# Integrative Structure Validation Report

## July 22, 2024 - 04:10 PM PDT

**The following software was used in the production of this report:**

*Python-IHM Version 1.3*
*MolProbity Version 4.5.2*
*Integrative Modeling Validation Version 1.2*

| | |
|---|---|
| PDB ID | 9A0J |
| PDB-Dev ID | PDBDEV_00000055 |
| Structure Title | Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM |
| Structure Authors | Farrell DP; Anishchenko I; Shakeel S; Lauko A; Passmore LA; Baker D; DiMaio F |

*This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.*

*We welcome your comments at pdb-dev@mail.wwpdb.org*

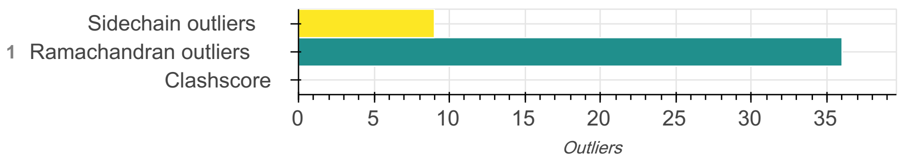
*A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the* ? symbol.

*List of references used to build this report is available here.*

## Overall quality

*This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.*

Model Quality: MolProbity Analysis



## Ensemble information

*This entry consists of 0 distinct ensemble(s).*

## Summary

*This entry consists of 1 unique models, with 11 subunits in each model. A total of 93 datasets or restraints were used to build this entry. Each model is represented by 76 rigid bodies and 4 flexible or non-rigid units.*

## Entry composition

*There is 1 unique type of models in this entry.This model is titled Top Model/Best scoring model.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Chain ID [auth] | Total residues |
|---|---|---|---|---|---|---|
| 1 | 1 | 1 | fancB | B | B | 867 |
| 1 | 2 | 1 | fancB | b | b | 867 |
| 1 | 3 | 2 | fancC | C | C | 595 |
| 1 | 4 | 3 | fancE | E | E | 520 |
| 1 | 5 | 4 | fancF | F | F | 350 |
| 1 | 6 | 5 | fancG | G | G | 648 |
| 1 | 7 | 5 | fancG | g | g | 648 |
| 1 | 8 | 6 | fancL | L | L | 373 |
| 1 | 9 | 6 | fancL | l | l | 373 |
| 1 | 10 | 7 | faap100 | P | P | 888 |
| 1 | 11 | 7 | faap100 | p | p | 888 |

## Datasets used for modeling

*There are 93 unique datasets used to build the models in this entry.*

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 1 | De Novo model | File | 10.5281/zenodo.3979898 |
| 2 | De Novo model | File | 10.5281/zenodo.3979898 |
| 3 | De Novo model | File | 10.5281/zenodo.3979898 |
| 4 | De Novo model | File | 10.5281/zenodo.3979898 |
| 5 | De Novo model | File | 10.5281/zenodo.3979898 |
| 6 | De Novo model | File | 10.5281/zenodo.3979898 |
| 7 | De Novo model | File | 10.5281/zenodo.3979898 |

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 8 | De Novo model | File | 10.5281/zenodo.3979898 |
| 9 | De Novo model | File | 10.5281/zenodo.3979898 |
| 10 | De Novo model | File | 10.5281/zenodo.3979898 |
| 11 | De Novo model | File | 10.5281/zenodo.3979898 |
| 12 | De Novo model | File | 10.5281/zenodo.3979898 |
| 13 | De Novo model | File | 10.5281/zenodo.3979898 |
| 14 | De Novo model | File | 10.5281/zenodo.3979898 |
| 15 | De Novo model | File | 10.5281/zenodo.3979898 |
| 16 | De Novo model | File | 10.5281/zenodo.3979898 |
| 17 | De Novo model | File | 10.5281/zenodo.3979898 |
| 18 | De Novo model | File | 10.5281/zenodo.3979898 |
| 19 | De Novo model | File | 10.5281/zenodo.3979898 |
| 20 | De Novo model | File | 10.5281/zenodo.3979898 |
| 21 | De Novo model | File | 10.5281/zenodo.3979898 |
| 22 | De Novo model | File | 10.5281/zenodo.3979898 |
| 23 | De Novo model | File | 10.5281/zenodo.3979898 |
| 24 | De Novo model | File | 10.5281/zenodo.3979898 |
| 25 | De Novo model | File | 10.5281/zenodo.3979898 |
| 26 | De Novo model | File | 10.5281/zenodo.3979898 |
| 27 | De Novo model | File | 10.5281/zenodo.3979898 |
| 28 | De Novo model | File | 10.5281/zenodo.3979898 |
| 29 | De Novo model | File | 10.5281/zenodo.3979898 |
| 30 | De Novo model | File | 10.5281/zenodo.3979898 |
| 31 | De Novo model | File | 10.5281/zenodo.3979898 |
| 32 | De Novo model | File | 10.5281/zenodo.3979898 |
| 33 | De Novo model | File | 10.5281/zenodo.3979898 |
| 34 | De Novo model | File | 10.5281/zenodo.3979898 |
| 35 | De Novo model | File | 10.5281/zenodo.3979898 |

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 36 | 3DEM volume | EMDB | EMDB-10291 |
| 37 | 3DEM volume | EMDB | EMDB-10292 |
| 38 | 3DEM volume | EMDB | EMDB-10293 |
| 39 | Crosslinking-MS data | PRIDE | PXD014282 |
| 40 | Comparative model | File | 10.5281/zenodo.3979898 |
| 41 | Comparative model | File | 10.5281/zenodo.3979898 |
| 42 | Comparative model | File | 10.5281/zenodo.3979898 |
| 43 | Comparative model | File | 10.5281/zenodo.3979898 |
| 44 | Comparative model | File | 10.5281/zenodo.3979898 |
| 45 | Comparative model | File | 10.5281/zenodo.3979898 |
| 46 | Comparative model | File | 10.5281/zenodo.3979898 |
| 47 | Comparative model | File | 10.5281/zenodo.3979898 |
| 48 | Comparative model | File | 10.5281/zenodo.3979898 |
| 49 | Comparative model | File | 10.5281/zenodo.3979898 |
| 50 | Comparative model | File | 10.5281/zenodo.3979898 |
| 51 | Experimental model | PDB | 4ccg |
| 52 | Experimental model | PDB | 4zdt |
| 53 | Experimental model | PDB | 5o6c |
| 54 | Experimental model | PDB | 2d8s |
| 55 | Experimental model | PDB | 1vyx |
| 56 | Experimental model | PDB | 3k1l |
| 57 | Experimental model | PDB | 2iqc |
| 58 | Experimental model | PDB | 1r5m |
| 59 | Experimental model | PDB | 5m23 |
| 60 | Experimental model | PDB | 6chg |
| 61 | Experimental model | PDB | 6f9n |
| 62 | Experimental model | PDB | 2pbi |

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 63 | Experimental model | PDB | 5m89 |
| 64 | Experimental model | PDB | 4ggc |
| 65 | Experimental model | PDB | 6eoj |
| 66 | Experimental model | PDB | 5kdo |
| 67 | Experimental model | PDB | 5oql |
| 68 | Experimental model | PDB | 5opt |
| 69 | Experimental model | PDB | 3odt |
| 70 | Experimental model | PDB | 5a31 |
| 71 | Experimental model | PDB | 5xyi |
| 72 | Experimental model | PDB | 2ilr |
| 73 | Experimental model | PDB | 5orq |
| 74 | Experimental model | PDB | 1fch |
| 75 | Experimental model | PDB | 3hym |
| 76 | Experimental model | PDB | 3fp2 |
| 77 | Experimental model | PDB | 2gw1 |
| 78 | Experimental model | PDB | 6c9m |
| 79 | Experimental model | PDB | 6eou |
| 80 | Experimental model | PDB | 3ieg |
| 81 | Experimental model | PDB | 4rg9 |
| 82 | Experimental model | PDB | 2xpi |
| 83 | Experimental model | PDB | 3cvp |
| 84 | Experimental model | PDB | 5i9f |
| 85 | Experimental model | PDB | 5aio |
| 86 | Experimental model | PDB | 5dse |
| 87 | Experimental model | PDB | 4g1t |
| 88 | Experimental model | PDB | 4zlh |
| 89 | Experimental model | PDB | 2y4t |

| ID | Dataset type | Database name | Data access code |
|---|---|---|---|
| 90 | Experimental model | PDB | 3u4t |
| 91 | Experimental model | PDB | 4pjr |
| 92 | Experimental model | PDB | 4buj |
| 93 | 3DEM volume | File | 10.5281/zenodo.3979898 |

## Representation

*This entry has only one representation and includes 76 rigid bodies and 4 flexible units*

| Chain ID | Rigid bodies | Non-rigid segments |
|---|---|---|
| B | 378-434, 1-370, 441-780, 231-365, 441-660, 651-770, 1-235, 466-626 | 435-440 |
| b | 378-434, 1-370, 441-780, 231-365, 441-660, 651-770, 1-235, 466-626 | 435-440 |
| C | 331-570, 176-335, 1-335, 1-175 | - |
| E | 266-520, 1-150, 261-520 | 151-170 |
| F | 140-341 | 342-350 |
| G | 44-645, 1-320, 181-320, 201-435, 204-315, 1-175, 321-648 | - |
| g | 44-645, 1-320, 181-320, 201-435, 204-315, 1-175, 321-648 | - |
| L | 191-300, 301-373, 104-373, 101-300, 2-91, 101-205, 1-100 | - |
| l | 191-300, 301-373, 104-373, 101-300, 2-91, 101-205, 1-100 | - |
| P | 28-442, 1-300, 711-820, 1-200, 186-480, 301-480, 510-609, 491-615, 714-803, 804-888, 453-507, 491-820 | - |
| p | 28-442, 1-300, 711-820, 1-200, 186-480, 301-480, 510-609, 491-615, 714-803, 804-888, 453-507, 491-820 | - |

## Methodology and software

*This entry is a result of 1 distinct protocol(s).*

| Step number | Protocol ID | Method name | Method type | Method description | Number of computed models | Multi state modeling | Multi scale modeling |
|---|---|---|---|---|---|---|---|
| 1 | 1 | Monte Carlo | Production sampling | None | None | False | False |

| Step number | Protocol ID | Method name | Method type | Method description | Number of computed models | Multi state modeling | Multi scale modeling |
|---|---|---|---|---|---|---|---|
| 2 | 1 | Rosetta Hybridize | Rosetta Hybridize | None | None | False | False |

*There are 3 software packages reported in this entry.*

| ID | Software name | Software version | Software classification | Software location |
|---|---|---|---|---|
| 1 | Rosetta | Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa87 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git | RosettaCM/hybridize and unpublished 'complex assembly' | https://www.rosettacommons.org/ |
| 2 | trRosetta | 1.0.0 | trRosetta | https://github.com/gjoni/trRosetta |
| 3 | HHpred | website | protein homology detection | https://toolkit.tuebingen.mpg.de/hhpred |

## Data quality ?

### 3DEM volume

Validation for this section is under development.

### Crosslinking-MS

Validation for this section is under development.

## Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Standard geometry: bond outliers ?

*There are 39748 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be foundhere.*

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CB--1HB | 1.05 | 0.97 | 45 |
| CG--HG | 1.05 | 0.97 | 17 |
| CD1--1HD1 | 1.05 | 0.97 | 11 |
| CG--1HG | 1.05 | 0.97 | 14 |
| CB--HB | 1.05 | 0.97 | 15 |
| CB--2HB | 1.05 | 0.97 | 51 |
| CD1--2HD1 | 1.05 | 0.97 | 15 |
| CB--3HB | 1.05 | 0.97 | 7 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CG2--3HG2 | 1.05 | 0.97 | 8 |
| CD1--3HD1 | 1.05 | 0.97 | 16 |
| CD2--2HD2 | 1.05 | 0.97 | 11 |
| CD2--3HD2 | 1.05 | 0.97 | 10 |
| CD2--1HD2 | 1.05 | 0.97 | 7 |
| CG1--3HG1 | 1.05 | 0.97 | 7 |
| CG1--1HG1 | 1.05 | 0.97 | 5 |
| CG2--2HG2 | 1.05 | 0.97 | 12 |
| CD--1HD | 1.05 | 0.97 | 6 |
| CD--2HD | 1.05 | 0.97 | 3 |
| CG1--2HG1 | 1.05 | 0.97 | 10 |
| CG--2HG | 1.05 | 0.97 | 4 |
| CE--1HE | 1.05 | 0.97 | 2 |
| CD1--HD1 | 1.01 | 0.93 | 1 |
| CA--2HA | 1.05 | 0.97 | 1 |
| CE--2HE | 1.05 | 0.97 | 1 |
| CG2--1HG2 | 1.05 | 0.97 | 3 |
| CA--HA | 1.05 | 0.97 | 1 |
| CB--1HB | 1.06 | 0.97 | 169 |
| CG1--2HG1 | 1.06 | 0.97 | 35 |
| CD2--2HD2 | 1.06 | 0.97 | 25 |
| CB--3HB | 1.06 | 0.97 | 29 |
| CD1--3HD1 | 1.06 | 0.97 | 60 |
| CD2--1HD2 | 1.06 | 0.97 | 32 |
| CG2--1HG2 | 1.06 | 0.97 | 33 |
| CD1--1HD1 | 1.06 | 0.97 | 51 |
| CB--2HB | 1.06 | 0.97 | 176 |
| CD1--2HD1 | 1.06 | 0.97 | 46 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CG1--1HG1 | 1.06 | 0.97 | 29 |
| CG2--3HG2 | 1.06 | 0.97 | 37 |
| CG--2HG | 1.06 | 0.97 | 31 |
| CG--1HG | 1.06 | 0.97 | 41 |
| CD2--3HD2 | 1.06 | 0.97 | 48 |
| CB--HB | 1.06 | 0.97 | 48 |
| CA--1HA | 1.06 | 0.97 | 3 |
| CG2--2HG2 | 1.06 | 0.97 | 44 |
| CG--HG | 1.06 | 0.97 | 50 |
| CG1--3HG1 | 1.06 | 0.97 | 15 |
| CA--2HA | 1.06 | 0.97 | 3 |
| CD--2HD | 1.06 | 0.97 | 21 |
| CA--HA | 1.06 | 0.97 | 34 |
| CD--1HD | 1.06 | 0.97 | 22 |
| CE--2HE | 1.06 | 0.97 | 7 |
| CE3--HE3 | 1.02 | 0.93 | 1 |
| CE--3HE | 1.06 | 0.97 | 3 |
| CD2--HD2 | 1.02 | 0.93 | 1 |
| CE--1HE | 1.06 | 0.97 | 6 |
| CB--1HB | 1.07 | 0.97 | 327 |
| CB--2HB | 1.07 | 0.97 | 330 |
| CZ--HZ | 1.03 | 0.93 | 1 |
| CD1--3HD1 | 1.07 | 0.97 | 147 |
| CA--HA | 1.07 | 0.97 | 183 |
| CG2--3HG2 | 1.07 | 0.97 | 93 |
| CG2--1HG2 | 1.07 | 0.97 | 76 |
| CD2--2HD2 | 1.07 | 0.97 | 87 |
| CD--1HD | 1.07 | 0.97 | 33 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CE--3HE | 1.07 | 0.97 | 7 |
| CB--3HB | 1.07 | 0.97 | 44 |
| CD2--1HD2 | 1.07 | 0.97 | 75 |
| CD2--3HD2 | 1.07 | 0.97 | 124 |
| CG1--3HG1 | 1.07 | 0.97 | 36 |
| CG--HG | 1.07 | 0.97 | 97 |
| CD1--2HD1 | 1.07 | 0.97 | 155 |
| CG1--1HG1 | 1.07 | 0.97 | 76 |
| CB--HB | 1.07 | 0.97 | 77 |
| CG1--2HG1 | 1.07 | 0.97 | 69 |
| CG2--2HG2 | 1.07 | 0.97 | 93 |
| CD--2HD | 1.07 | 0.97 | 50 |
| CG--1HG | 1.07 | 0.97 | 83 |
| CD1--1HD1 | 1.07 | 0.97 | 97 |
| CA--2HA | 1.07 | 0.97 | 15 |
| CE--2HE | 1.07 | 0.97 | 19 |
| CG--2HG | 1.07 | 0.97 | 84 |
| CE--1HE | 1.07 | 0.97 | 16 |
| CA--1HA | 1.07 | 0.97 | 7 |
| CE1--HE1 | 1.03 | 0.93 | 1 |
| CD2--HD2 | 1.03 | 0.93 | 1 |
| CD1--1HD1 | 1.08 | 0.97 | 278 |
| CD--1HD | 1.08 | 0.97 | 113 |
| CG--2HG | 1.08 | 0.97 | 278 |
| CD1--3HD1 | 1.08 | 0.97 | 318 |
| CB--1HB | 1.08 | 0.97 | 773 |
| CG2--1HG2 | 1.08 | 0.97 | 251 |
| CG2--3HG2 | 1.08 | 0.97 | 235 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CE--3HE | 1.08 | 0.97 | 28 |
| CD2--1HD2 | 1.08 | 0.97 | 175 |
| CB--2HB | 1.08 | 0.97 | 724 |
| CA--HA | 1.08 | 0.97 | 1202 |
| CG--HG | 1.08 | 0.97 | 180 |
| CG--1HG | 1.08 | 0.97 | 205 |
| CA--1HA | 1.08 | 0.97 | 34 |
| CD1--2HD1 | 1.08 | 0.97 | 318 |
| CD2--3HD2 | 1.08 | 0.97 | 313 |
| CD2--2HD2 | 1.08 | 0.97 | 163 |
| CD--2HD | 1.08 | 0.97 | 103 |
| CB--HB | 1.08 | 0.97 | 166 |
| CE--2HE | 1.08 | 0.97 | 43 |
| CG1--1HG1 | 1.08 | 0.97 | 141 |
| CB--3HB | 1.08 | 0.97 | 143 |
| CG1--2HG1 | 1.08 | 0.97 | 175 |
| CA--2HA | 1.08 | 0.97 | 46 |
| CG1--3HG1 | 1.08 | 0.97 | 93 |
| CG2--2HG2 | 1.08 | 0.97 | 194 |
| CE--1HE | 1.08 | 0.97 | 57 |
| NZ--3HZ | 1.00 | 0.89 | 29 |
| CE1--HE1 | 1.04 | 0.93 | 2 |
| NZ--2HZ | 1.00 | 0.89 | 30 |
| NZ--1HZ | 1.00 | 0.89 | 25 |
| OG1--HG1 | 0.95 | 0.84 | 1 |
| CD1--HD1 | 1.04 | 0.93 | 4 |
| CE3--HE3 | 1.04 | 0.93 | 1 |
| CD2--HD2 | 1.04 | 0.93 | 1 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| OG--HG | 0.95 | 0.84 | 7 |
| OH--HH | 0.95 | 0.84 | 6 |
| CZ--HZ | 1.04 | 0.93 | 1 |
| CE2--HE2 | 1.04 | 0.93 | 2 |
| CZ3--HZ3 | 1.04 | 0.93 | 2 |
| CH2--HH2 | 1.04 | 0.93 | 1 |
| CA--HA | 1.09 | 0.97 | 3225 |
| CB--2HB | 1.09 | 0.97 | 2458 |
| CD2--3HD2 | 1.09 | 0.97 | 249 |
| CB--1HB | 1.09 | 0.97 | 2399 |
| CG1--1HG1 | 1.09 | 0.97 | 270 |
| CG1--3HG1 | 1.09 | 0.97 | 165 |
| CG2--3HG2 | 1.09 | 0.97 | 350 |
| NZ--3HZ | 1.01 | 0.89 | 165 |
| CG2--1HG2 | 1.09 | 0.97 | 369 |
| CG1--2HG1 | 1.09 | 0.97 | 231 |
| CG2--2HG2 | 1.09 | 0.97 | 382 |
| CD1--1HD1 | 1.09 | 0.97 | 505 |
| CA--1HA | 1.09 | 0.97 | 251 |
| CD2--1HD2 | 1.09 | 0.97 | 450 |
| CD1--3HD1 | 1.09 | 0.97 | 405 |
| NZ--1HZ | 1.01 | 0.89 | 174 |
| CG--2HG | 1.09 | 0.97 | 861 |
| CD2--2HD2 | 1.09 | 0.97 | 437 |
| CD--1HD | 1.09 | 0.97 | 456 |
| CE--1HE | 1.09 | 0.97 | 253 |
| CD--2HD | 1.09 | 0.97 | 431 |
| CD1--2HD1 | 1.09 | 0.97 | 416 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CB--3HB | 1.09 | 0.97 | 181 |
| OG--HG | 0.96 | 0.84 | 252 |
| CG--1HG | 1.09 | 0.97 | 905 |
| CB--HB | 1.09 | 0.97 | 391 |
| CA--2HA | 1.09 | 0.97 | 232 |
| CG--HG | 1.09 | 0.97 | 346 |
| CE--2HE | 1.09 | 0.97 | 260 |
| CE--3HE | 1.09 | 0.97 | 52 |
| NZ--2HZ | 1.01 | 0.89 | 161 |
| CD2--HD2 | 1.05 | 0.93 | 9 |
| CD1--HD1 | 1.05 | 0.93 | 10 |
| OH--HH | 0.96 | 0.84 | 59 |
| OG1--HG1 | 0.96 | 0.84 | 55 |
| CZ3--HZ3 | 1.05 | 0.93 | 2 |
| N--2H | 1.01 | 0.89 | 8 |
| CH2--HH2 | 1.05 | 0.93 | 2 |
| CE3--HE3 | 1.05 | 0.93 | 4 |
| CE1--HE1 | 1.05 | 0.93 | 3 |
| NE2--2HE2 | 0.98 | 0.86 | 1 |
| CE2--HE2 | 1.05 | 0.93 | 5 |
| N--1H | 1.01 | 0.89 | 8 |
| ND2--1HD2 | 0.98 | 0.86 | 1 |
| CZ--HZ | 1.05 | 0.93 | 2 |
| N--3H | 1.01 | 0.89 | 6 |
| CG--HG | 1.10 | 0.97 | 34 |
| CD1--2HD1 | 1.10 | 0.97 | 9 |
| CB--1HB | 1.10 | 0.97 | 259 |
| CD--2HD | 1.10 | 0.97 | 107 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CD--1HD | 1.10 | 0.97 | 90 |
| OG1--HG1 | 0.97 | 0.84 | 77 |
| CA--HA | 1.10 | 0.97 | 189 |
| CG1--3HG1 | 1.10 | 0.97 | 6 |
| CG2--2HG2 | 1.10 | 0.97 | 4 |
| CD1--1HD1 | 1.10 | 0.97 | 13 |
| CD2--2HD2 | 1.10 | 0.97 | 15 |
| CB--2HB | 1.10 | 0.97 | 213 |
| CZ2--HZ2 | 1.06 | 0.93 | 7 |
| CD2--HD2 | 1.06 | 0.93 | 17 |
| CD1--3HD1 | 1.10 | 0.97 | 5 |
| OG--HG | 0.97 | 0.84 | 62 |
| CB--HB | 1.10 | 0.97 | 21 |
| CG--1HG | 1.10 | 0.97 | 172 |
| CG--2HG | 1.10 | 0.97 | 183 |
| NZ--3HZ | 1.02 | 0.89 | 20 |
| NZ--2HZ | 1.02 | 0.89 | 22 |
| CG2--3HG2 | 1.10 | 0.97 | 10 |
| CD2--1HD2 | 1.10 | 0.97 | 10 |
| CG1--2HG1 | 1.10 | 0.97 | 4 |
| NZ--1HZ | 1.02 | 0.89 | 19 |
| N--3H | 1.02 | 0.89 | 2 |
| CE--2HE | 1.10 | 0.97 | 3 |
| CE2--HE2 | 1.06 | 0.93 | 9 |
| OH--HH | 0.97 | 0.84 | 9 |
| CG2--1HG2 | 1.10 | 0.97 | 2 |
| CD2--3HD2 | 1.10 | 0.97 | 2 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| CD1--HD1 | 1.06 | 0.93 | 17 |
| CE1--HE1 | 1.06 | 0.93 | 17 |
| CZ--HZ | 1.06 | 0.93 | 5 |
| SG--HG | 1.33 | 1.20 | 22 |
| CA--1HA | 1.10 | 0.97 | 1 |
| CE3--HE3 | 1.06 | 0.93 | 3 |
| NE--HE | 0.99 | 0.86 | 1 |
| CZ3--HZ3 | 1.06 | 0.93 | 2 |
| CB--3HB | 1.10 | 0.97 | 1 |
| ND1--HD1 | 0.99 | 0.86 | 3 |
| NE2--1HE2 | 0.99 | 0.86 | 11 |
| CH2--HH2 | 1.06 | 0.93 | 1 |
| ND2--2HD2 | 0.99 | 0.86 | 4 |
| ND2--1HD2 | 0.99 | 0.86 | 7 |
| N--H | 0.99 | 0.86 | 2 |
| NE1--HE1 | 0.99 | 0.86 | 1 |
| NE2--2HE2 | 0.99 | 0.86 | 4 |
| OG--HG | 0.98 | 0.84 | 40 |
| NE2--1HE2 | 1.00 | 0.86 | 214 |
| CG--2HG | 1.11 | 0.97 | 14 |
| ND2--1HD2 | 1.00 | 0.86 | 105 |
| SG--HG | 1.34 | 1.20 | 47 |
| CG--1HG | 1.11 | 0.97 | 23 |
| CD--1HD | 1.11 | 0.97 | 8 |
| ND2--2HD2 | 1.00 | 0.86 | 100 |
| CE1--HE1 | 1.07 | 0.93 | 25 |
| CD--2HD | 1.11 | 0.97 | 18 |
| CA--HA | 1.11 | 0.97 | 4 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| OG1--HG1 | 0.98 | 0.84 | 53 |
| CD2--HD2 | 1.07 | 0.93 | 32 |
| CD1--HD1 | 1.07 | 0.93 | 51 |
| CZ--HZ | 1.07 | 0.93 | 17 |
| CB--1HB | 1.11 | 0.97 | 21 |
| CZ3--HZ3 | 1.07 | 0.93 | 12 |
| NH1--1HH1 | 1.00 | 0.86 | 54 |
| CH2--HH2 | 1.07 | 0.93 | 6 |
| N--H | 1.00 | 0.86 | 96 |
| CE3--HE3 | 1.07 | 0.93 | 15 |
| CB--2HB | 1.11 | 0.97 | 10 |
| NE2--2HE2 | 1.00 | 0.86 | 190 |
| NZ--1HZ | 1.03 | 0.89 | 14 |
| NH1--2HH1 | 1.00 | 0.86 | 11 |
| OH--HH | 0.98 | 0.84 | 8 |
| NZ--3HZ | 1.03 | 0.89 | 8 |
| NZ--2HZ | 1.03 | 0.89 | 13 |
| CZ2--HZ2 | 1.07 | 0.93 | 5 |
| NE1--HE1 | 1.00 | 0.86 | 11 |
| NH2--2HH2 | 1.00 | 0.86 | 35 |
| ND1--HD1 | 1.00 | 0.86 | 28 |
| CE2--HE2 | 1.07 | 0.93 | 26 |
| NH2--1HH2 | 1.00 | 0.86 | 6 |
| NE--HE | 1.00 | 0.86 | 2 |
| NE2--HE2 | 1.00 | 0.86 | 1 |
| NH2--2HH2 | 1.01 | 0.86 | 184 |
| NE2--1HE2 | 1.01 | 0.86 | 30 |
| NH1--1HH1 | 1.01 | 0.86 | 143 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| NZ--2HZ | 1.04 | 0.89 | 11 |
| NH2--1HH2 | 1.01 | 0.86 | 150 |
| N--H | 1.01 | 0.86 | 1353 |
| CH2--HH2 | 1.08 | 0.93 | 24 |
| CZ--HZ | 1.08 | 0.93 | 45 |
| OG--HG | 0.99 | 0.84 | 30 |
| NH1--2HH1 | 1.01 | 0.86 | 178 |
| ND1--HD1 | 1.01 | 0.86 | 13 |
| NE2--2HE2 | 1.01 | 0.86 | 23 |
| NE1--HE1 | 1.01 | 0.86 | 40 |
| CZ3--HZ3 | 1.08 | 0.93 | 20 |
| OG1--HG1 | 0.99 | 0.84 | 16 |
| CD1--HD1 | 1.08 | 0.93 | 95 |
| SG--HG | 1.35 | 1.20 | 51 |
| ND2--2HD2 | 1.01 | 0.86 | 8 |
| CE3--HE3 | 1.08 | 0.93 | 24 |
| CE1--HE1 | 1.08 | 0.93 | 75 |
| ND2--1HD2 | 1.01 | 0.86 | 5 |
| CE2--HE2 | 1.08 | 0.93 | 67 |
| NE--HE | 1.01 | 0.86 | 142 |
| CZ2--HZ2 | 1.08 | 0.93 | 14 |
| NZ--1HZ | 1.04 | 0.89 | 6 |
| CG--2HG | 1.12 | 0.97 | 1 |
| CD2--HD2 | 1.08 | 0.93 | 77 |
| CG--1HG | 1.12 | 0.97 | 1 |
| NZ--3HZ | 1.04 | 0.89 | 14 |
| OH--HH | 0.99 | 0.84 | 15 |
| NE2--HE2 | 1.01 | 0.86 | 42 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| N--H | 1.02 | 0.86 | 2439 |
| NE2--2HE2 | 1.02 | 0.86 | 30 |
| CZ2--HZ2 | 1.09 | 0.93 | 50 |
| CD1--HD1 | 1.09 | 0.93 | 149 |
| CE3--HE3 | 1.09 | 0.93 | 28 |
| CE1--HE1 | 1.09 | 0.93 | 258 |
| CD2--HD2 | 1.09 | 0.93 | 245 |
| NE2--HE2 | 1.02 | 0.86 | 11 |
| SG--HG | 1.36 | 1.20 | 30 |
| CH2--HH2 | 1.09 | 0.93 | 41 |
| NH1--1HH1 | 1.02 | 0.86 | 21 |
| NH1--2HH1 | 1.02 | 0.86 | 33 |
| NE--HE | 1.02 | 0.86 | 49 |
| NE2--1HE2 | 1.02 | 0.86 | 16 |
| CE2--HE2 | 1.09 | 0.93 | 147 |
| CZ--HZ | 1.09 | 0.93 | 81 |
| CZ3--HZ3 | 1.09 | 0.93 | 38 |
| NH2--2HH2 | 1.02 | 0.86 | 14 |
| NH2--1HH2 | 1.02 | 0.86 | 36 |
| NE1--HE1 | 1.02 | 0.86 | 8 |
| OG--HG | 1.00 | 0.84 | 15 |
| ND2--1HD2 | 1.02 | 0.86 | 8 |
| ND1--HD1 | 1.02 | 0.86 | 11 |
| OH--HH | 1.00 | 0.84 | 8 |
| OG1--HG1 | 1.00 | 0.84 | 9 |
| ND2--2HD2 | 1.02 | 0.86 | 10 |
| NZ--3HZ | 1.05 | 0.89 | 5 |
| NZ--1HZ | 1.05 | 0.89 | 4 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| NZ--2HZ | 1.05 | 0.89 | 3 |
| N--H | 1.03 | 0.86 | 986 |
| CE1--HE1 | 1.10 | 0.93 | 11 |
| CD2--HD2 | 1.10 | 0.93 | 9 |
| CD1--HD1 | 1.10 | 0.93 | 12 |
| CE2--HE2 | 1.10 | 0.93 | 7 |
| NH1--1HH1 | 1.03 | 0.86 | 34 |
| NH2--1HH2 | 1.03 | 0.86 | 39 |
| NH2--2HH2 | 1.03 | 0.86 | 18 |
| OG1--HG1 | 1.01 | 0.84 | 3 |
| NE2--1HE2 | 1.03 | 0.86 | 11 |
| NE--HE | 1.03 | 0.86 | 36 |
| NH1--2HH1 | 1.03 | 0.86 | 28 |
| SG--HG | 1.37 | 1.20 | 9 |
| CH2--HH2 | 1.10 | 0.93 | 1 |
| ND2--1HD2 | 1.03 | 0.86 | 1 |
| ND2--2HD2 | 1.03 | 0.86 | 6 |
| NZ--2HZ | 1.06 | 0.89 | 2 |
| ND1--HD1 | 1.03 | 0.86 | 6 |
| NE2--HE2 | 1.03 | 0.86 | 6 |
| NE2--2HE2 | 1.03 | 0.86 | 30 |
| NE1--HE1 | 1.03 | 0.86 | 7 |
| CZ--HZ | 1.10 | 0.93 | 4 |
| OG--HG | 1.01 | 0.84 | 7 |
| OH--HH | 1.01 | 0.84 | 2 |
| NZ--3HZ | 1.06 | 0.89 | 1 |
| NH2--2HH2 | 1.04 | 0.86 | 11 |
| N--H | 1.04 | 0.86 | 16 |

| Bond type | Observed distance (Å) | Ideal distance (Å) | Number of outliers |
|---|---|---|---|
| NH2--1HH2 | 1.04 | 0.86 | 29 |
| NE2--1HE2 | 1.04 | 0.86 | 4 |
| NE--HE | 1.04 | 0.86 | 28 |
| NH1--1HH1 | 1.04 | 0.86 | 9 |
| NE2--2HE2 | 1.04 | 0.86 | 8 |
| SG--HG | 1.38 | 1.20 | 1 |
| NH1--2HH1 | 1.04 | 0.86 | 10 |
| NE2--HE2 | 1.04 | 0.86 | 4 |
| OG--HG | 1.02 | 0.84 | 1 |
| NE1--HE1 | 1.04 | 0.86 | 5 |
| OG1--HG1 | 1.02 | 0.84 | 4 |
| ND2--1HD2 | 1.04 | 0.86 | 1 |
| ND1--HD1 | 1.04 | 0.86 | 1 |
| NH1--2HH1 | 1.05 | 0.86 | 2 |
| NH2--1HH2 | 1.05 | 0.86 | 2 |
| NE2--HE2 | 1.05 | 0.86 | 3 |
| NH1--1HH1 | 1.05 | 0.86 | 1 |
| NE--HE | 1.05 | 0.86 | 4 |
| NE1--HE1 | 1.05 | 0.86 | 3 |
| NE1--HE1 | 1.06 | 0.86 | 1 |
| N--2H | 1.86 | 0.96 | 1 |
| N--1H | 1.88 | 0.96 | 1 |
| N--1H | 1.89 | 0.96 | 1 |
| N--2H | 1.89 | 0.96 | 1 |
| N--2H | 1.92 | 0.96 | 1 |
| N--1H | 1.93 | 0.96 | 1 |

## Standard geometry: angle outliers ?

*There are 260 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be foundhere.*

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-CB-CG | 113.80 | 101.00 | 1 |
| C-N-CA | 121.70 | 140.14 | 1 |
| N-CA-CB | 103.00 | 92.73 | 1 |
| C-N-CA | 121.70 | 138.30 | 1 |
| CA-CB-CG | 112.60 | 121.80 | 1 |
| C-N-CA | 121.70 | 137.98 | 1 |
| N-CA-CB | 103.00 | 93.71 | 1 |
| C-N-CA | 121.70 | 136.20 | 1 |
| C-N-CA | 121.70 | 136.02 | 1 |
| CA-CB-CG | 113.80 | 121.68 | 2 |
| C-N-CA | 121.70 | 135.66 | 1 |
| C-N-CA | 121.70 | 135.28 | 1 |
| C-N-CA | 121.70 | 135.22 | 1 |
| N-CA-C | 111.00 | 131.72 | 1 |
| C-N-CA | 121.70 | 134.75 | 1 |
| N-CA-C | 111.00 | 130.93 | 1 |
| C-N-CA | 121.70 | 134.46 | 1 |
| CA-CB-CG | 113.80 | 120.83 | 1 |
| CA-CB-CG | 113.80 | 106.82 | 1 |
| CA-CB-CG | 113.80 | 106.88 | 1 |
| C-N-CA | 121.70 | 133.58 | 1 |
| N-CA-C | 111.00 | 129.35 | 1 |
| CA-CB-CG | 113.80 | 120.34 | 1 |
| CA-CB-CG | 113.80 | 120.30 | 1 |
| CA-CB-CG | 112.60 | 119.09 | 2 |
| O-C-N | 123.00 | 112.71 | 1 |
| C-N-CA | 121.70 | 133.11 | 1 |
| N-CA-C | 111.00 | 93.37 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| C-CA-CB | 110.10 | 98.26 | 1 |
| N-CA-C | 111.00 | 128.34 | 1 |
| C-N-CA | 121.70 | 132.83 | 1 |
| CA-CB-CG | 113.80 | 119.96 | 1 |
| N-CA-C | 112.10 | 127.34 | 1 |
| C-N-CA | 121.70 | 132.64 | 1 |
| C-N-CA | 121.70 | 132.58 | 1 |
| C-N-CA | 121.70 | 132.44 | 1 |
| C-N-CA | 121.70 | 132.37 | 1 |
| C-N-CA | 121.70 | 132.30 | 1 |
| CA-CB-CG | 112.60 | 118.46 | 1 |
| N-CA-CB | 110.50 | 120.45 | 1 |
| C-N-CA | 121.70 | 132.22 | 1 |
| CA-CB-CG | 113.80 | 119.64 | 1 |
| CA-CB-CG | 113.80 | 119.62 | 1 |
| CA-CB-CG | 113.80 | 119.61 | 1 |
| CA-CB-CG | 113.80 | 108.02 | 1 |
| CA-CB-CG | 113.80 | 119.56 | 1 |
| C-N-CA | 121.70 | 131.99 | 1 |
| CA-CB-CG | 112.60 | 106.88 | 1 |
| CA-CB-CG | 113.80 | 119.42 | 1 |
| N-CA-CB | 110.50 | 120.01 | 1 |
| CA-CB-CG | 113.80 | 119.37 | 1 |
| C-CA-CB | 110.10 | 120.68 | 1 |
| C-N-CA | 121.70 | 131.66 | 1 |
| CA-CB-CG | 113.80 | 108.27 | 1 |
| CA-CB-CG | 112.60 | 118.10 | 1 |
| CA-CB-CG | 113.90 | 104.00 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-CB-CG | 113.80 | 119.26 | 1 |
| CA-CB-CG | 113.80 | 108.34 | 1 |
| C-N-CA | 121.70 | 131.49 | 1 |
| C-CA-CB | 111.60 | 100.73 | 1 |
| CA-C-N | 116.90 | 124.99 | 1 |
| C-CA-CB | 110.10 | 120.35 | 1 |
| C-CA-CB | 110.10 | 99.99 | 1 |
| CA-C-N | 116.90 | 124.81 | 1 |
| CA-CB-CG | 113.80 | 119.07 | 1 |
| N-CA-C | 111.00 | 125.73 | 1 |
| C-N-CA | 121.70 | 131.14 | 1 |
| C-N-CA | 121.70 | 131.03 | 1 |
| CA-CB-CG | 112.60 | 117.78 | 1 |
| C-N-CA | 121.70 | 131.02 | 1 |
| CA-CB-CG | 113.80 | 118.98 | 1 |
| CA-C-O | 120.80 | 112.09 | 1 |
| C-CA-CB | 110.10 | 119.81 | 1 |
| C-N-CA | 121.70 | 112.51 | 1 |
| CA-C-N | 116.20 | 126.38 | 1 |
| C-N-CA | 121.70 | 130.85 | 1 |
| C-N-CA | 121.70 | 130.84 | 1 |
| CA-CB-CG | 112.60 | 117.68 | 1 |
| N-CA-C | 111.00 | 125.15 | 1 |
| C-N-CA | 121.70 | 130.77 | 1 |
| CA-CB-CG | 113.80 | 118.83 | 1 |
| CA-C-N | 116.20 | 126.24 | 1 |
| C-N-CA | 121.70 | 130.72 | 1 |
| CA-C-N | 116.20 | 126.22 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| N-CA-C | 111.00 | 97.00 | 1 |
| C-CA-CB | 110.10 | 119.57 | 1 |
| N-CA-C | 113.30 | 98.86 | 1 |
| CA-CB-CG | 113.80 | 108.84 | 1 |
| CA-CB-CG | 112.60 | 117.56 | 1 |
| C-CA-CB | 111.60 | 101.72 | 1 |
| C-N-CA | 121.70 | 112.86 | 1 |
| CA-CB-CG | 113.80 | 108.89 | 1 |
| CA-CB-CG | 113.80 | 118.71 | 1 |
| N-CA-C | 111.00 | 124.71 | 1 |
| C-N-CA | 121.70 | 130.51 | 1 |
| CA-C-N | 116.20 | 125.98 | 1 |
| N-CA-C | 111.00 | 97.39 | 1 |
| N-CA-C | 111.00 | 97.40 | 1 |
| CA-CB-CG | 113.80 | 118.62 | 1 |
| C-N-CA | 121.70 | 130.37 | 1 |
| CA-C-N | 116.90 | 124.12 | 1 |
| C-N-CA | 121.70 | 130.35 | 1 |
| N-CA-C | 111.00 | 124.40 | 2 |
| C-CA-CB | 110.10 | 119.18 | 1 |
| CA-CB-CG | 112.60 | 117.37 | 1 |
| CA-CB-CG | 113.80 | 109.04 | 1 |
| CA-C-N | 116.90 | 124.02 | 1 |
| CA-CB-CG | 113.80 | 109.07 | 1 |
| N-CA-C | 111.00 | 124.08 | 1 |
| C-N-CA | 121.70 | 130.10 | 1 |
| CA-CB-CG | 112.60 | 117.26 | 1 |
| CA-CB-CG | 113.80 | 118.45 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-C-N | 116.90 | 123.88 | 1 |
| N-CA-C | 111.00 | 123.95 | 1 |
| CA-C-N | 116.90 | 123.83 | 1 |
| C-CA-CB | 110.10 | 118.85 | 1 |
| N-CA-C | 111.00 | 98.12 | 1 |
| CA-C-N | 116.90 | 123.80 | 1 |
| C-N-CA | 121.70 | 129.96 | 2 |
| N-CA-C | 112.10 | 100.63 | 1 |
| C-CA-CB | 110.10 | 118.82 | 1 |
| CA-CB-CG | 113.80 | 109.21 | 1 |
| CA-CB-CG | 113.90 | 122.14 | 1 |
| C-CA-CB | 110.10 | 101.41 | 1 |
| CA-CB-CG | 113.80 | 109.23 | 1 |
| CA-C-N | 116.90 | 123.76 | 1 |
| C-N-CA | 121.70 | 129.91 | 1 |
| C-N-CA | 121.70 | 113.50 | 1 |
| C-N-CA | 121.70 | 129.89 | 1 |
| CA-C-N | 116.20 | 125.30 | 1 |
| N-CA-C | 111.00 | 98.26 | 1 |
| C-N-CA | 121.70 | 129.88 | 1 |
| CA-CB-CG | 113.80 | 109.27 | 2 |
| CA-C-N | 116.90 | 123.68 | 1 |
| CA-CB-CG | 113.80 | 109.29 | 1 |
| CA-CB-CG | 112.60 | 108.09 | 1 |
| CA-CB-CG | 112.60 | 117.10 | 1 |
| C-N-CA | 121.70 | 113.63 | 1 |
| C-N-CA | 121.70 | 113.67 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| NE-CZ-NH2 | 119.20 | 123.20 | 1 |
| C-CA-CB | 110.10 | 118.55 | 1 |
| C-CA-CB | 110.10 | 101.66 | 1 |
| C-N-CA | 121.70 | 129.68 | 1 |
| CA-CB-CG | 112.60 | 108.18 | 2 |
| N-CA-C | 112.10 | 101.07 | 1 |
| C-N-CA | 121.70 | 113.79 | 1 |
| N-CA-C | 112.10 | 123.08 | 1 |
| C-N-CA | 121.70 | 129.60 | 1 |
| NE-CZ-NH2 | 119.20 | 123.14 | 1 |
| CA-CB-CG | 113.80 | 109.42 | 1 |
| CA-CB-CG | 112.60 | 116.98 | 1 |
| C-CA-CB | 110.10 | 118.40 | 1 |
| N-CA-C | 111.00 | 98.77 | 1 |
| NE-CZ-NH2 | 119.20 | 115.27 | 1 |
| NE-CZ-NH2 | 119.20 | 115.28 | 1 |
| C-N-CA | 121.70 | 113.86 | 1 |
| N-CA-CB | 110.50 | 117.90 | 1 |
| CA-CB-CG | 113.80 | 109.45 | 1 |
| N-CA-C | 112.10 | 101.29 | 1 |
| C-N-CA | 121.70 | 129.48 | 1 |
| C-N-CA | 121.70 | 113.93 | 1 |
| C-N-CA | 121.70 | 129.46 | 1 |
| C-N-CA | 121.70 | 129.45 | 2 |
| N-CA-CB | 111.50 | 104.18 | 1 |
| CA-CB-CG | 112.60 | 116.90 | 2 |
| CA-CB-CG | 112.60 | 108.30 | 1 |
| C-N-CA | 121.70 | 129.43 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| C-N-CA | 121.70 | 113.98 | 1 |
| CA-CB-CG | 113.80 | 118.08 | 1 |
| CA-CB-CG | 113.90 | 121.60 | 1 |
| N-CA-C | 111.00 | 122.97 | 1 |
| C-N-CA | 121.70 | 129.39 | 1 |
| CA-C-N | 116.20 | 124.74 | 1 |
| CA-CB-CG | 113.80 | 109.53 | 1 |
| C-N-CA | 121.70 | 129.38 | 1 |
| CA-CB-CG | 113.80 | 109.54 | 1 |
| C-N-CA | 121.70 | 114.04 | 1 |
| C-N-CA | 121.70 | 129.35 | 1 |
| N-CA-C | 111.00 | 122.90 | 1 |
| C-N-CA | 121.70 | 114.05 | 1 |
| C-CA-CB | 110.10 | 102.02 | 1 |
| CA-CB-CG | 112.60 | 116.84 | 1 |
| CA-C-N | 116.90 | 123.26 | 1 |
| C-N-CA | 121.70 | 129.31 | 1 |
| CA-CB-CG | 113.80 | 118.03 | 1 |
| CA-CB-CG | 113.90 | 106.31 | 1 |
| C-N-CA | 121.70 | 129.27 | 1 |
| C-N-CA | 121.70 | 129.26 | 1 |
| NE-CZ-NH2 | 119.20 | 115.43 | 1 |
| CA-CB-CG | 113.80 | 117.98 | 2 |
| C-N-CA | 121.70 | 129.23 | 1 |
| CA-CB-CG | 113.90 | 106.38 | 1 |
| CB-CG-CD | 112.60 | 119.70 | 1 |
| N-CA-CB | 110.50 | 103.41 | 1 |
| C-N-CA | 121.70 | 114.22 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| N-CA-C | 111.00 | 99.38 | 1 |
| C-N-CA | 121.70 | 129.17 | 1 |
| CA-CB-CG | 113.80 | 117.95 | 1 |
| CA-C-N | 116.20 | 124.49 | 1 |
| C-N-CA | 121.70 | 114.26 | 1 |
| C-CA-CB | 110.10 | 117.95 | 1 |
| C-N-CA | 121.70 | 114.27 | 1 |
| C-N-CA | 121.70 | 129.12 | 1 |
| C-N-CA | 121.70 | 129.11 | 1 |
| CA-CB-CG | 112.60 | 116.71 | 1 |
| CA-CB-CG | 113.80 | 117.91 | 1 |
| C-N-CA | 121.70 | 129.10 | 1 |
| N-CA-C | 111.00 | 122.51 | 1 |
| NE-CZ-NH2 | 119.20 | 122.90 | 1 |
| C-N-CA | 121.70 | 129.09 | 1 |
| C-N-CA | 121.70 | 129.07 | 1 |
| CA-CB-CG | 112.60 | 116.69 | 1 |
| N-CA-C | 112.10 | 101.88 | 1 |
| CA-CB-CG | 113.80 | 109.72 | 1 |
| C-N-CA | 121.70 | 129.04 | 1 |
| CA-CB-CG | 113.80 | 109.73 | 3 |
| CA-C-N | 116.90 | 123.00 | 1 |
| C-N-CA | 121.70 | 128.97 | 1 |
| C-N-CA | 121.70 | 114.44 | 1 |
| C-N-CA | 121.70 | 114.46 | 1 |
| C-N-CA | 121.70 | 128.92 | 1 |
| N-CA-C | 111.00 | 122.22 | 1 |
| CA-C-N | 116.90 | 122.91 | 1 |

| Angle type | Observed angle (°) | Ideal angle (°) | Number of outliers |
|---|---|---|---|
| CA-CB-CG | 113.80 | 109.80 | 2 |
| C-N-H | 112.29 | 124.30 | 1 |
| C-N-H | 112.06 | 124.30 | 1 |
| C-N-H | 111.98 | 124.30 | 1 |
| C-N-H | 111.93 | 124.30 | 1 |
| C-N-H | 111.70 | 124.30 | 1 |
| C-N-H | 111.59 | 124.30 | 1 |
| C-N-H | 111.56 | 124.30 | 1 |
| CA-N-2H | 96.36 | 109.47 | 1 |
| CA-N-2H | 96.10 | 109.47 | 1 |
| C-N-H | 110.69 | 124.30 | 1 |
| C-N-H | 110.63 | 124.30 | 1 |
| C-N-H | 109.60 | 124.30 | 1 |
| CA-N-1H | 88.89 | 109.47 | 1 |
| CA-N-1H | 88.64 | 109.47 | 1 |
| CA-N-2H | 87.61 | 109.47 | 1 |
| CD-N-1H | 133.47 | 109.47 | 1 |
| CD-N-2H | 134.82 | 109.47 | 1 |
| CD-N-1H | 138.86 | 109.47 | 1 |
| CD-N-2H | 143.60 | 109.47 | 1 |
| CD-N-2H | 145.89 | 109.47 | 1 |
| CD-N-1H | 146.52 | 109.47 | 1 |
| 1H-N-2H | 52.87 | 109.47 | 1 |
| 1H-N-2H | 52.69 | 109.47 | 1 |
| 1H-N-2H | 52.38 | 109.47 | 1 |

## Too-close contacts?

*The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.*

| Model ID | Clash score | Number of clashes |
|---|---|---|

| Model ID | Clash score | Number of clashes |
|---|---|---|
| 1 | 0.00 | 0 |

*All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.*

### Torsion angles: Protein backbone?

*In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 5079 | 4875 | 168 | 36 |

*Detailed list of outliers are tabulated below.*

### Torsion angles: Protein sidechains ?

*In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.*

| Model ID | Analyzed | Favored | Allowed | Outliers |
|---|---|---|---|---|
| 1 | 4426 | 4367 | 50 | 9 |

*Detailed list of outliers are tabulated below.*

| Model ID | Chain | Residue ID | Residue type |
|---|---|---|---|
| 1 | B | 427 | 0ILE |
| 1 | G | 33 | 0ARG |
| 1 | P | 100 | 0THR |
| 1 | P | 240 | 0CYS |
| 1 | b | 427 | 0ILE |
| 1 | b | 441 | 0LYS |
| 1 | b | 669 | 0MET |
| 1 | g | 213 | 0THR |
| 1 | p | 150 | 0MET |

## Fit of model to data used for modeling ?

### 3DEM volume

Validation for this section is under development.

### Crosslinking-MS

Validation for this section is under development.

## Fit of model to data used for validation ?

Validation for this section is under development.

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