AI | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AN | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BC | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BN | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BS | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CC | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | CN | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CS | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | DC | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AC | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | AN | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AS | 201 | Y43 | CAB-CAF-CAG-OAH |
| 3 | BN | 201 | Y43 | OAE-CAD-N9-C4 |
| 3 | CN | 201 | Y43 | OAE-CAD-N9-C4 |
| 3 | AN | 201 | Y43 | OAE-CAD-N9-C4 |
| 3 | BN | 201 | Y43 | OAE-CAD-N9-C8 |
| 3 | CN | 201 | Y43 | OAE-CAD-N9-C8 |
| 3 | AN | 201 | Y43 | OAE-CAD-N9-C8 |
| 3 | BO | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | CO | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | AO | 201 | Y43 | OAE-CAF-CAG-OAH |
| 3 | BO | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | CO | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | AO | 201 | Y43 | CAF-CAG-OAH-PAI |
| 3 | BN | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | CN | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | AN | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | BC | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | BG | 201 | Y43 | CAG-OAH-PAI-OAK |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | BN | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | BO | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | CB | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | CC | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | AB | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | CG | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | CN | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | CO | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | DB | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | DC | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | AC | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | DG | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | AG | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | AN | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | AO | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | BB | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | BU | 201 | Y43 | PAM-OAL-PAI-OAJ |
| 3 | BU | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | CB | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | AB | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | CU | 201 | Y43 | PAM-OAL-PAI-OAJ |
| 3 | CU | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | DB | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | AU | 201 | Y43 | PAM-OAL-PAI-OAJ |
| 3 | AU | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | BB | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | BC | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | CC | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | DC | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | AC | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | BG | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | CG | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | DG | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | AG | 201 | Y43 | CAG-OAH-PAI-OAL |
| 3 | BI | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | BN | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | BS | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | AB | 201 | Y43 | PAI-OAL-PAM-OAN |
| 3 | CI | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | CN | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | CS | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | DB | 201 | Y43 | PAI-OAL-PAM-OAN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | DI | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | AI | 201 | Y43 | PAM-OAL-PAI-OAK |
| 3 | AN | 201 | Y43 | PAQ-OAP-PAM-OAO |
| 3 | AS | 201 | Y43 | PAI-OAL-PAM-OAO |
| 3 | BS | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | CB | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | AB | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | CS | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | DB | 201 | Y43 | CAG-OAH-PAI-OAJ |
| 3 | AS | 201 | Y43 | CAG-OAH-PAI-OAK |
| 3 | BB | 201 | Y43 | CAG-OAH-PAI-OAJ |

There are no ring outliers.

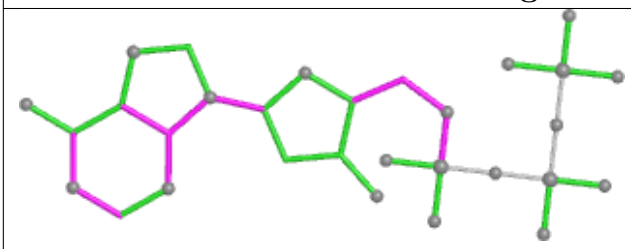
17 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | BS | 201 | Y43 | 2 | 0 |
| 3 | AU | 201 | Y43 | 1 | 0 |
| 3 | DI | 201 | Y43 | 1 | 0 |
| 3 | BN | 201 | Y43 | 1 | 0 |
| 3 | CI | 201 | Y43 | 1 | 0 |
| 3 | CU | 201 | Y43 | 1 | 0 |
| 3 | AG | 201 | Y43 | 1 | 0 |
| 3 | BU | 201 | Y43 | 1 | 0 |
| 3 | CN | 201 | Y43 | 1 | 0 |
| 3 | AN | 201 | Y43 | 1 | 0 |
| 3 | CS | 201 | Y43 | 2 | 0 |
| 3 | AO | 201 | Y43 | 1 | 0 |
| 3 | AC | 201 | Y43 | 1 | 0 |
| 3 | CG | 201 | Y43 | 1 | 0 |
| 3 | CO | 201 | Y43 | 1 | 0 |
| 3 | BO | 201 | Y43 | 1 | 0 |
| 3 | AI | 201 | Y43 | 1 | 0 |

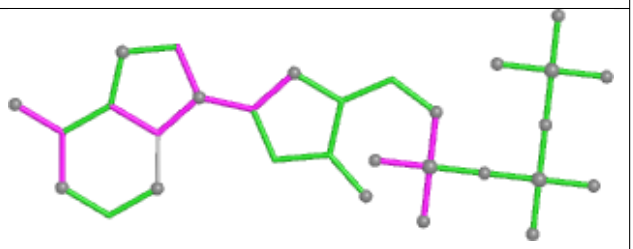
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

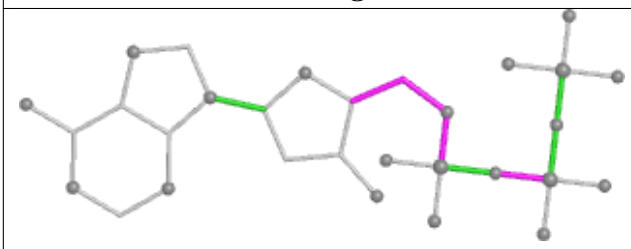
**Ligand Y43 BS 201**



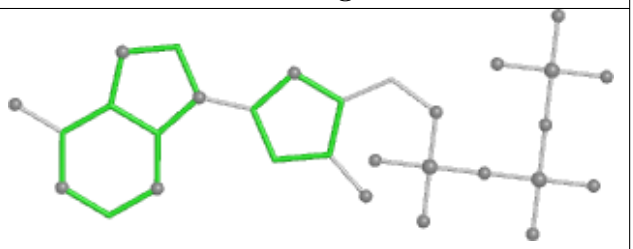
Bond lengths



Bond angles

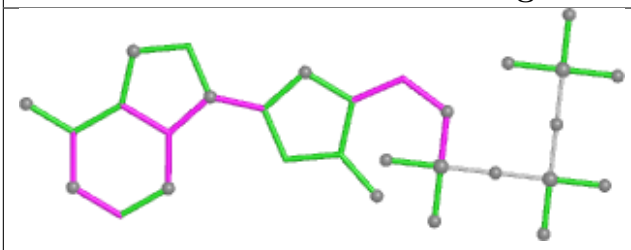


Torsions

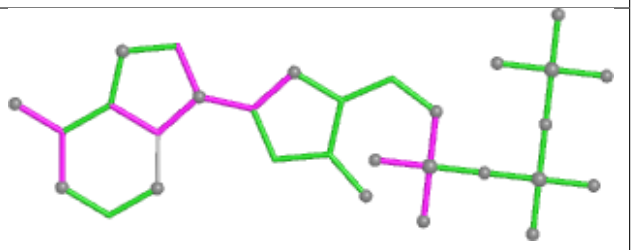


Rings

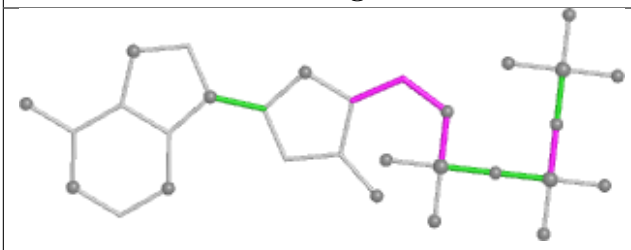
**Ligand Y43 CC 201**



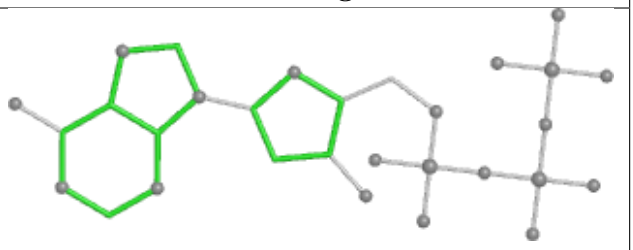
Bond lengths



Bond angles

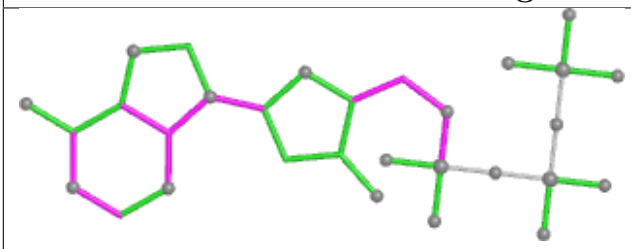


Torsions

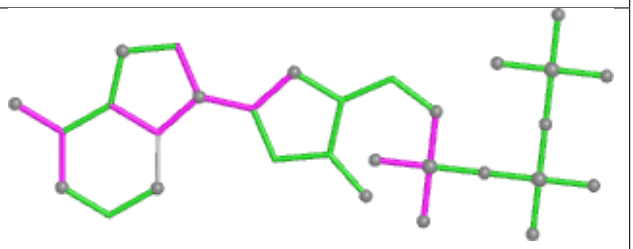


Rings

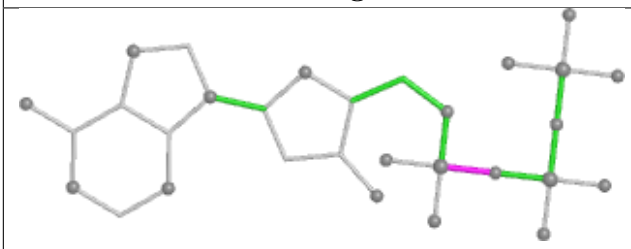
## Ligand Y43 AU 201



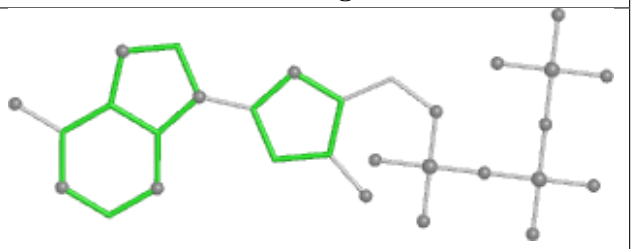
Bond lengths



Bond angles

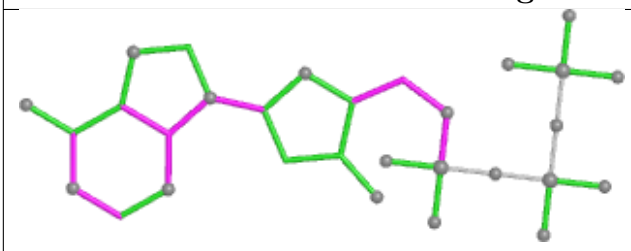


Torsions

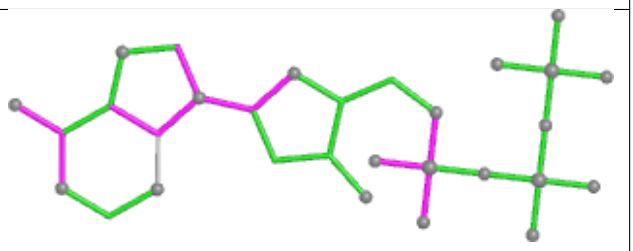


Rings

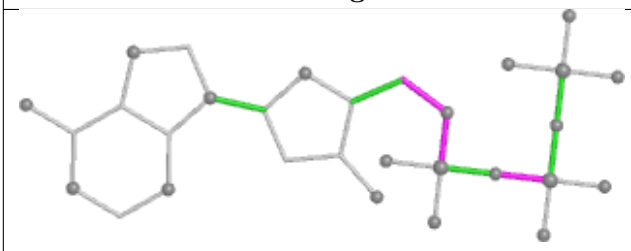
## Ligand Y43 AB 201



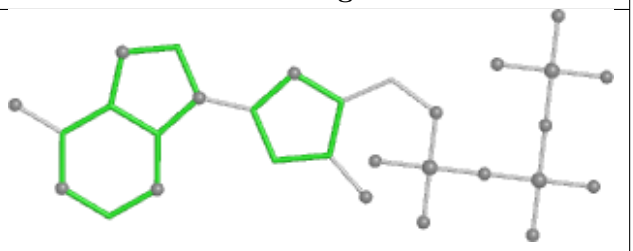
Bond lengths



Bond angles

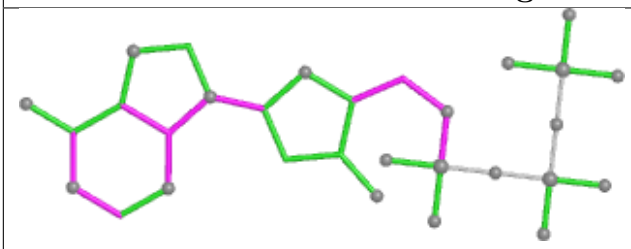


Torsions

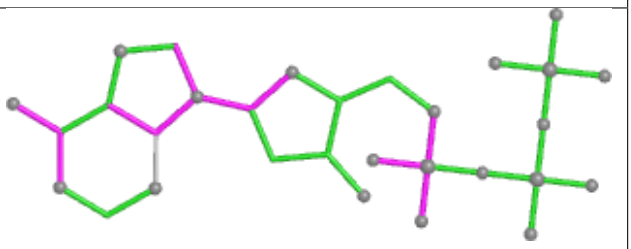


Rings

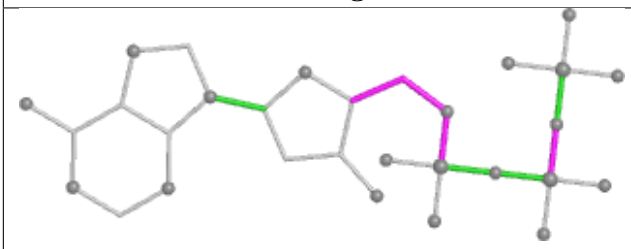
## Ligand Y43 DC 201



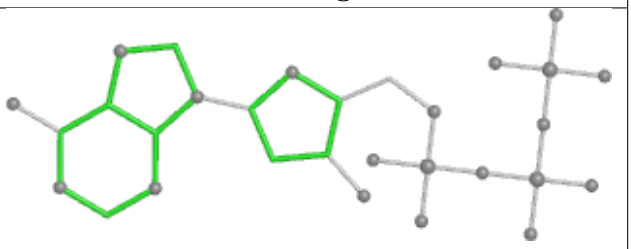
Bond lengths



Bond angles

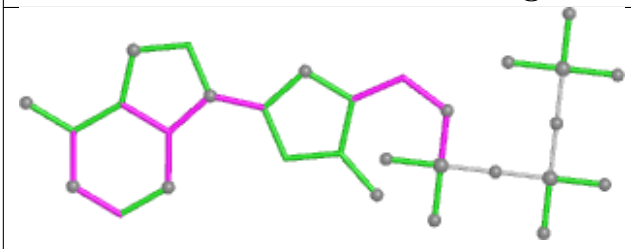


Torsions

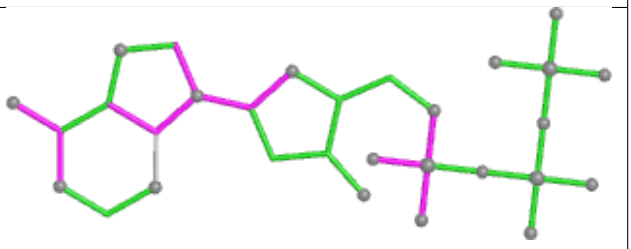


Rings

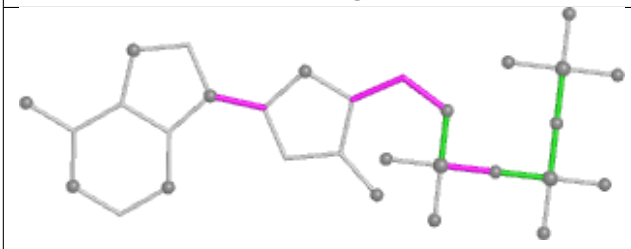
## Ligand Y43 DI 201



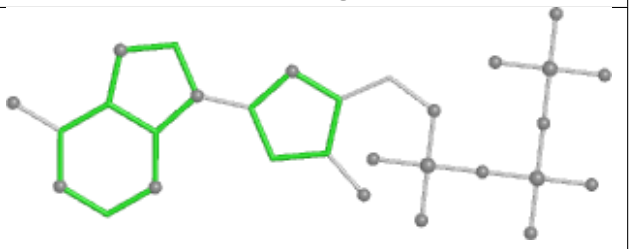
Bond lengths



Bond angles

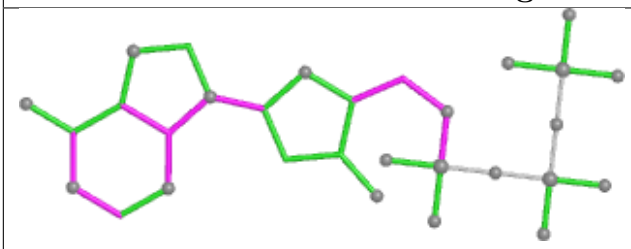


Torsions

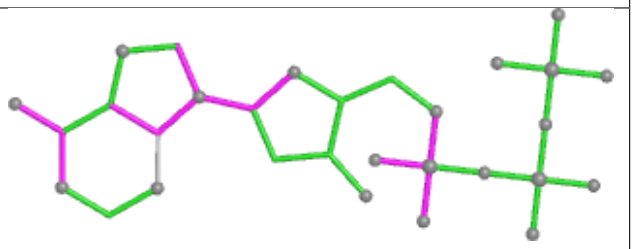


Rings

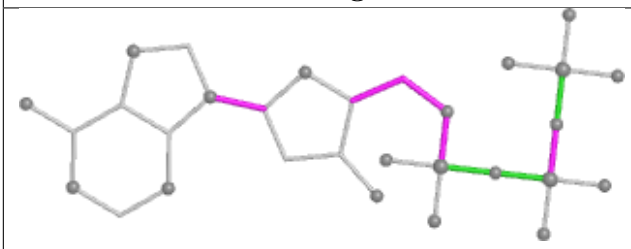
## Ligand Y43 BN 201



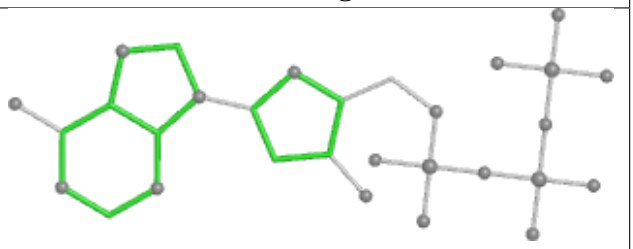
Bond lengths



Bond angles

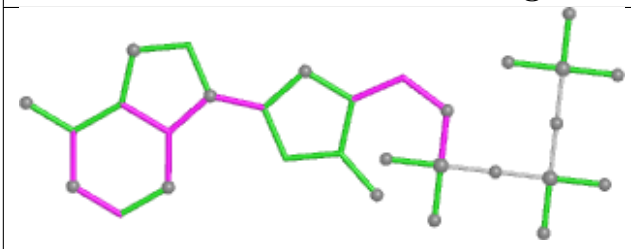


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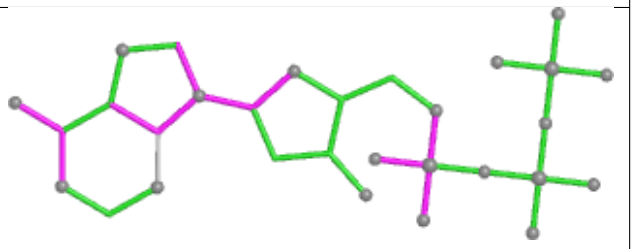


Rings

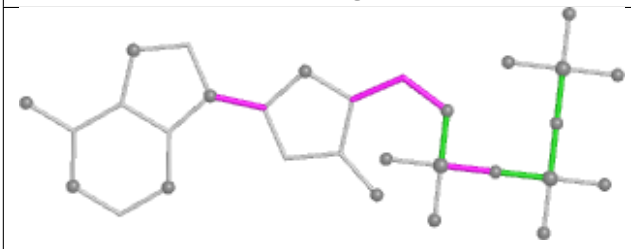
## Ligand Y43 CI 201



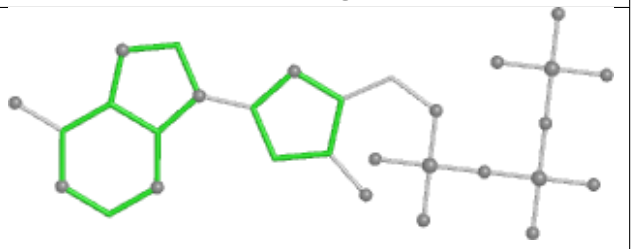
Bond lengths



Bond angles

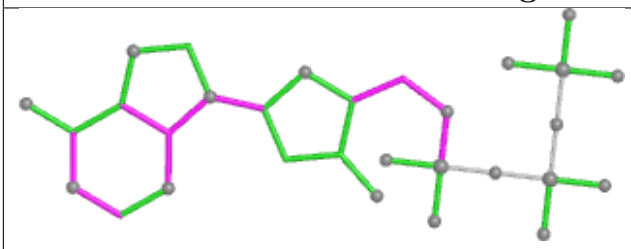


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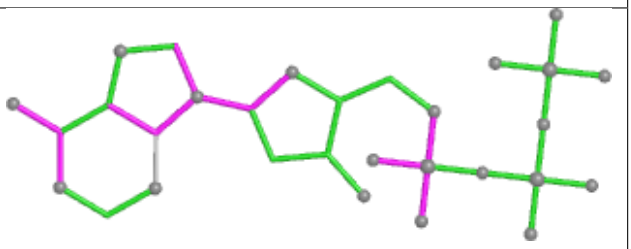


Rings

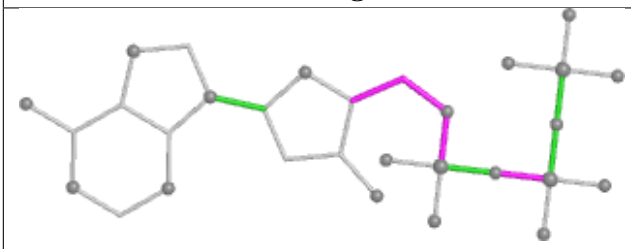
## Ligand Y43 AS 201



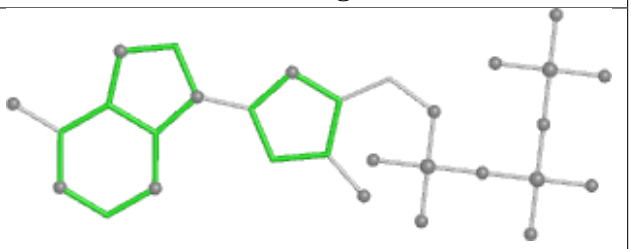
Bond lengths



Bond angles

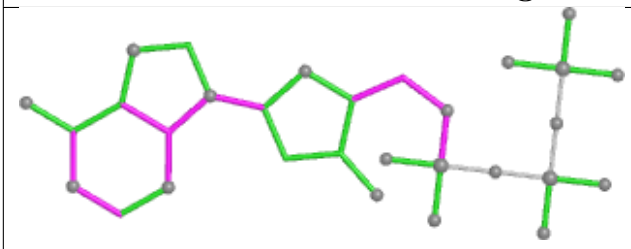


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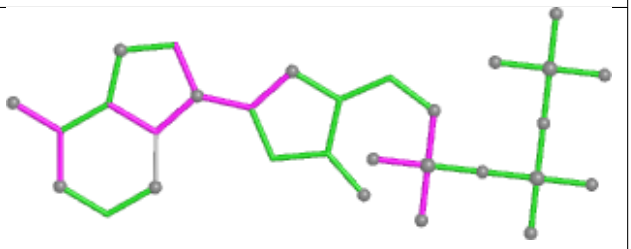


Rings

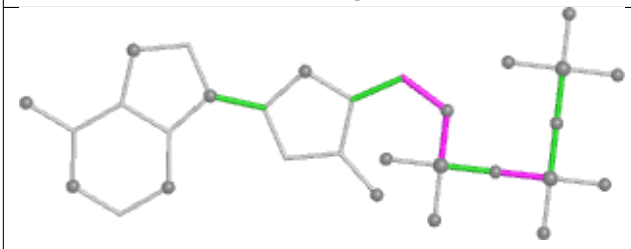
## Ligand Y43 DB 201



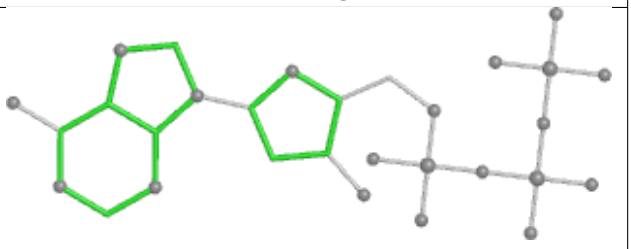
Bond lengths



Bond angles

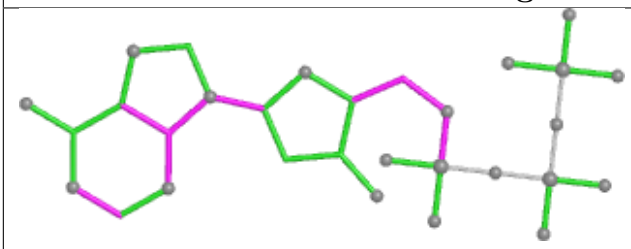


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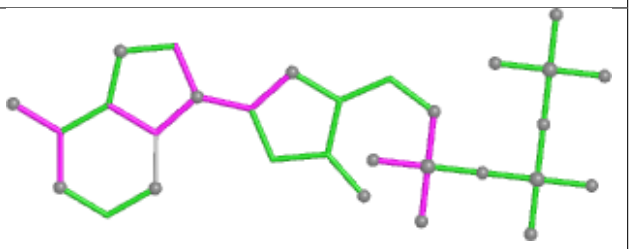


Rings

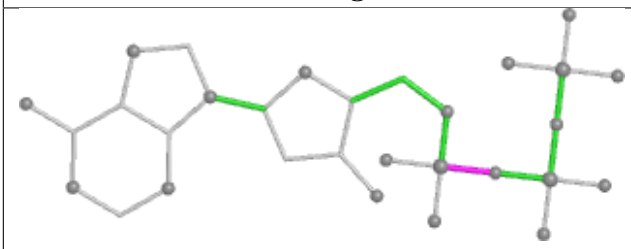
## Ligand Y43 CU 201



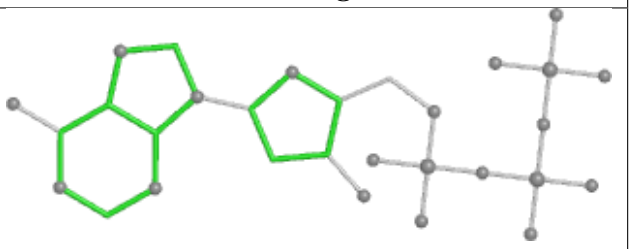
Bond lengths



Bond angles

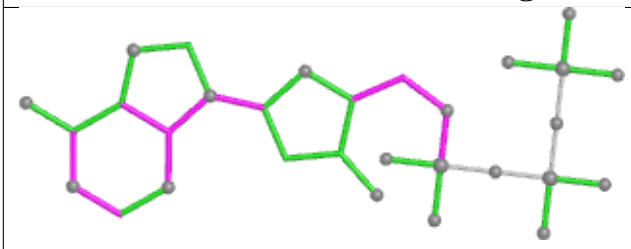


Torsions

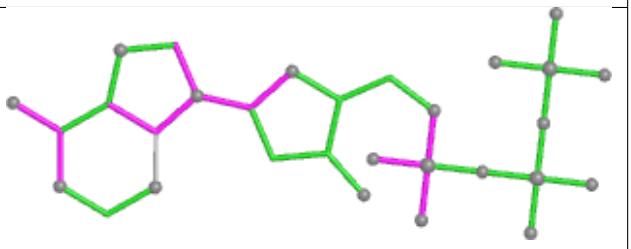


Rings

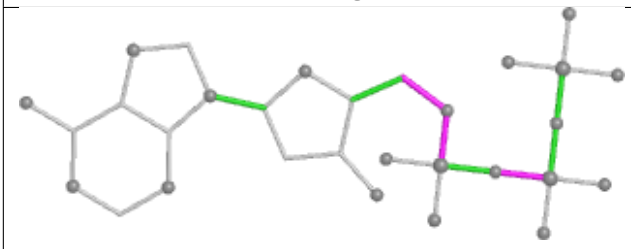
## Ligand Y43 BB 201



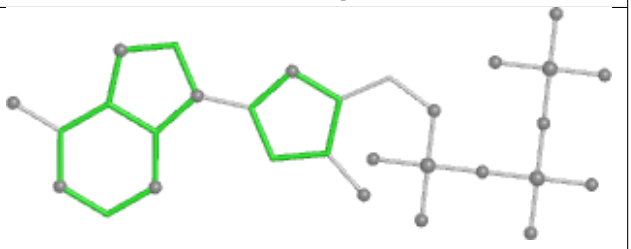
Bond lengths



Bond angles

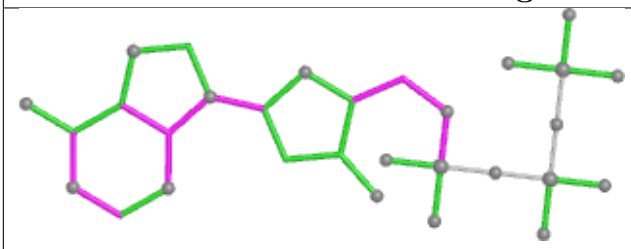


Torsions

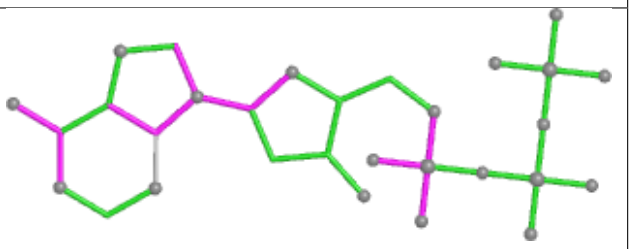


Rings

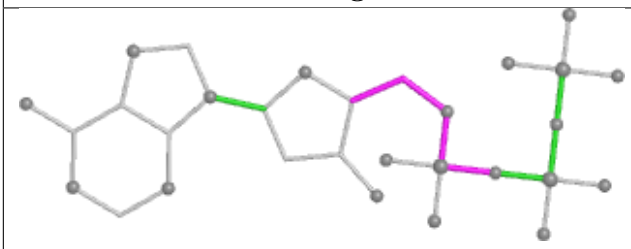
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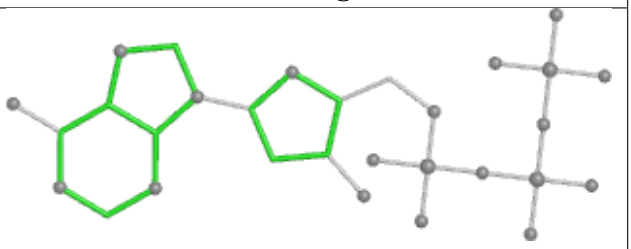
Bond lengths



Bond angles

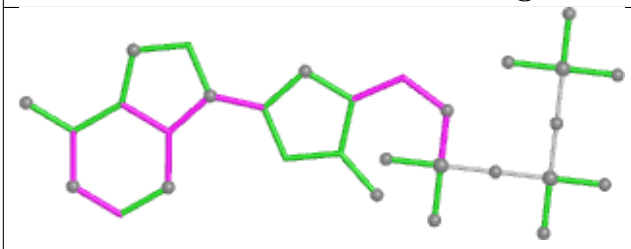


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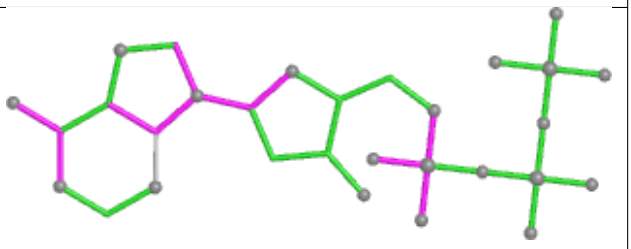


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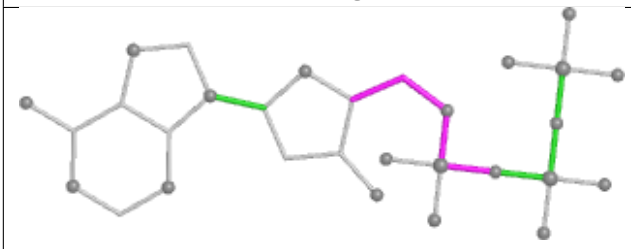
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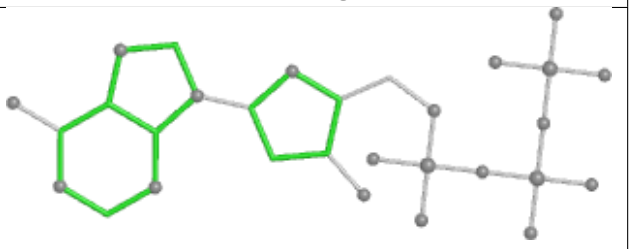
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Bond angles

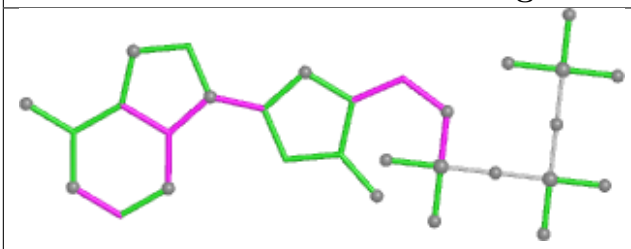


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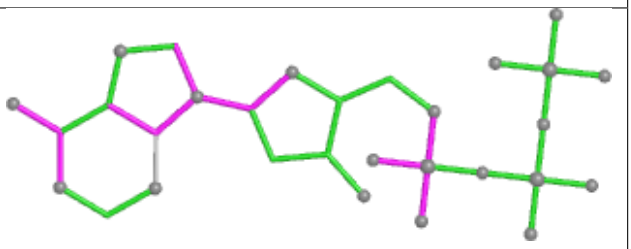


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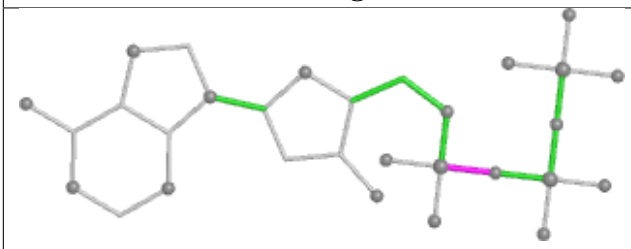
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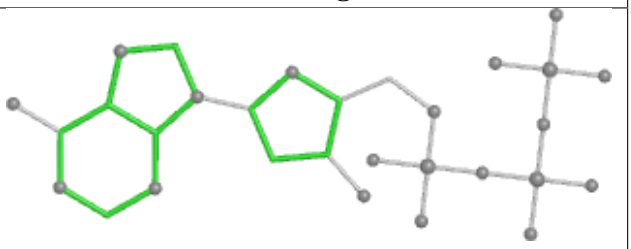
Bond lengths



Bond angles

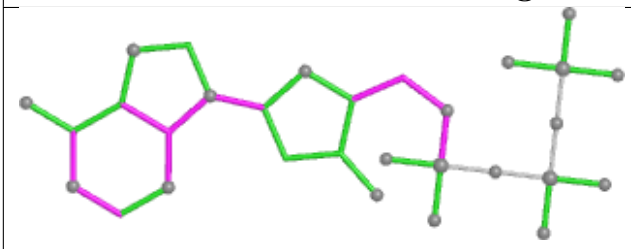


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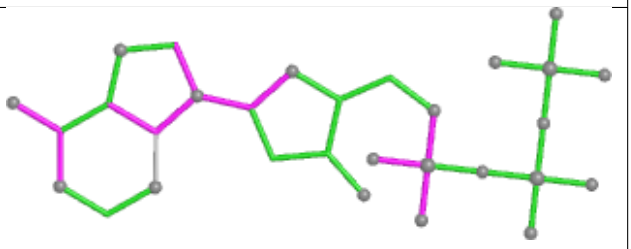


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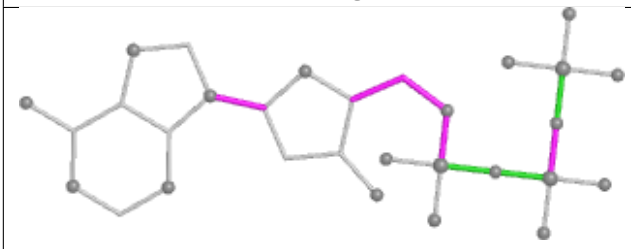
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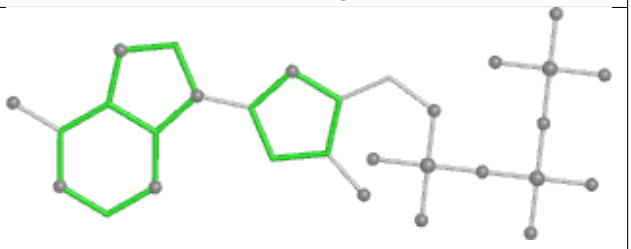
Bond lengths



Bond angles

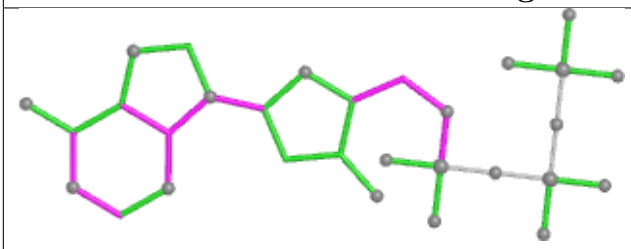


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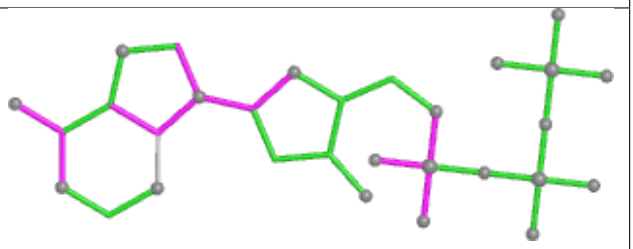


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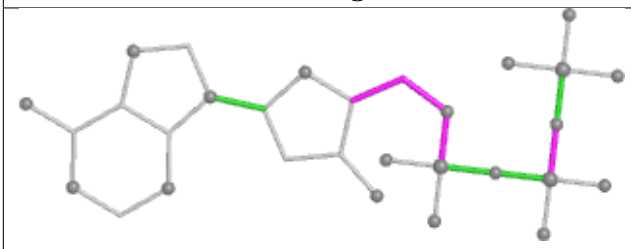
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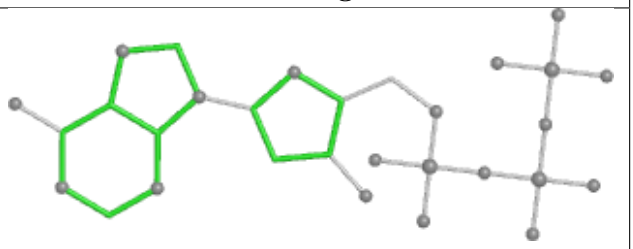
Bond lengths



Bond angles

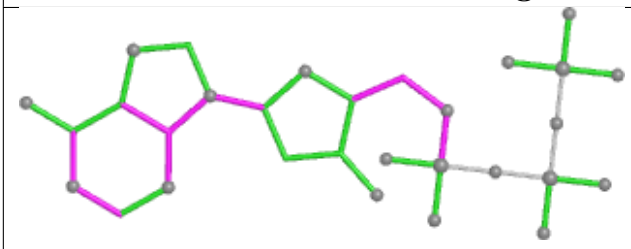


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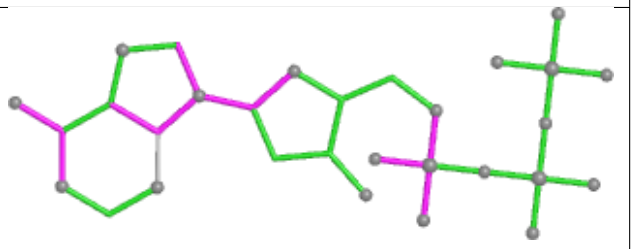


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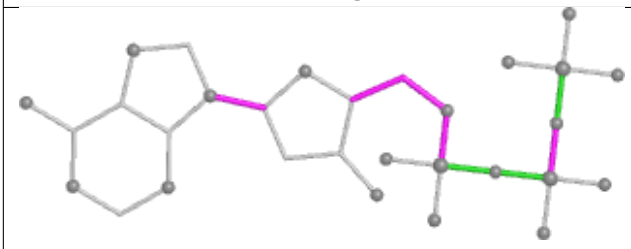
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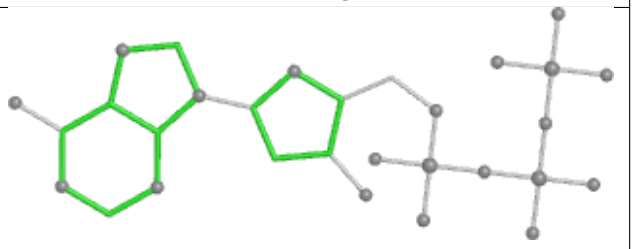
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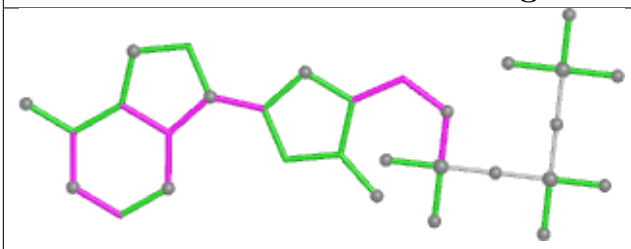


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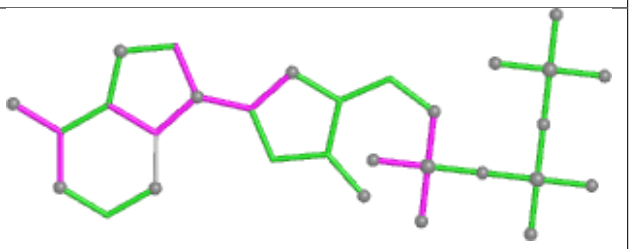


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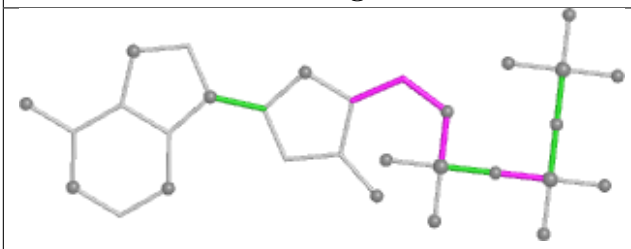
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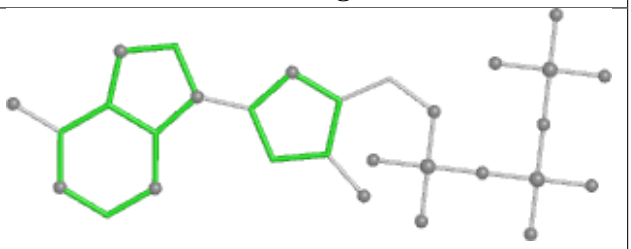
Bond lengths



Bond angles

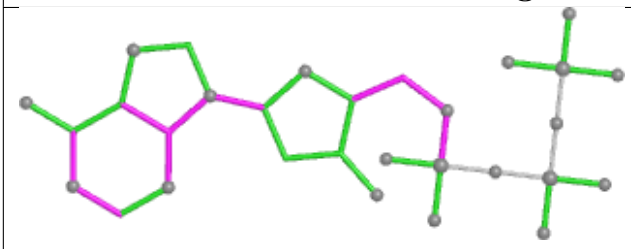


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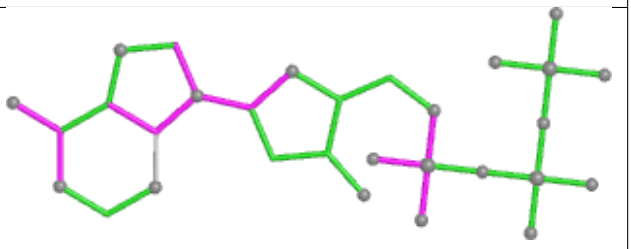


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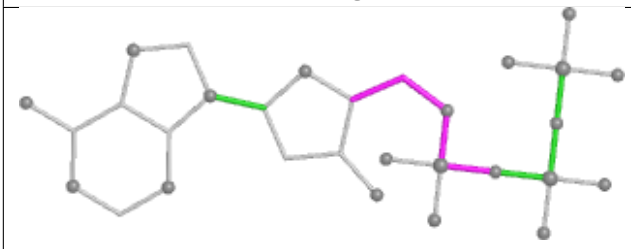
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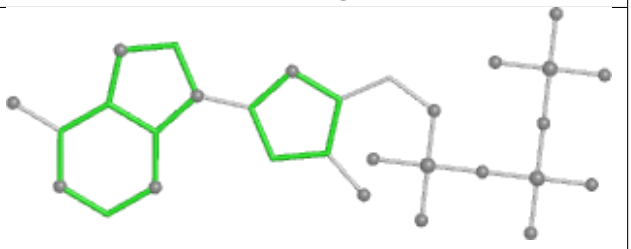
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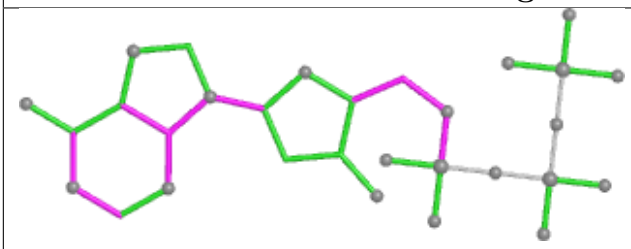


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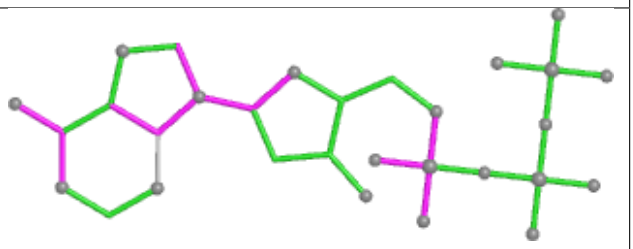


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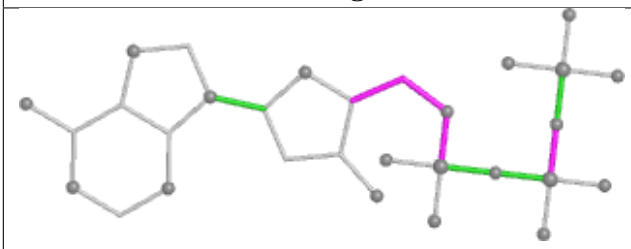
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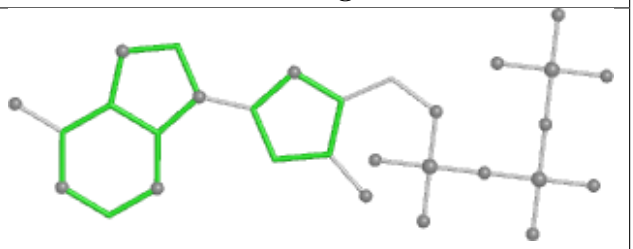
Bond lengths



Bond angles

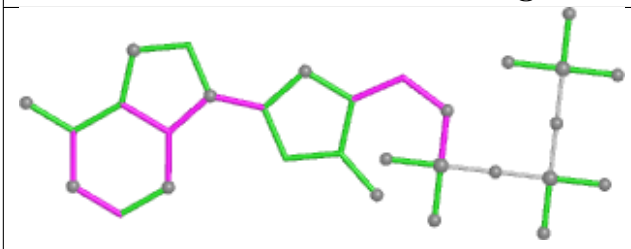


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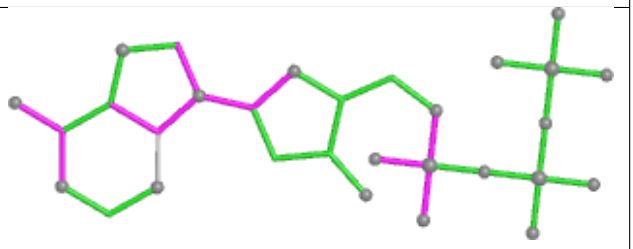


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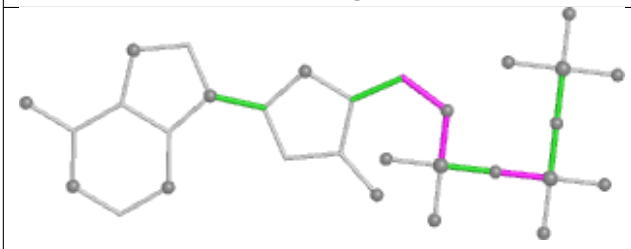
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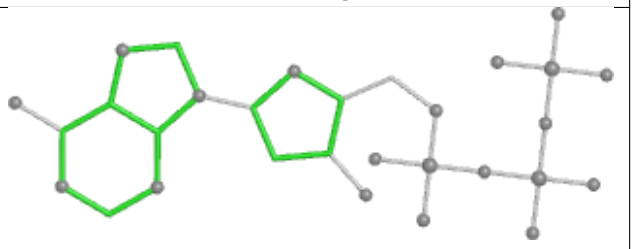
Bond lengths



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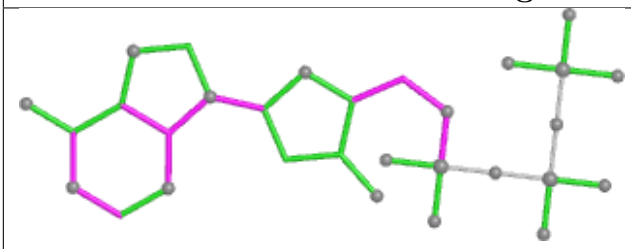


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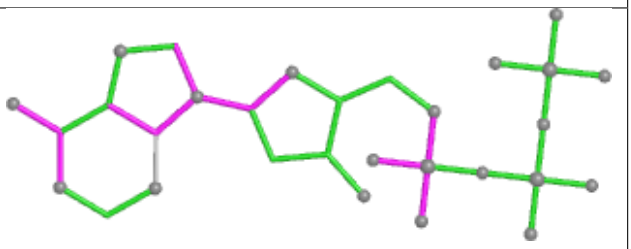


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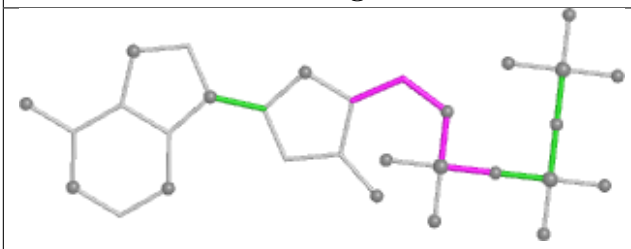
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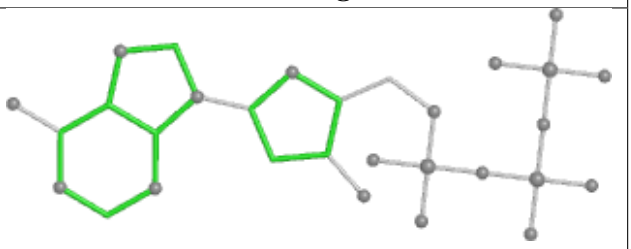
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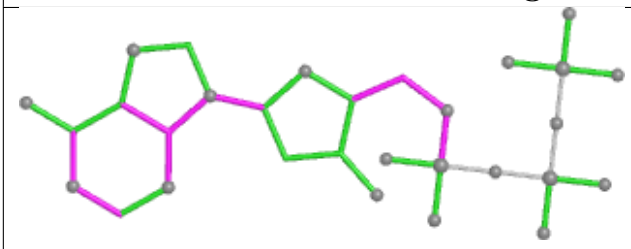


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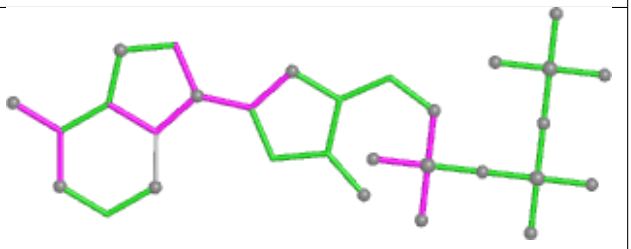


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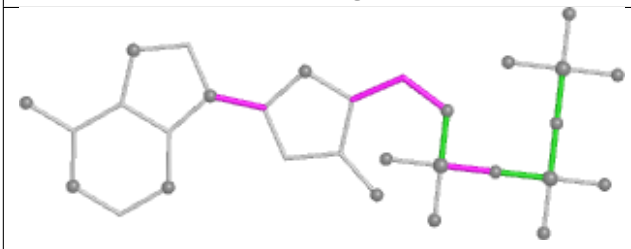
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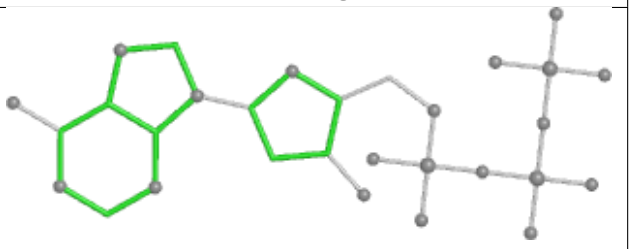
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Bond angles

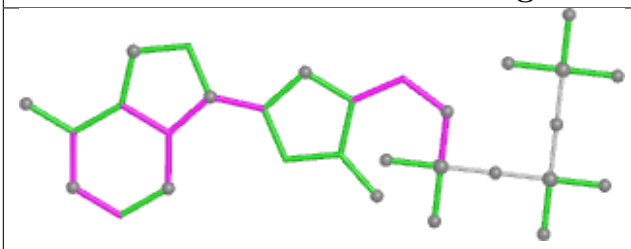


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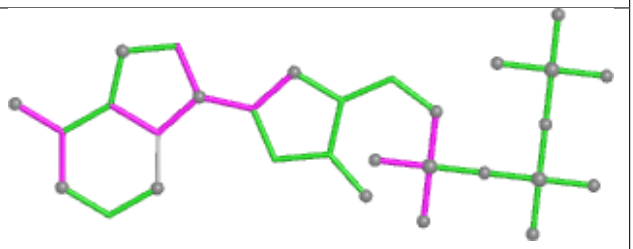


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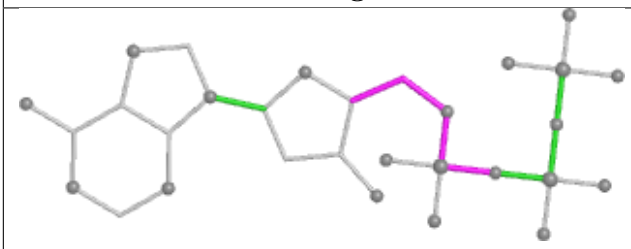
## Ligand Y43 CO 201



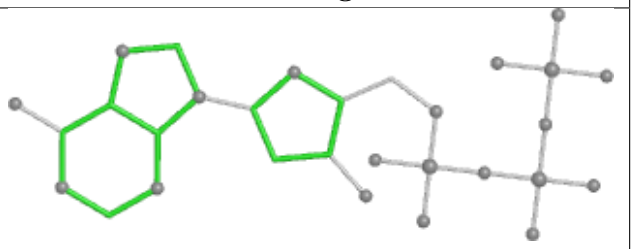
Bond lengths



Bond angles

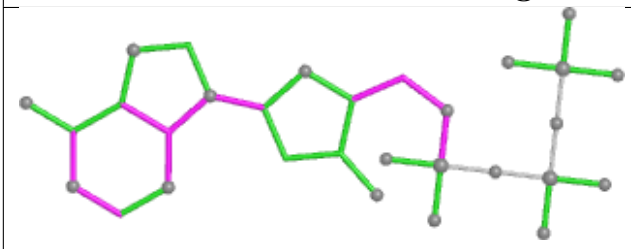


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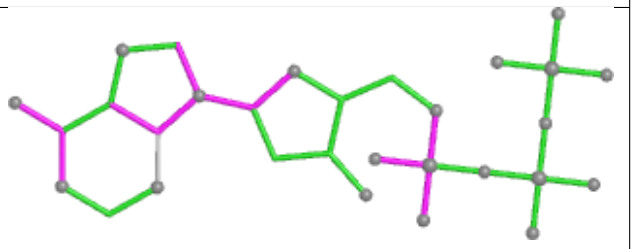


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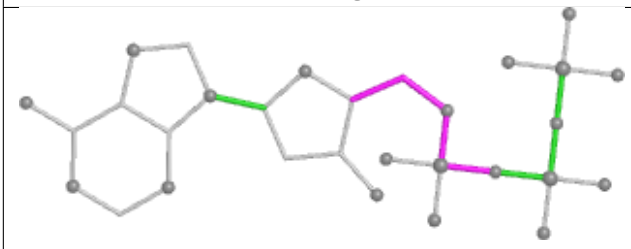
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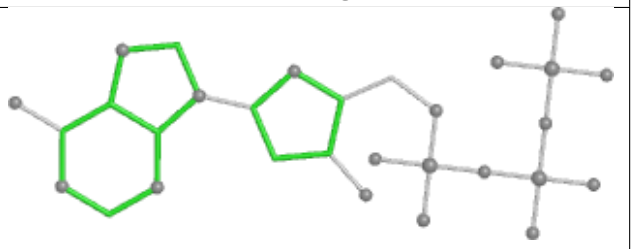
Bond lengths



Bond angles

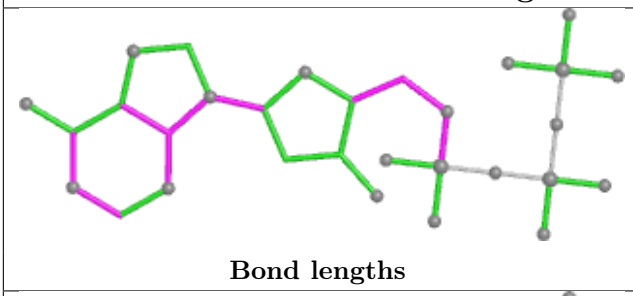


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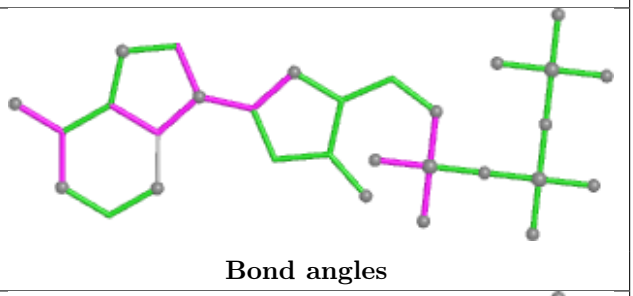


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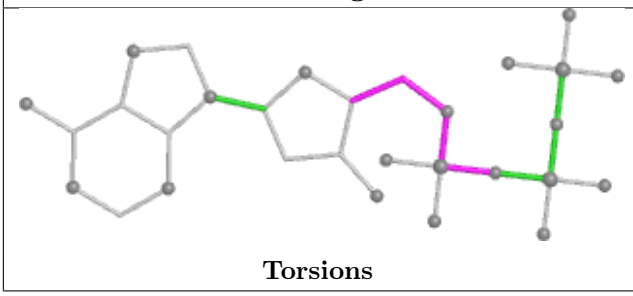
**Ligand Y43 BO 201**



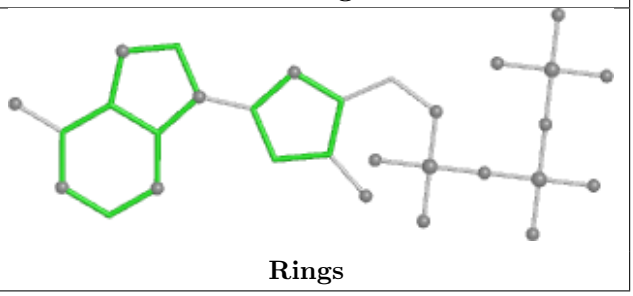
Bond lengths



Bond angles

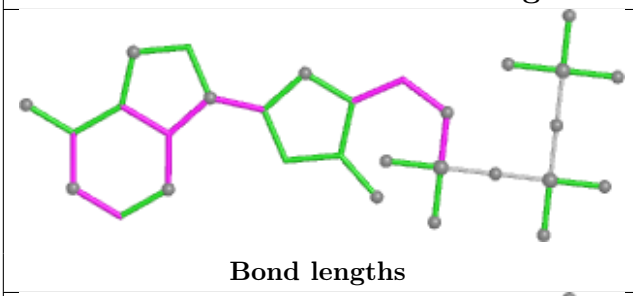


Torsions

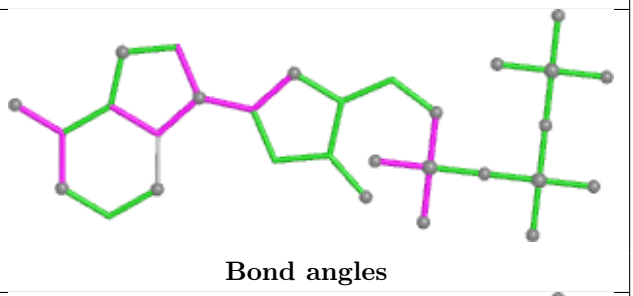


Rings

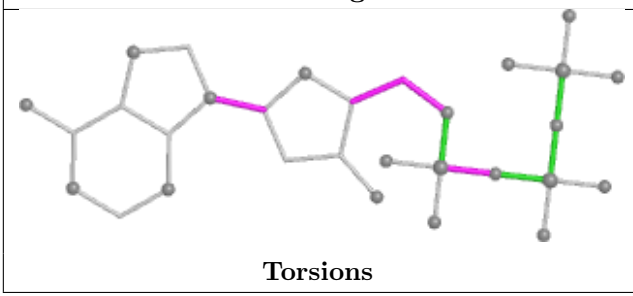
**Ligand Y43 AI 201**



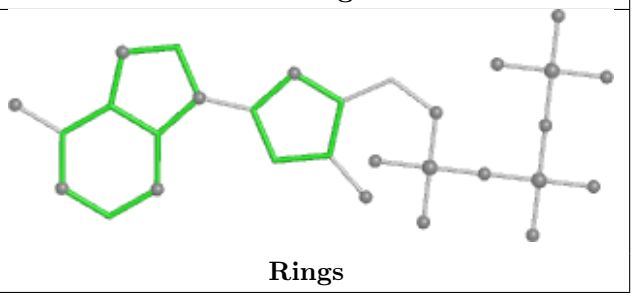
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

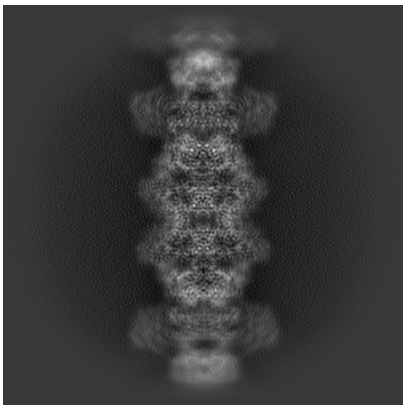
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66453. These allow visual inspection of the internal detail of the map and identification of artifacts.

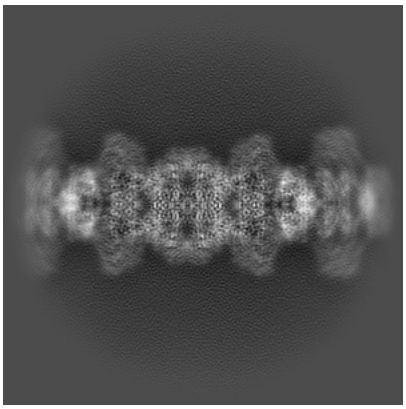
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

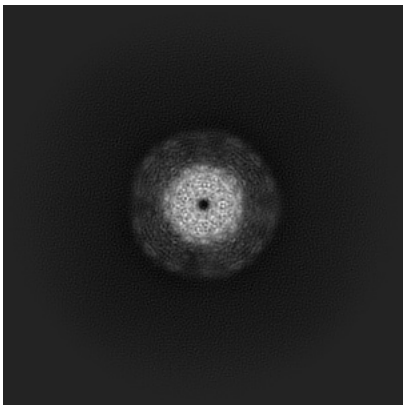
### 6.1.1 Primary map



X

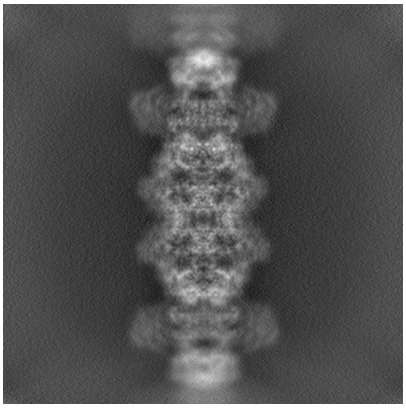


Y

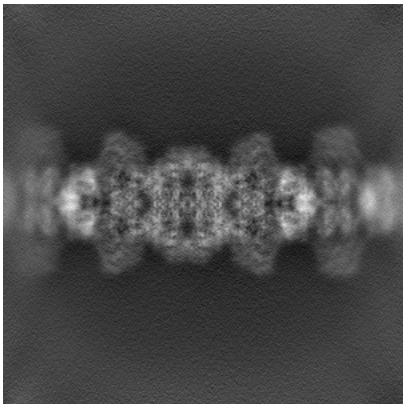


Z

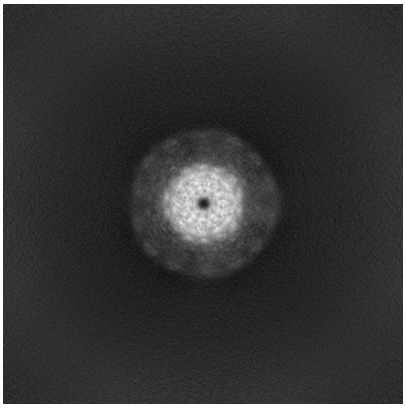
### 6.1.2 Raw map



X



Y

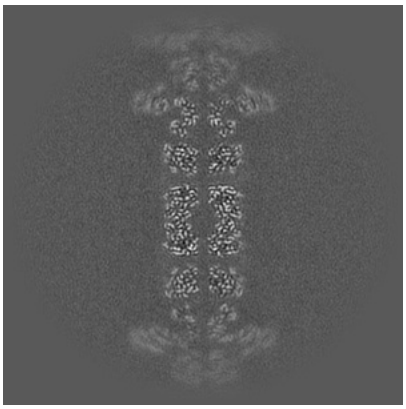


Z

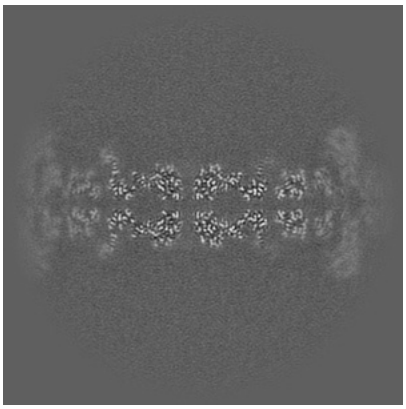
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

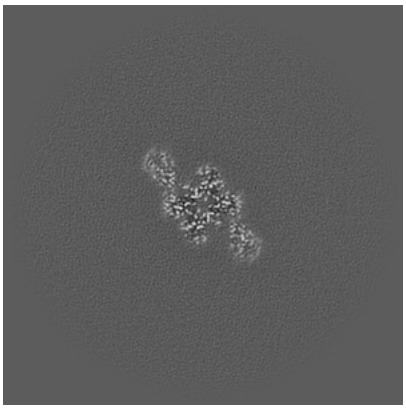
### 6.2.1 Primary map



X Index: 300

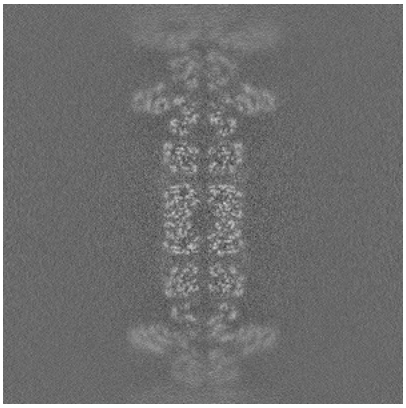


Y Index: 300

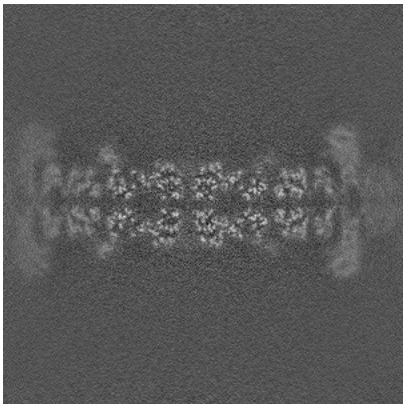


Z Index: 300

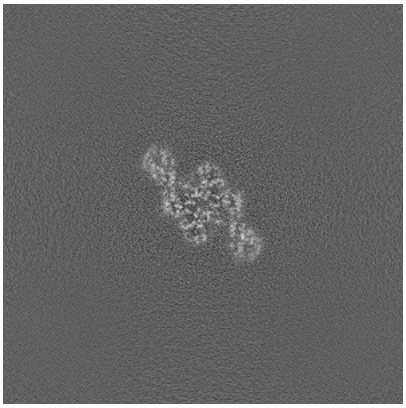
### 6.2.2 Raw map



X Index: 300



Y Index: 300

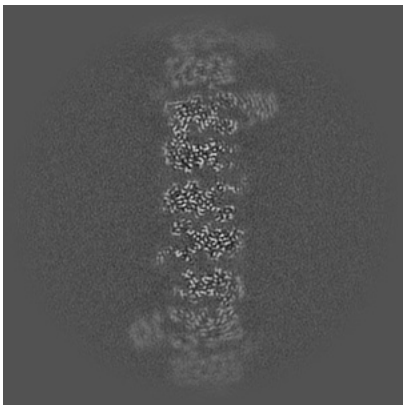


Z Index: 300

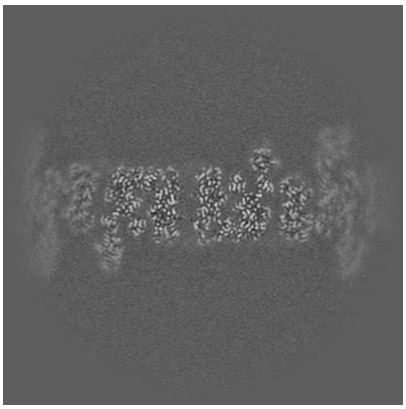
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

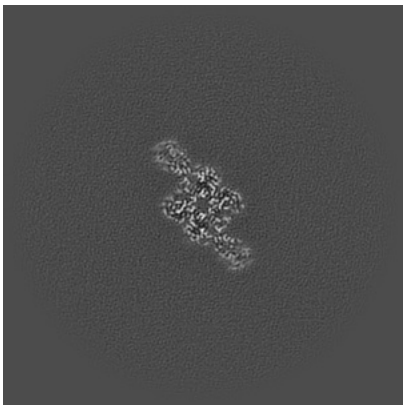
### 6.3.1 Primary map



X Index: 286

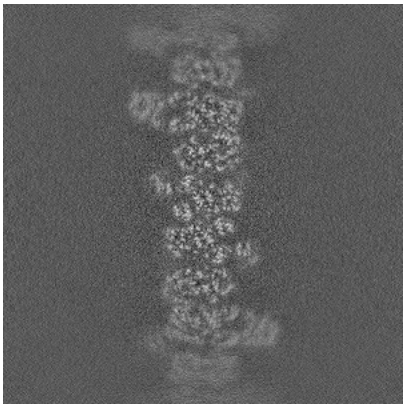


Y Index: 313

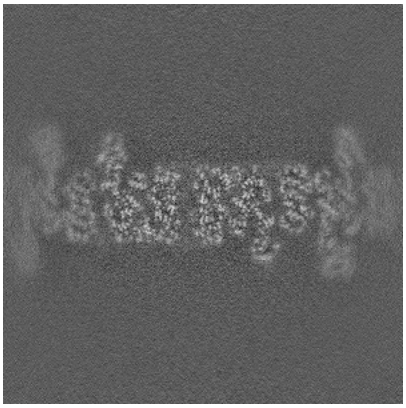


Z Index: 319

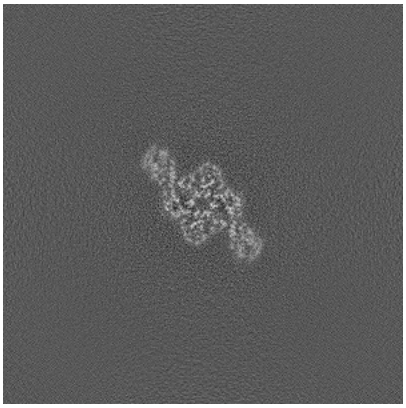
### 6.3.2 Raw map



X Index: 318



Y Index: 287

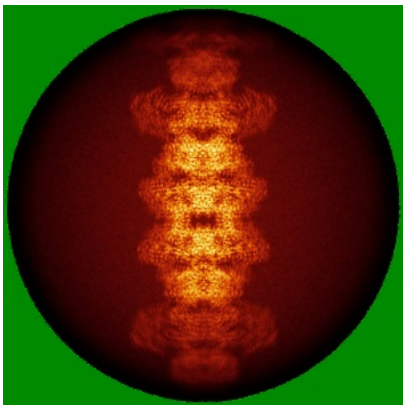


Z Index: 298

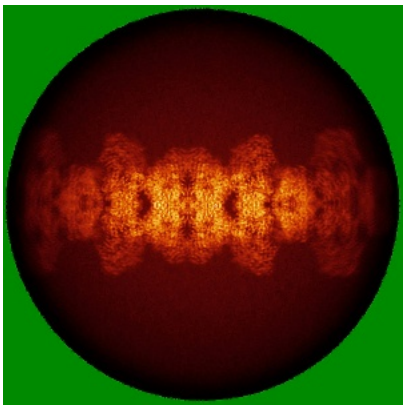
The images above show the largest variance slices of the map in three orthogonal directions.

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

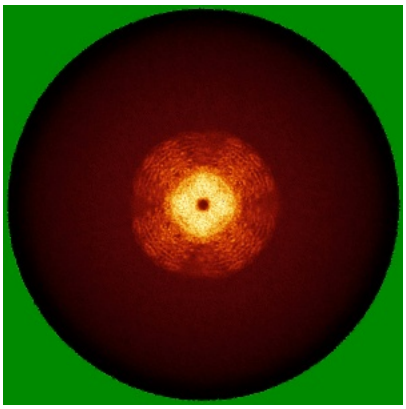
### 6.4.1 Primary map



X

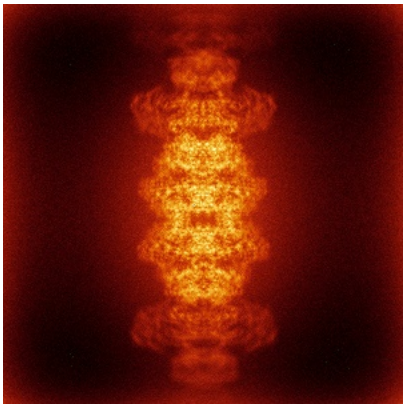


Y

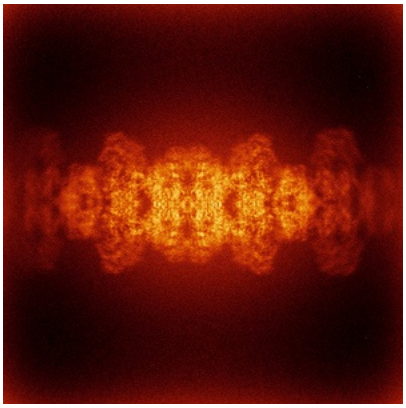


Z

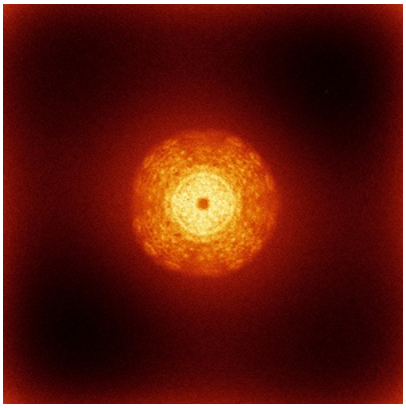
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

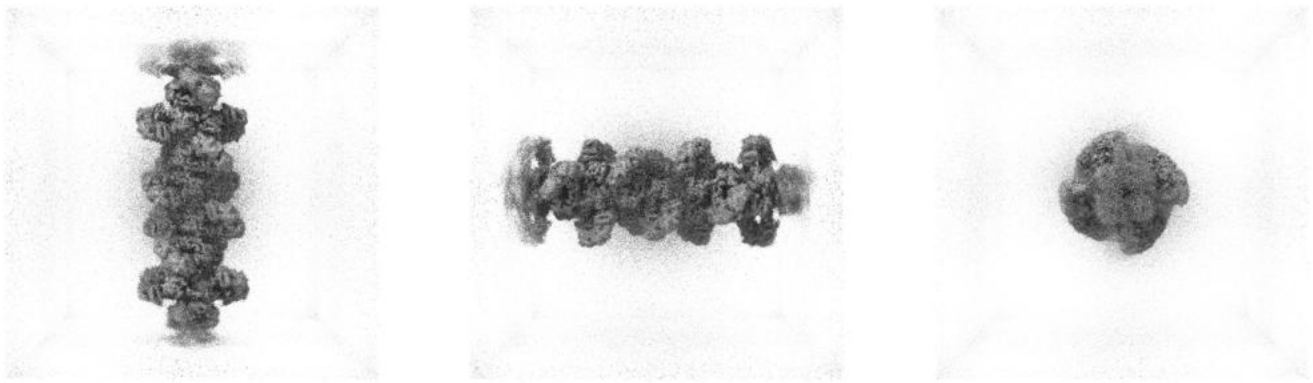
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

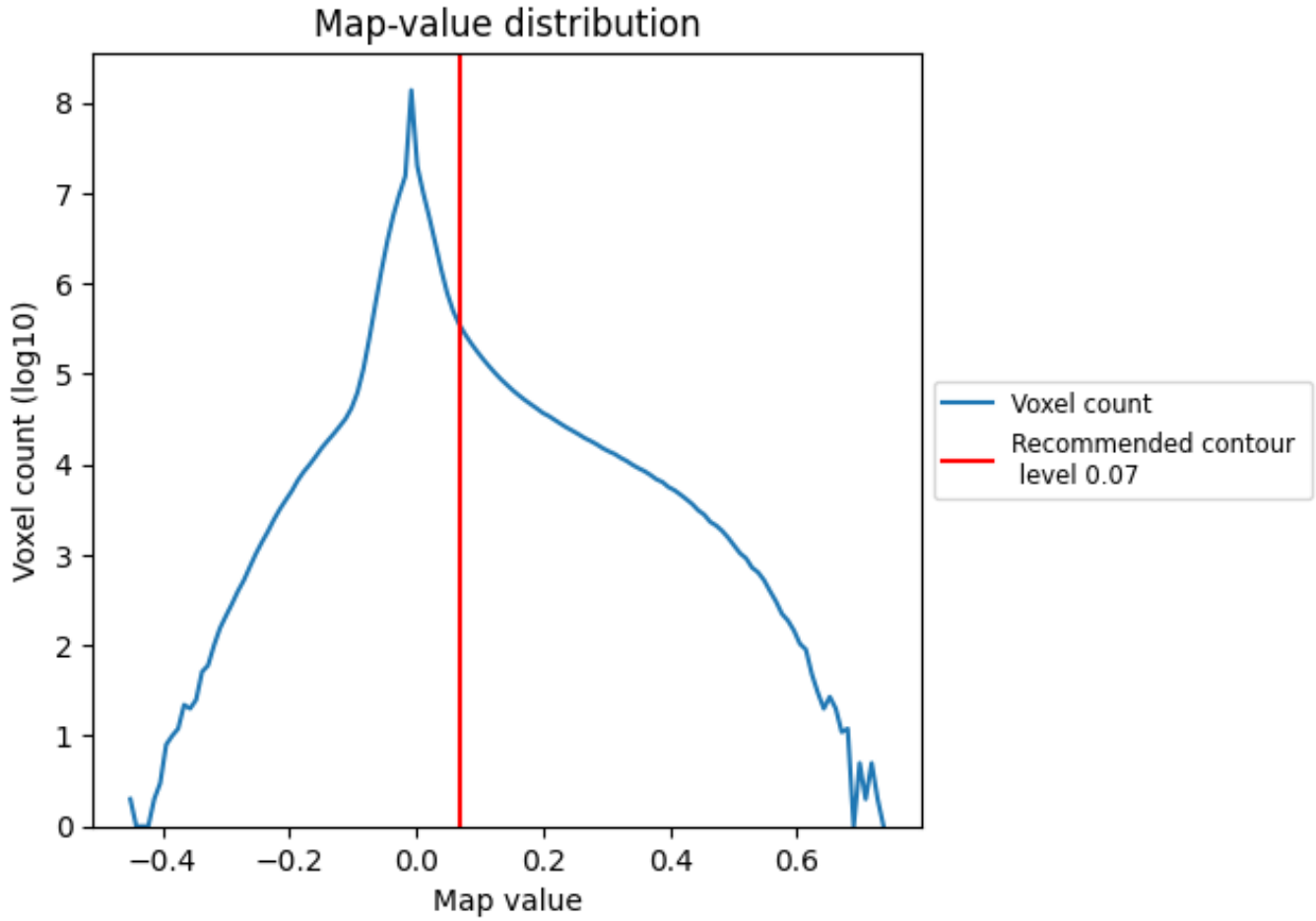
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

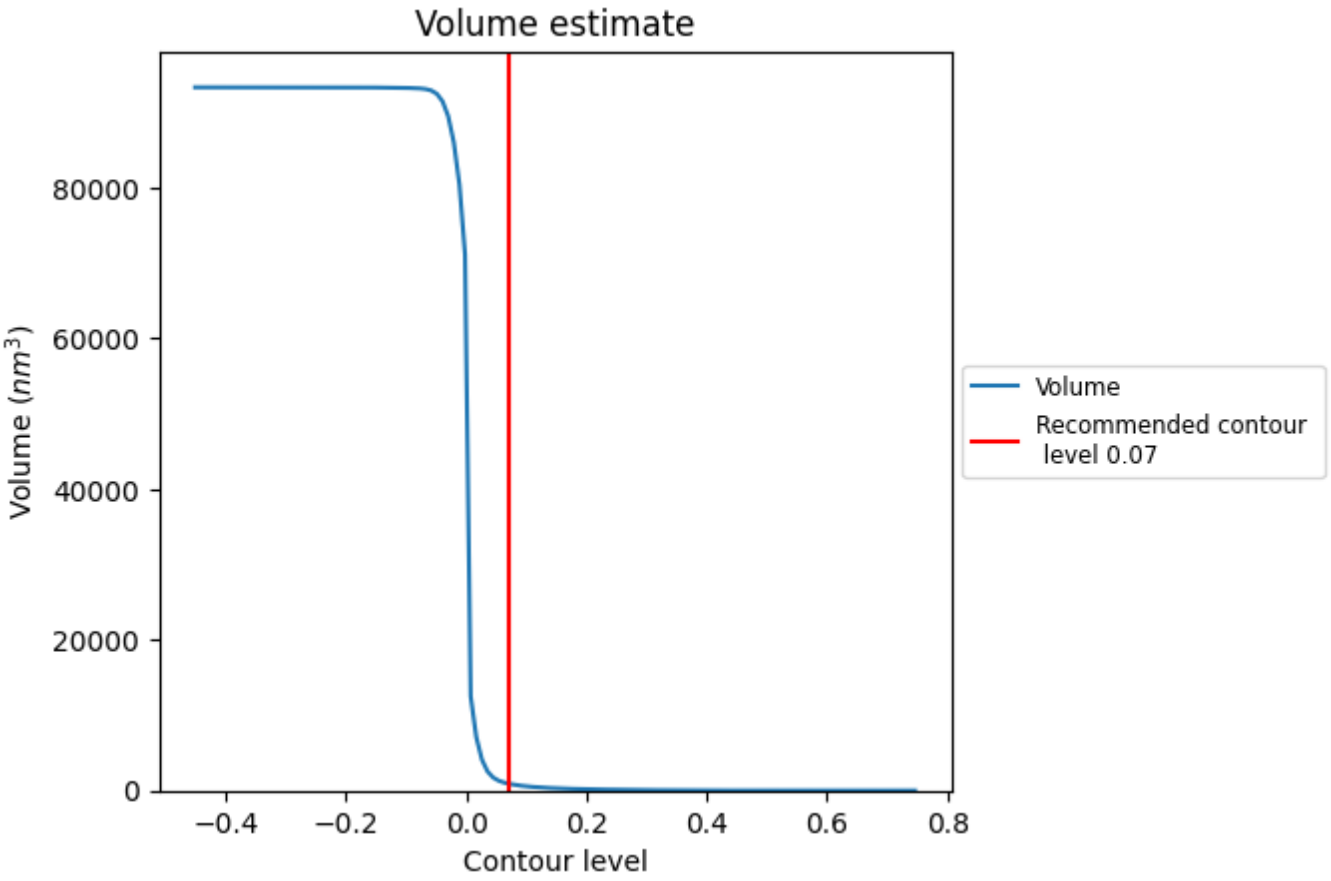
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

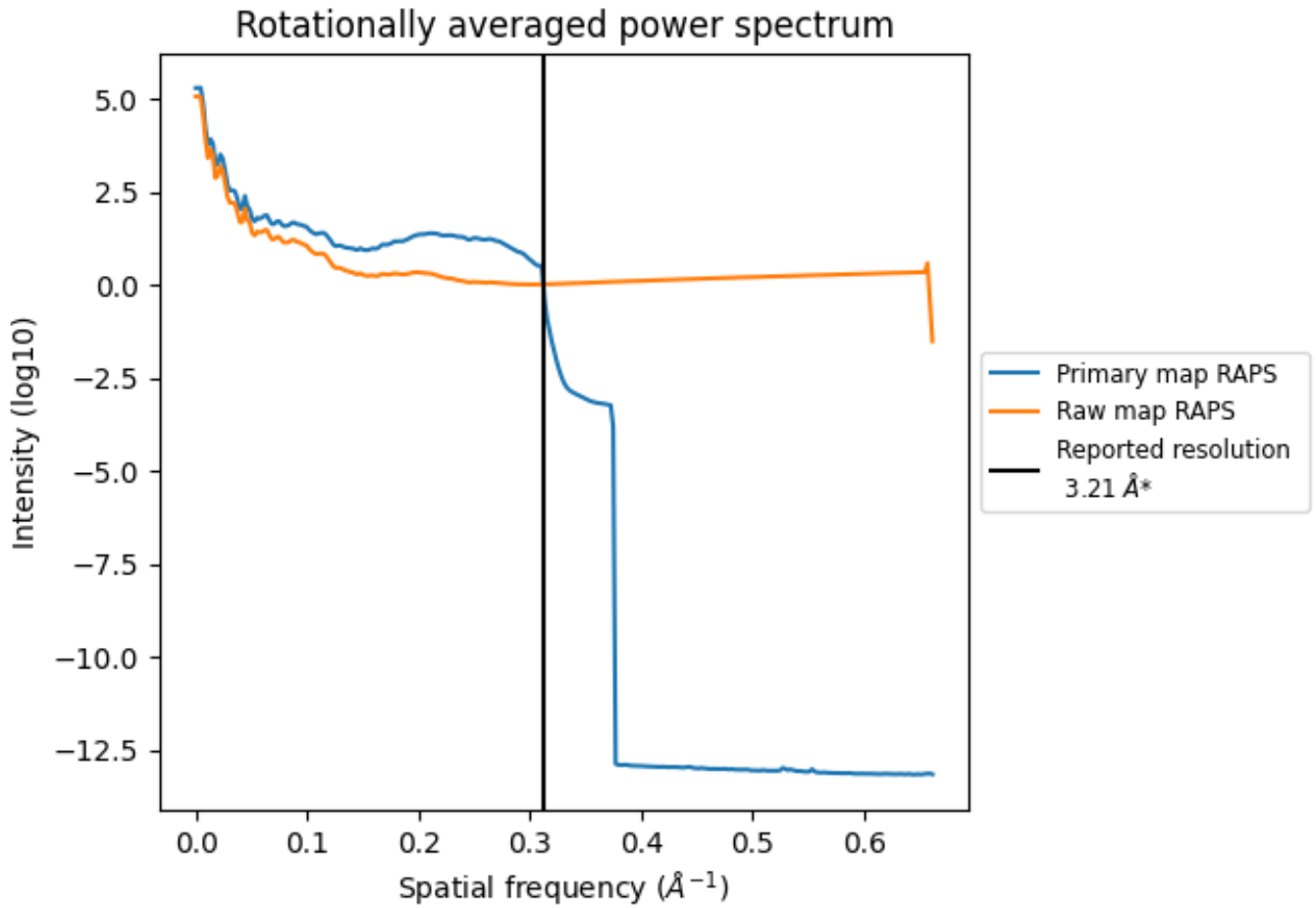
## 7.2 Volume estimate




The volume at the recommended contour level is 927 $nm^3$; this corresponds to an approximate mass of 837 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

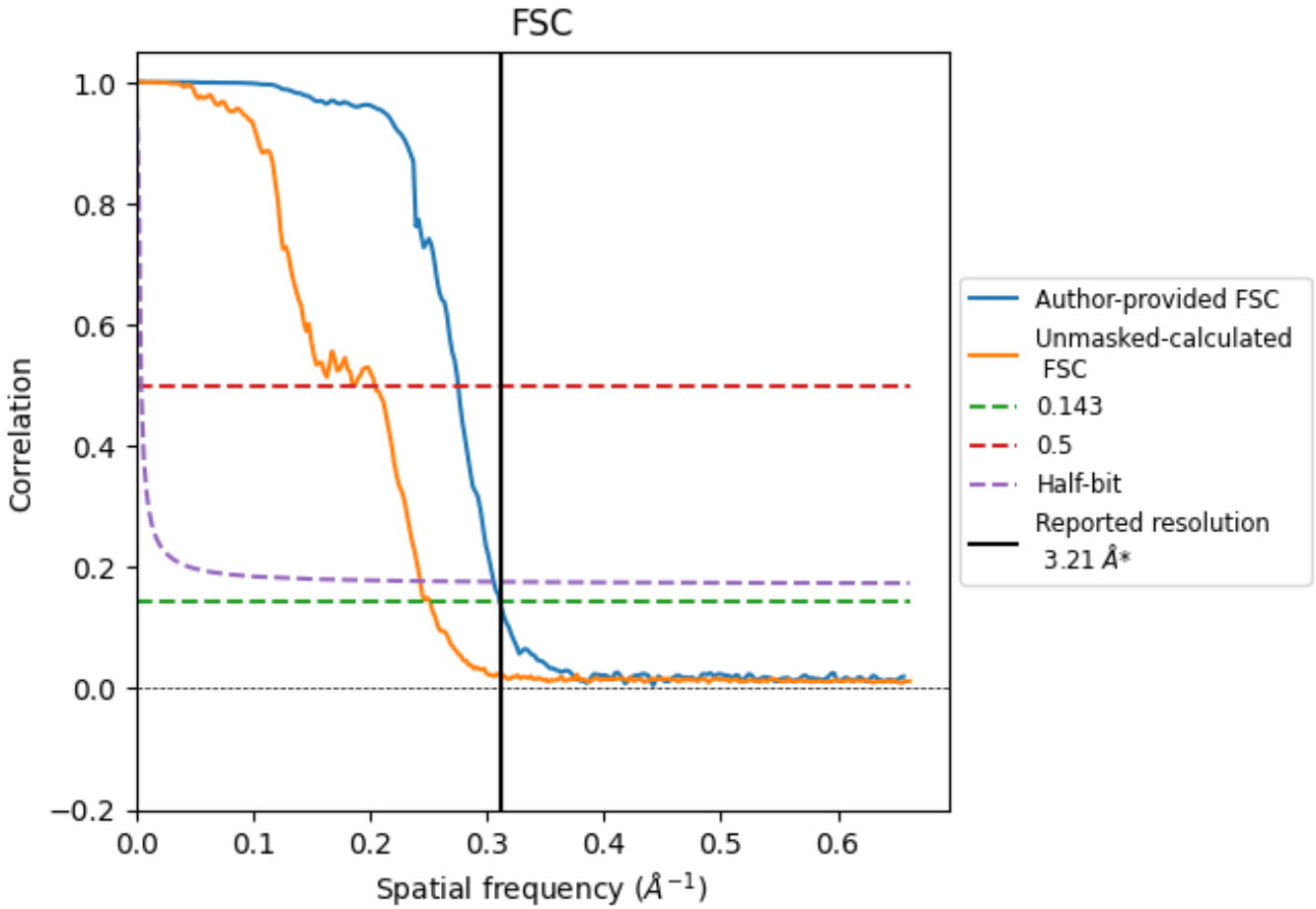



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.312 Å$^{-1}$

## 8.2 Resolution estimates (i)

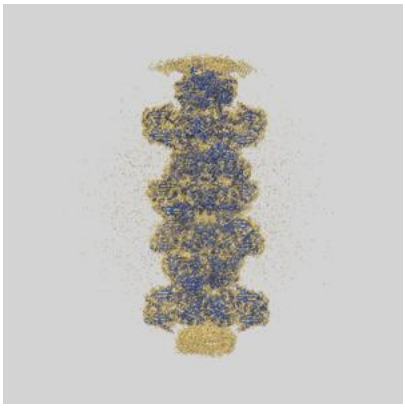
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.21 | - | - |
| Author-provided FSC curve | 3.21 | 3.63 | 3.27 |
| Unmasked-calculated* | 3.98 | 5.35 | 4.12 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.21 by more than 10 %

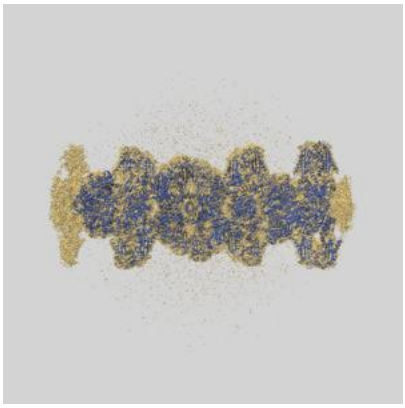
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66453 and PDB model 9X17. Per-residue inclusion information can be found in section 3 on page 11.

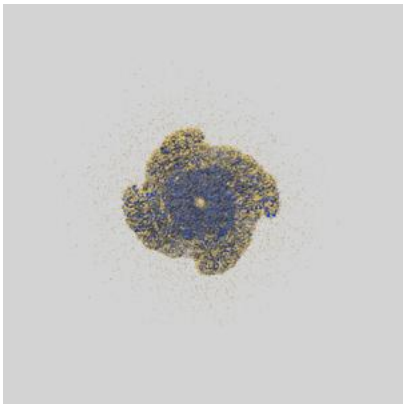
## 9.1 Map-model overlay



X



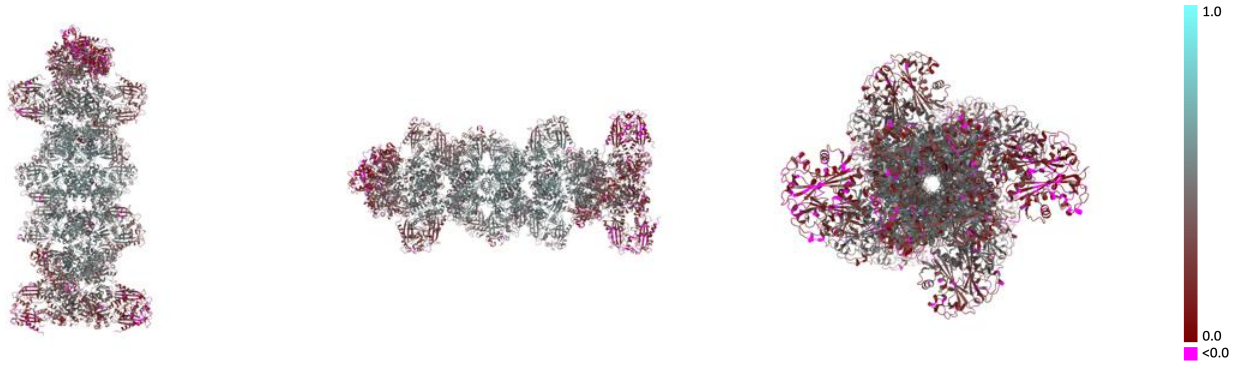
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

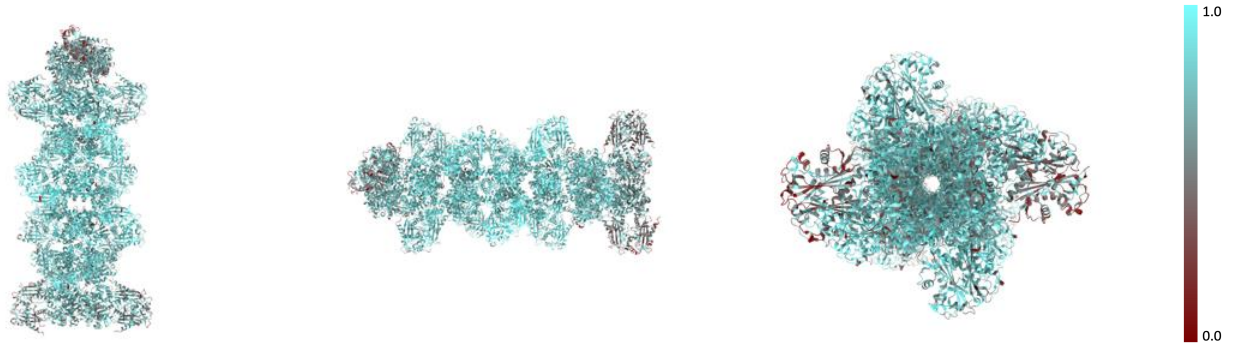
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

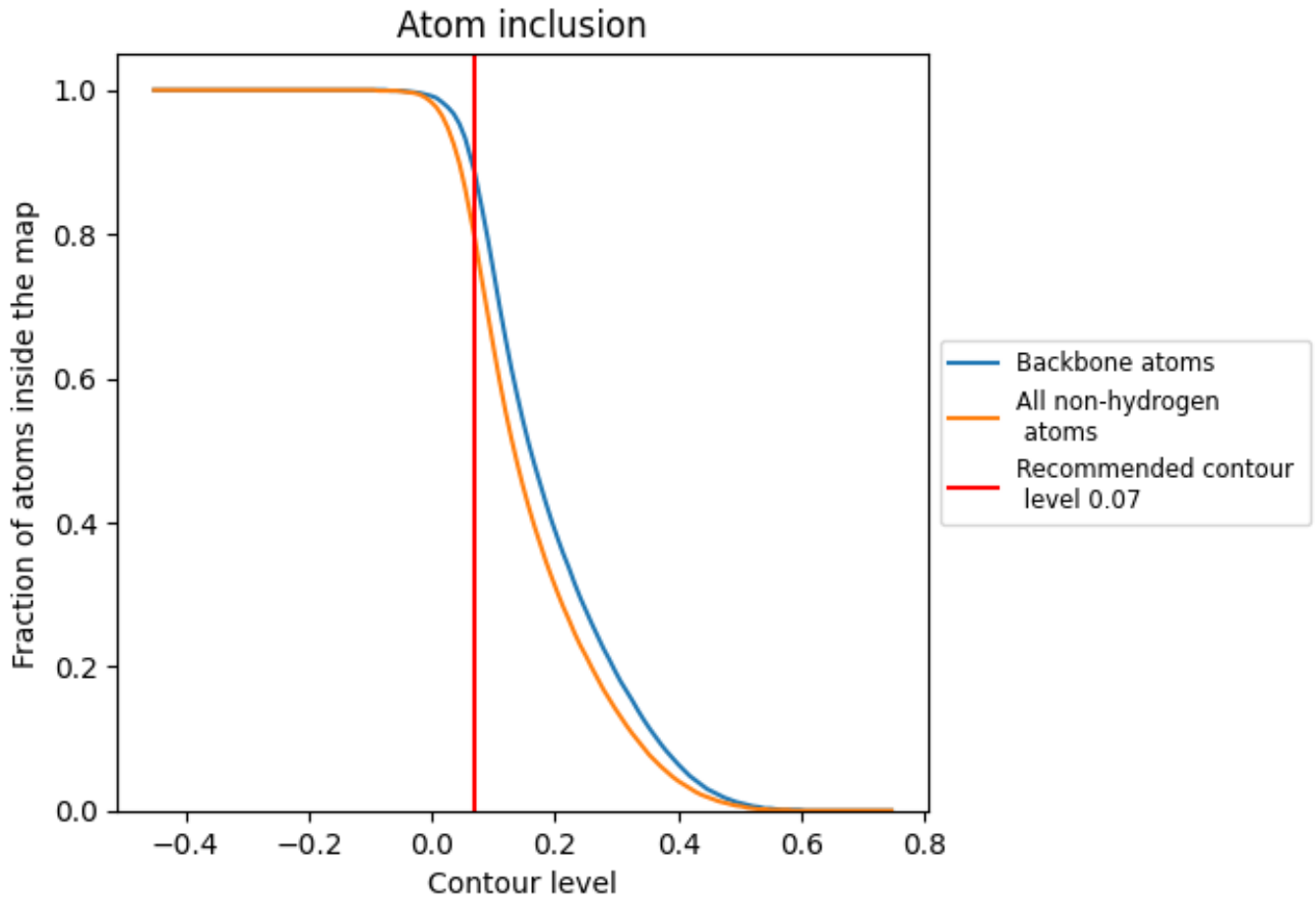
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

## 9.4 Atom inclusion (i)




At the recommended contour level, 88% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7930 | 0.3910 |
| AB | 0.5250 | 0.1370 |
| AC | 0.4480 | 0.0980 |
| AD | 0.6040 | 0.2240 |
| AE | 0.6810 | 0.3030 |
| AG | 0.5480 | 0.1620 |
| AI | 0.4680 | 0.1130 |
| AK | 0.6840 | 0.3090 |
| AL | 0.6130 | 0.2430 |
| AN | 0.7460 | 0.2960 |
| AO | 0.7460 | 0.2920 |
| AP | 0.8520 | 0.4550 |
| AQ | 0.8810 | 0.4880 |
| AS | 0.7300 | 0.2730 |
| AU | 0.7580 | 0.2780 |
| AW | 0.8470 | 0.4660 |
| AX | 0.8560 | 0.4590 |
| BB | 0.8720 | 0.4420 |
| BC | 0.8760 | 0.4460 |
| BD | 0.8890 | 0.5140 |
| BE | 0.8940 | 0.5270 |
| BG | 0.8770 | 0.4360 |
| BI | 0.8760 | 0.4460 |
| BK | 0.9030 | 0.5280 |
| BL | 0.9100 | 0.5350 |
| BN | 0.8970 | 0.4580 |
| BO | 0.8970 | 0.4730 |
| BP | 0.9310 | 0.5450 |
| BQ | 0.9250 | 0.5440 |
| BS | 0.8990 | 0.4490 |
| BU | 0.9100 | 0.4620 |
| BW | 0.9110 | 0.5300 |
| BX | 0.9210 | 0.5410 |
| CB | 0.8380 | 0.4080 |
| CC | 0.8420 | 0.4110 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| CD | 0.8670 | 0.4890 |
| CE | 0.8650 | 0.4910 |
| CG | 0.8390 | 0.3880 |
| CI | 0.8480 | 0.4030 |
| CK | 0.8810 | 0.4990 |
| CL | 0.9000 | 0.5180 |
| CN | 0.7840 | 0.3220 |
| CO | 0.7540 | 0.2950 |
| CP | 0.8770 | 0.4890 |
| CQ | 0.8570 | 0.4520 |
| CS | 0.7970 | 0.3280 |
| CU | 0.7720 | 0.3220 |
| CW | 0.8610 | 0.4760 |
| CX | 0.8880 | 0.5030 |
| DB | 0.5480 | 0.1310 |
| DC | 0.6110 | 0.1960 |
| DD | 0.7400 | 0.3610 |
| DE | 0.6690 | 0.2900 |
| DG | 0.5250 | 0.1100 |
| DI | 0.6030 | 0.1830 |
| DK | 0.6880 | 0.3140 |
| DL | 0.7470 | 0.3740 |