



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:25 AM UTC

PDB ID : 3PCI / pdb\_00003pci  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 3-iodo-4-HYDROXYBENZOATE  
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.  
Deposited on : 1997-07-02  
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

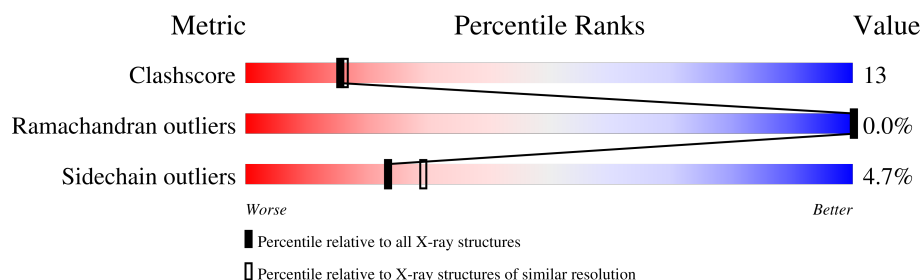
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 8402 (2.24-2.20)                                      |
| Ramachandran outliers | 187476                      | 8303 (2.24-2.20)                                      |
| Sidechain outliers    | 187428                      | 8304 (2.24-2.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 200    | 70% 26% .        |
| 1   | B     | 200    | 64% 30% 6%       |
| 1   | C     | 200    | 68% 26% 6%       |
| 1   | D     | 200    | 68% 26% 6%       |
| 1   | E     | 200    | 63% 28% 8%       |
| 1   | F     | 200    | 58% 34% 7% .     |
| 2   | M     | 238    | 62% 30% 5% ..    |
| 2   | N     | 238    | 68% 25% 5% ..    |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 2   | O     | 238    | <div><div></div><div>69%26%<div><div></div><div></div><div></div></div></div></div>   |
| 2   | P     | 238    | <div><div></div><div>67%25%5%<div><div></div><div></div><div></div></div></div></div> |
| 2   | Q     | 238    | <div><div></div><div>63%26%8%<div><div></div><div></div><div></div></div></div></div> |
| 2   | R     | 238    | <div><div></div><div>61%31%6%<div><div></div><div></div><div></div></div></div></div> |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22104 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PROTOCATECHUATE 3,4-DIOXYGENASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | B     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | C     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | D     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | E     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | F     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |

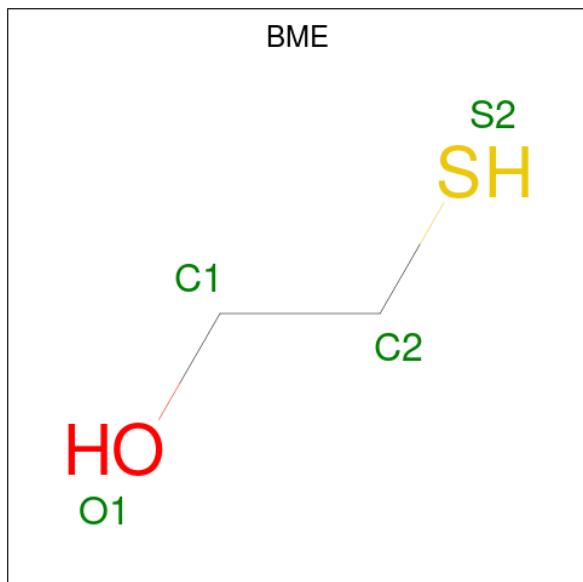
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | M     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | N     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | O     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | P     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | Q     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | R     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

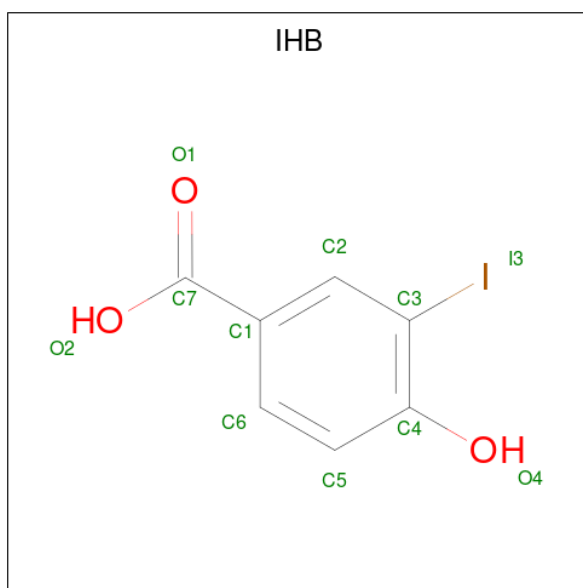
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | M     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | N     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | O     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | P     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | Q     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | R     | 1        | Total Fe<br>1 1 | 0       | 0       |

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula:  $C_2H_6OS$ ).



| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 4   | M     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | N     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | O     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | P     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | Q     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | R     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |

- Molecule 5 is 3-iodo-4-hydroxybenzoic acid (CCD ID: IHB) (formula:  $C_7H_5IO_3$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | M     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | M     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | N     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | N     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | O     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | O     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | P     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | P     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | Q     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | Q     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | R     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |
| 5   | R     | 1        | Total | C | I | O | 0       | 0       |
|     |       |          | 11    | 7 | 1 | 3 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6   | A     | 82       | Total O<br>82 82   | 0       | 0       |
| 6   | M     | 163      | Total O<br>163 163 | 0       | 0       |
| 6   | B     | 85       | Total O<br>85 85   | 0       | 0       |
| 6   | N     | 167      | Total O<br>167 167 | 0       | 0       |
| 6   | C     | 82       | Total O<br>82 82   | 0       | 0       |
| 6   | O     | 162      | Total O<br>162 162 | 0       | 0       |
| 6   | D     | 81       | Total O<br>81 81   | 0       | 0       |
| 6   | P     | 157      | Total O<br>157 157 | 0       | 0       |
| 6   | E     | 84       | Total O<br>84 84   | 0       | 0       |
| 6   | Q     | 165      | Total O<br>165 165 | 0       | 0       |
| 6   | F     | 81       | Total O<br>81 81   | 0       | 0       |
| 6   | R     | 167      | Total O<br>167 167 | 0       | 0       |

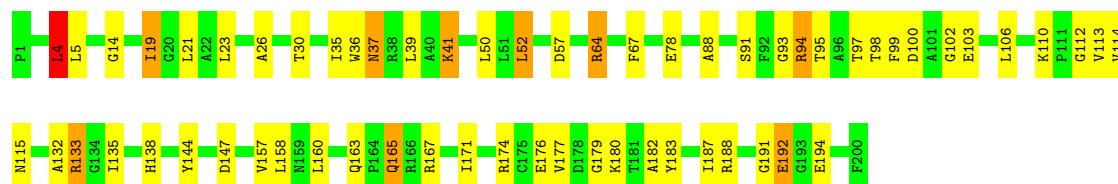
### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

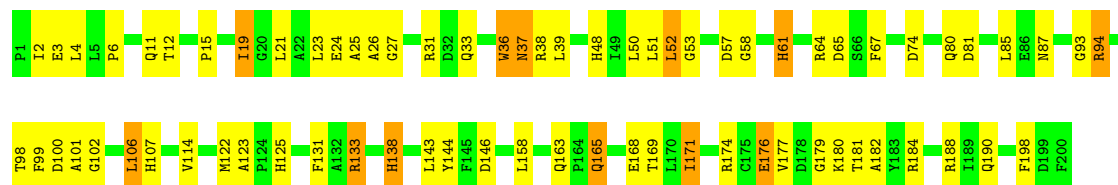
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



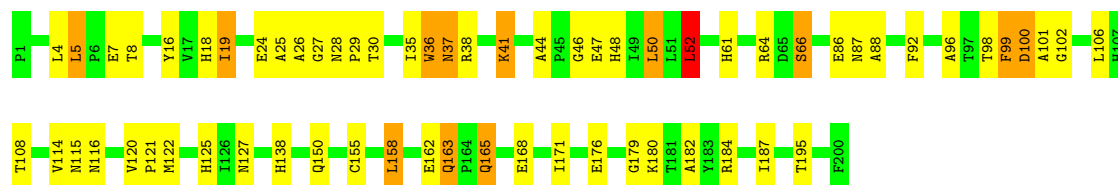
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 





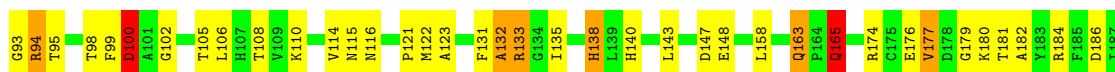
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 63% 28% 8%



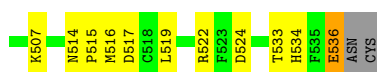
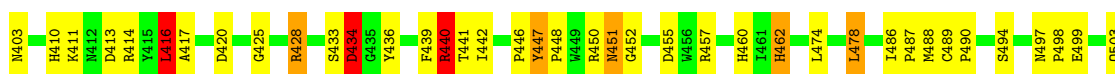
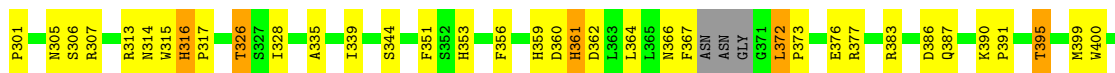
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 58% 34% 7%



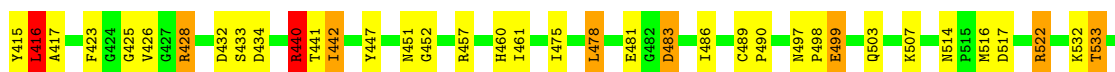
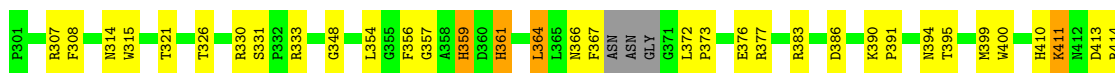
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 62% 30% 5%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N: 68% 25% 5%



E536  
ASN  
CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O: 69% 26% • •

P301 D304 R305 S306 N314 W315 K318 I328 Q334 I339 I343 H353 L354 H361 D362 L363 L364 N366 F367 ASN GLY G371 L372 P373 E376 I379 R383 V384 Q387 K390 N394 T395 W400 R409 H410 K411 N412 L416 D420

G425 R428 D434 C435 Y436 R440 T441 I442 Y447 R450 N451 G452 P453 N454 H460 F463 G464 I465 K473 E481 P484 L486 P487 M488 C489 P490 V492 S494 N497 P498 E499 Q502 Q503 K507 L508 N514 R522 R528

T533 H534 F535 E536 ASN CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 67% 25% 5% •

P301 S306 R307 F308 N314 K318 Y324 K325 T326 R330 R333 I343 N350 F351 S352 H353 F356 H359 D360 H361 L364 F367 ASN GLY G371 L372 P373 E376 D386 K390 P391 V392 P393 N394 T395 W400 Q401 G405 K411 L416

D420 P421 G424 G425 V426 G427 S433 Y436 R440 T441 I442 K443 N451 G452 P453 R457 I475 L478 Y479 F480 G482 D483 L485 C489 P490 A496 N497 P498 E499 I505 L508 N512 A513 P515 M516 L527 R528 G529 T533

H534 F535 E536 ASN CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 63% 26% 8% •

P301 R307 W315 K325 T326 I339 I343 H353 L354 F356 H359 D360 H361 N366 F367 ASN GLY G371 L372 E376 R383 V384 V385 K390 P391 V392 T395 M399 W400 Y408 R409 H410 N412 D413 N414 Y415 L416 A417 D420 P421 F423

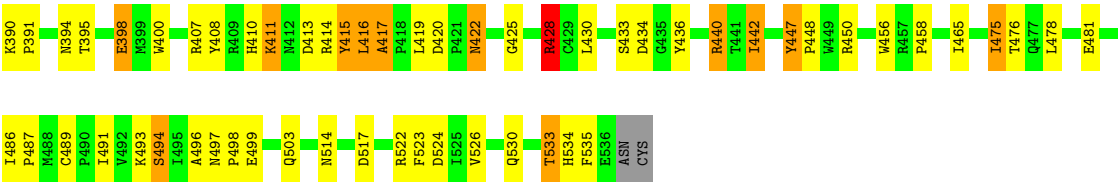
G424 G425 R428 G429 L430 T431 D432 S433 G435 Y436 S438 F439 R440 T441 I442 Y447 P448 W449 R450 N451 G452 P453 N454 R457 H462 F463 G464 I465 L478 E481 G482 D483 I486 P487 M488 C489 P490 S494 I495 A496 N497 D498 E499 A500 Q503 L504 I505 A506 K507

N512 A513 N514 C518 R522 F523 D524 V526 T533 E536 ASN CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 61% 31% 6% • •

P301 D304 N305 S306 R307 R311 W315 P322 T326 S327 I328 A329 R330 S331 P332 A335 Q341 S342 I343 T346 T347 G348 P349 N350 F351 S352 H353 F356 H359 D360 H361 L364 L365 N366 F367 ASN GLY G371 L372 E376 R383 V385 D386 Q387



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                                      | Source    |
|----------------------------------------------------------|------------------------------------------------------------|-----------|
| Space group                                              | I 1 2 1                                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 197.00 Å   127.07 Å   134.08 Å<br>90.00°   97.53°   90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.21                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 83.0 (6.00-2.21)                                           | Depositor |
| $R_{merge}$                                              | (Not available)                                            | Depositor |
| $R_{sym}$                                                | 0.06                                                       | Depositor |
| Refinement program                                       | PROLSQ                                                     | Depositor |
| R, $R_{free}$                                            | 0.159 , (Not available)                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                     | Xtriage   |
| Total number of atoms                                    | 22104                                                      | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 22.0                                                       | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME, FE, IHB

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   | A     | 1.37         | 3/1611 (0.2%)   | 1.88        | 40/2195 (1.8%)   |
| 1   | B     | 1.37         | 4/1611 (0.2%)   | 1.86        | 32/2195 (1.5%)   |
| 1   | C     | 1.42         | 3/1611 (0.2%)   | 1.77        | 24/2195 (1.1%)   |
| 1   | D     | 1.34         | 2/1611 (0.1%)   | 1.77        | 24/2195 (1.1%)   |
| 1   | E     | 1.46         | 7/1611 (0.4%)   | 1.83        | 30/2195 (1.4%)   |
| 1   | F     | 1.46         | 5/1611 (0.3%)   | 1.81        | 32/2195 (1.5%)   |
| 2   | M     | 1.50         | 6/1895 (0.3%)   | 1.82        | 36/2580 (1.4%)   |
| 2   | N     | 1.47         | 6/1895 (0.3%)   | 1.84        | 44/2580 (1.7%)   |
| 2   | O     | 1.49         | 5/1895 (0.3%)   | 1.88        | 37/2580 (1.4%)   |
| 2   | P     | 1.46         | 6/1895 (0.3%)   | 1.86        | 41/2580 (1.6%)   |
| 2   | Q     | 1.51         | 3/1895 (0.2%)   | 1.88        | 36/2580 (1.4%)   |
| 2   | R     | 1.44         | 6/1895 (0.3%)   | 1.87        | 37/2580 (1.4%)   |
| All | All   | 1.44         | 56/21036 (0.3%) | 1.84        | 413/28650 (1.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | D     | 0                   | 1                   |

All (56) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | N     | 451 | ASN  | CA-C  | 10.77 | 1.57        | 1.52     |
| 2   | P     | 451 | ASN  | CA-C  | 9.40  | 1.56        | 1.52     |
| 2   | Q     | 441 | THR  | CA-CB | 7.75  | 1.64        | 1.53     |
| 2   | N     | 428 | ARG  | CD-NE | -6.59 | 1.37        | 1.46     |
| 1   | C     | 195 | THR  | CA-CB | 6.46  | 1.64        | 1.53     |
| 1   | B     | 12  | THR  | CA-CB | 6.40  | 1.64        | 1.53     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | M     | 441 | THR  | CA-CB  | 6.39  | 1.62        | 1.54     |
| 2   | M     | 428 | ARG  | CD-NE  | -6.35 | 1.37        | 1.46     |
| 1   | E     | 5   | LEU  | CA-C   | 6.31  | 1.60        | 1.53     |
| 1   | D     | 108 | THR  | CA-CB  | 6.20  | 1.62        | 1.54     |
| 2   | N     | 440 | ARG  | CD-NE  | -6.16 | 1.37        | 1.46     |
| 1   | A     | 171 | ILE  | CA-CB  | 6.07  | 1.61        | 1.53     |
| 2   | O     | 379 | ILE  | CA-C   | 6.07  | 1.59        | 1.52     |
| 2   | M     | 462 | HIS  | N-CA   | 6.06  | 1.53        | 1.46     |
| 1   | B     | 94  | ARG  | CD-NE  | -6.05 | 1.37        | 1.46     |
| 2   | P     | 527 | LEU  | N-CA   | 6.04  | 1.52        | 1.45     |
| 1   | C     | 108 | THR  | CA-CB  | 5.85  | 1.62        | 1.54     |
| 1   | E     | 108 | THR  | CA-CB  | 5.84  | 1.61        | 1.53     |
| 1   | F     | 106 | LEU  | N-CA   | 5.79  | 1.52        | 1.46     |
| 2   | O     | 441 | THR  | CA-CB  | 5.75  | 1.61        | 1.54     |
| 1   | F     | 108 | THR  | CA-CB  | 5.72  | 1.61        | 1.53     |
| 2   | M     | 452 | GLY  | CA-C   | 5.71  | 1.59        | 1.51     |
| 1   | B     | 36  | TRP  | CA-C   | -5.70 | 1.47        | 1.53     |
| 2   | P     | 452 | GLY  | N-CA   | 5.67  | 1.52        | 1.44     |
| 2   | R     | 428 | ARG  | CD-NE  | -5.66 | 1.38        | 1.46     |
| 2   | P     | 343 | ILE  | CA-CB  | 5.62  | 1.63        | 1.54     |
| 1   | E     | 171 | ILE  | CA-CB  | 5.56  | 1.60        | 1.54     |
| 1   | E     | 175 | CYS  | CA-CB  | -5.55 | 1.46        | 1.53     |
| 2   | P     | 505 | ILE  | CA-CB  | 5.52  | 1.60        | 1.53     |
| 2   | O     | 514 | ASN  | N-CA   | 5.51  | 1.52        | 1.45     |
| 1   | A     | 113 | VAL  | CA-CB  | 5.45  | 1.59        | 1.54     |
| 2   | M     | 524 | ASP  | N-CA   | 5.45  | 1.52        | 1.45     |
| 2   | Q     | 495 | ILE  | CA-CB  | 5.44  | 1.59        | 1.53     |
| 2   | N     | 517 | ASP  | CG-OD2 | 5.41  | 1.35        | 1.25     |
| 1   | A     | 94  | ARG  | CD-NE  | -5.41 | 1.38        | 1.46     |
| 1   | C     | 8   | THR  | CA-CB  | 5.40  | 1.61        | 1.53     |
| 2   | Q     | 417 | ALA  | N-CA   | 5.39  | 1.53        | 1.45     |
| 2   | R     | 322 | PRO  | C-O    | 5.38  | 1.30        | 1.24     |
| 1   | B     | 2   | ILE  | CA-CB  | 5.34  | 1.60        | 1.54     |
| 2   | N     | 377 | ARG  | N-CA   | 5.34  | 1.52        | 1.46     |
| 2   | P     | 528 | ARG  | NE-CZ  | 5.28  | 1.38        | 1.33     |
| 1   | E     | 196 | VAL  | CA-C   | 5.28  | 1.58        | 1.52     |
| 2   | R     | 476 | THR  | CA-CB  | 5.27  | 1.60        | 1.53     |
| 2   | O     | 452 | GLY  | N-CA   | 5.25  | 1.51        | 1.44     |
| 2   | O     | 440 | ARG  | NE-CZ  | 5.23  | 1.38        | 1.33     |
| 2   | M     | 416 | LEU  | C-O    | 5.21  | 1.30        | 1.24     |
| 1   | F     | 95  | THR  | CB-OG1 | 5.14  | 1.51        | 1.43     |
| 2   | N     | 441 | THR  | CA-CB  | 5.14  | 1.60        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | R     | 517 | ASP  | N-CA  | 5.11 | 1.52        | 1.46     |
| 1   | E     | 65  | ASP  | N-CA  | 5.11 | 1.51        | 1.46     |
| 2   | R     | 398 | GLU  | N-CA  | 5.09 | 1.52        | 1.45     |
| 1   | E     | 35  | ILE  | N-CA  | 5.08 | 1.52        | 1.46     |
| 2   | R     | 330 | ARG  | CD-NE | 5.08 | 1.53        | 1.46     |
| 1   | D     | 30  | THR  | CA-CB | 5.01 | 1.60        | 1.53     |
| 1   | F     | 93  | GLY  | N-CA  | 5.01 | 1.50        | 1.45     |
| 1   | F     | 123 | ALA  | N-CA  | 5.01 | 1.52        | 1.45     |

All (413) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | O     | 353 | HIS  | CA-CB-CG  | -12.84 | 100.96      | 113.80   |
| 2   | Q     | 451 | ASN  | O-C-N     | 12.14  | 129.81      | 120.83   |
| 2   | O     | 428 | ARG  | CD-NE-CZ  | 12.01  | 141.21      | 124.40   |
| 1   | B     | 87  | ASN  | CA-CB-CG  | 11.01  | 123.61      | 112.60   |
| 2   | Q     | 452 | GLY  | N-CA-C    | -10.82 | 99.13       | 112.23   |
| 2   | M     | 457 | ARG  | CD-NE-CZ  | 10.69  | 139.36      | 124.40   |
| 2   | P     | 440 | ARG  | NE-CZ-NH2 | -10.55 | 109.70      | 119.20   |
| 2   | N     | 440 | ARG  | NE-CZ-NH2 | -10.27 | 109.96      | 119.20   |
| 2   | Q     | 361 | HIS  | CA-CB-CG  | -10.26 | 103.55      | 113.80   |
| 2   | R     | 440 | ARG  | NE-CZ-NH2 | -10.08 | 110.13      | 119.20   |
| 2   | R     | 361 | HIS  | CA-CB-CG  | -9.74  | 104.06      | 113.80   |
| 2   | R     | 434 | ASP  | CA-CB-CG  | -9.69  | 102.92      | 112.60   |
| 2   | R     | 428 | ARG  | CD-NE-CZ  | 9.51   | 137.72      | 124.40   |
| 2   | O     | 339 | ILE  | O-C-N     | 9.25   | 127.52      | 121.69   |
| 2   | M     | 428 | ARG  | CD-NE-CZ  | 9.09   | 137.13      | 124.40   |
| 2   | O     | 514 | ASN  | CA-CB-CG  | 8.94   | 121.54      | 112.60   |
| 1   | D     | 37  | ASN  | N-CA-C    | 8.91   | 123.76      | 113.15   |
| 2   | P     | 361 | HIS  | CA-CB-CG  | -8.83  | 104.97      | 113.80   |
| 2   | N     | 434 | ASP  | CA-CB-CG  | -8.71  | 103.89      | 112.60   |
| 1   | B     | 133 | ARG  | CD-NE-CZ  | 8.68   | 136.56      | 124.40   |
| 1   | A     | 99  | PHE  | CA-CB-CG  | 8.65   | 122.45      | 113.80   |
| 2   | P     | 452 | GLY  | N-CA-C    | -8.59  | 101.83      | 112.23   |
| 1   | E     | 125 | HIS  | CA-CB-CG  | -8.59  | 105.21      | 113.80   |
| 2   | O     | 434 | ASP  | CA-CB-CG  | -8.52  | 104.08      | 112.60   |
| 2   | R     | 353 | HIS  | CA-CB-CG  | -8.50  | 105.30      | 113.80   |
| 2   | P     | 451 | ASN  | O-C-N     | 8.43   | 127.07      | 120.83   |
| 2   | M     | 452 | GLY  | N-CA-C    | -8.35  | 101.83      | 112.10   |
| 1   | C     | 47  | GLU  | CB-CG-CD  | 8.33   | 126.76      | 112.60   |
| 2   | P     | 536 | GLU  | CA-C-O    | 8.32   | 134.95      | 120.80   |
| 2   | P     | 359 | HIS  | CA-CB-CG  | -8.24  | 105.56      | 113.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 99  | PHE  | CA-CB-CG   | 8.23  | 122.03      | 113.80   |
| 1   | C     | 37  | ASN  | N-CA-C     | 8.13  | 122.82      | 113.15   |
| 1   | F     | 37  | ASN  | N-CA-C     | 8.13  | 122.77      | 113.02   |
| 1   | D     | 84  | ASN  | CA-CB-CG   | 8.10  | 120.70      | 112.60   |
| 2   | M     | 434 | ASP  | CA-CB-CG   | -8.03 | 104.57      | 112.60   |
| 2   | R     | 394 | ASN  | CA-CB-CG   | -8.02 | 104.58      | 112.60   |
| 2   | O     | 361 | HIS  | CA-CB-CG   | -7.94 | 105.86      | 113.80   |
| 1   | B     | 37  | ASN  | N-CA-C     | 7.89  | 122.49      | 113.02   |
| 1   | D     | 26  | ALA  | N-CA-C     | -7.88 | 102.93      | 112.54   |
| 1   | D     | 52  | LEU  | CB-CA-C    | 7.86  | 126.67      | 109.94   |
| 2   | O     | 460 | HIS  | CA-CB-CG   | -7.77 | 106.03      | 113.80   |
| 1   | B     | 184 | ARG  | NE-CZ-NH2  | -7.76 | 112.22      | 119.20   |
| 1   | A     | 112 | GLY  | CA-C-N     | 7.70  | 130.82      | 120.50   |
| 1   | A     | 112 | GLY  | C-N-CA     | 7.70  | 130.82      | 120.50   |
| 2   | M     | 439 | PHE  | CA-CB-CG   | 7.67  | 121.47      | 113.80   |
| 1   | E     | 37  | ASN  | N-CA-C     | 7.66  | 121.51      | 112.93   |
| 2   | N     | 452 | GLY  | N-CA-C     | -7.61 | 102.74      | 112.10   |
| 2   | N     | 361 | HIS  | CA-CB-CG   | -7.56 | 106.24      | 113.80   |
| 2   | M     | 536 | GLU  | CA-C-O     | 7.50  | 133.55      | 120.80   |
| 1   | E     | 5   | LEU  | N-CA-C     | -7.46 | 100.36      | 109.83   |
| 2   | Q     | 481 | GLU  | CB-CG-CD   | 7.45  | 125.27      | 112.60   |
| 1   | F     | 36  | TRP  | N-CA-C     | 7.43  | 118.32      | 108.07   |
| 1   | F     | 100 | ASP  | CA-CB-CG   | -7.39 | 105.21      | 112.60   |
| 2   | O     | 334 | GLN  | OE1-CD-NE2 | -7.38 | 115.22      | 122.60   |
| 2   | R     | 387 | GLN  | OE1-CD-NE2 | 7.31  | 129.91      | 122.60   |
| 1   | E     | 99  | PHE  | CA-CB-CG   | 7.31  | 121.11      | 113.80   |
| 2   | R     | 428 | ARG  | CG-CD-NE   | 7.27  | 127.99      | 112.00   |
| 2   | Q     | 353 | HIS  | CA-CB-CG   | -7.25 | 106.56      | 113.80   |
| 1   | A     | 30  | THR  | CA-CB-OG1  | -7.23 | 98.76       | 109.60   |
| 2   | Q     | 483 | ASP  | O-C-N      | 7.22  | 127.59      | 121.31   |
| 1   | A     | 94  | ARG  | CB-CG-CD   | 7.19  | 127.83      | 111.30   |
| 1   | E     | 28  | ASN  | O-C-N      | 7.17  | 127.15      | 121.55   |
| 1   | A     | 41  | LYS  | N-CA-C     | -7.11 | 99.86       | 110.24   |
| 1   | D     | 178 | ASP  | CA-CB-CG   | -7.10 | 105.50      | 112.60   |
| 2   | P     | 394 | ASN  | CA-CB-CG   | -7.09 | 105.51      | 112.60   |
| 2   | P     | 353 | HIS  | CA-CB-CG   | -7.09 | 106.71      | 113.80   |
| 2   | R     | 422 | ASN  | CA-CB-CG   | -7.09 | 105.51      | 112.60   |
| 1   | F     | 94  | ARG  | CB-CG-CD   | 7.06  | 127.53      | 111.30   |
| 2   | Q     | 512 | ASN  | CA-CB-CG   | -7.05 | 105.55      | 112.60   |
| 2   | Q     | 440 | ARG  | NE-CZ-NH2  | -7.03 | 112.87      | 119.20   |
| 1   | C     | 163 | GLN  | CA-C-O     | 7.03  | 124.52      | 119.32   |
| 1   | F     | 38  | ARG  | CA-CB-CG   | 7.02  | 128.13      | 114.10   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 333 | ARG  | CB-CA-C   | 7.01  | 120.80      | 109.02   |
| 2   | N     | 428 | ARG  | CG-CD-NE  | 7.00  | 127.40      | 112.00   |
| 2   | M     | 326 | THR  | CA-CB-OG1 | -6.97 | 99.14       | 109.60   |
| 2   | O     | 528 | ARG  | CD-NE-CZ  | 6.97  | 134.16      | 124.40   |
| 1   | E     | 52  | LEU  | CB-CA-C   | 6.97  | 125.41      | 110.07   |
| 2   | Q     | 454 | ASN  | CA-CB-CG  | 6.97  | 119.57      | 112.60   |
| 2   | M     | 460 | HIS  | CA-CB-CG  | -6.89 | 106.91      | 113.80   |
| 1   | B     | 94  | ARG  | CB-CG-CD  | 6.88  | 127.12      | 111.30   |
| 2   | M     | 361 | HIS  | CA-CB-CG  | -6.85 | 106.95      | 113.80   |
| 2   | R     | 494 | SER  | N-CA-C    | -6.84 | 104.20      | 112.54   |
| 1   | C     | 52  | LEU  | CB-CA-C   | 6.81  | 125.10      | 110.45   |
| 2   | M     | 494 | SER  | N-CA-C    | -6.80 | 103.89      | 111.71   |
| 2   | Q     | 533 | THR  | CA-CB-OG1 | -6.79 | 99.41       | 109.60   |
| 1   | A     | 171 | ILE  | N-CA-C    | 6.79  | 117.63      | 107.51   |
| 1   | A     | 37  | ASN  | N-CA-C    | 6.78  | 120.52      | 112.93   |
| 2   | P     | 434 | ASP  | CA-CB-CG  | -6.75 | 105.84      | 112.60   |
| 2   | P     | 440 | ARG  | NE-CZ-NH1 | 6.74  | 128.24      | 121.50   |
| 1   | A     | 133 | ARG  | CD-NE-CZ  | 6.74  | 133.83      | 124.40   |
| 2   | M     | 440 | ARG  | NE-CZ-NH2 | -6.71 | 113.16      | 119.20   |
| 2   | R     | 428 | ARG  | CB-CG-CD  | 6.69  | 126.69      | 111.30   |
| 2   | M     | 316 | HIS  | O-C-N     | 6.68  | 129.01      | 121.53   |
| 1   | E     | 158 | LEU  | CB-CA-C   | 6.68  | 121.88      | 110.79   |
| 1   | B     | 48  | HIS  | CA-CB-CG  | -6.63 | 107.17      | 113.80   |
| 1   | C     | 36  | TRP  | N-CA-C    | 6.62  | 117.21      | 108.07   |
| 2   | N     | 359 | HIS  | CA-CB-CG  | -6.62 | 107.18      | 113.80   |
| 2   | R     | 517 | ASP  | CA-CB-CG  | 6.61  | 119.21      | 112.60   |
| 1   | C     | 41  | LYS  | N-CA-C    | -6.60 | 101.18      | 110.29   |
| 2   | Q     | 325 | LYS  | N-CA-C    | 6.57  | 119.00      | 111.11   |
| 1   | F     | 198 | PHE  | CA-CB-CG  | 6.57  | 120.37      | 113.80   |
| 1   | C     | 5   | LEU  | N-CA-C    | -6.56 | 101.50      | 109.83   |
| 1   | F     | 186 | ASP  | CB-CA-C   | 6.52  | 120.29      | 109.53   |
| 1   | E     | 36  | TRP  | N-CA-C    | 6.52  | 117.07      | 108.07   |
| 1   | E     | 181 | THR  | N-CA-CB   | 6.51  | 119.56      | 109.85   |
| 1   | E     | 90  | ASN  | CA-CB-CG  | 6.47  | 119.08      | 112.60   |
| 1   | F     | 38  | ARG  | CB-CA-C   | 6.45  | 122.31      | 111.22   |
| 2   | P     | 392 | VAL  | O-C-N     | 6.45  | 127.15      | 120.96   |
| 2   | M     | 306 | SER  | N-CA-C    | 6.44  | 120.40      | 110.42   |
| 2   | M     | 417 | ALA  | N-CA-C    | -6.42 | 101.68      | 109.83   |
| 2   | R     | 533 | THR  | CA-CB-OG1 | -6.41 | 99.98       | 109.60   |
| 2   | N     | 451 | ASN  | O-C-N     | 6.41  | 125.57      | 120.83   |
| 1   | C     | 125 | HIS  | CA-CB-CG  | -6.40 | 107.40      | 113.80   |
| 1   | A     | 5   | LEU  | N-CA-C    | -6.39 | 101.25      | 110.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 94  | ARG  | NE-CZ-NH2 | -6.32 | 113.51      | 119.20   |
| 2   | R     | 348 | GLY  | O-C-N     | 6.31  | 128.08      | 121.77   |
| 2   | P     | 428 | ARG  | CG-CD-NE  | 6.30  | 125.86      | 112.00   |
| 1   | B     | 107 | HIS  | CA-CB-CG  | -6.30 | 107.50      | 113.80   |
| 2   | N     | 333 | ARG  | N-CA-C    | -6.30 | 106.19      | 114.31   |
| 2   | O     | 420 | ASP  | CB-CA-C   | 6.30  | 117.39      | 110.15   |
| 1   | E     | 189 | ILE  | O-C-N     | 6.29  | 127.97      | 121.87   |
| 2   | O     | 409 | ARG  | NE-CZ-NH2 | 6.29  | 124.86      | 119.20   |
| 2   | N     | 415 | TYR  | N-CA-C    | -6.28 | 101.13      | 110.23   |
| 1   | D     | 112 | GLY  | N-CA-C    | -6.27 | 102.75      | 112.85   |
| 1   | E     | 181 | THR  | O-C-N     | 6.27  | 130.65      | 122.93   |
| 2   | O     | 494 | SER  | N-CA-C    | -6.27 | 104.50      | 111.71   |
| 1   | C     | 66  | SER  | CA-CB-OG  | 6.26  | 123.63      | 111.10   |
| 1   | B     | 31  | ARG  | CD-NE-CZ  | 6.26  | 133.17      | 124.40   |
| 1   | F     | 94  | ARG  | CG-CD-NE  | 6.25  | 125.76      | 112.00   |
| 1   | A     | 64  | ARG  | CD-NE-CZ  | -6.25 | 115.65      | 124.40   |
| 2   | P     | 386 | ASP  | CB-CA-C   | 6.18  | 123.96      | 111.60   |
| 2   | O     | 454 | ASN  | CA-C-O    | -6.17 | 114.87      | 121.78   |
| 2   | Q     | 505 | ILE  | N-CA-C    | 6.17  | 116.99      | 107.99   |
| 2   | Q     | 463 | PHE  | O-C-N     | 6.16  | 130.82      | 123.24   |
| 1   | C     | 187 | ILE  | CA-C-O    | -6.15 | 113.99      | 120.39   |
| 2   | Q     | 372 | LEU  | N-CA-CB   | -6.15 | 99.89       | 110.10   |
| 1   | A     | 115 | ASN  | CA-CB-CG  | 6.12  | 118.72      | 112.60   |
| 2   | N     | 483 | ASP  | O-C-N     | 6.11  | 126.63      | 121.31   |
| 2   | M     | 372 | LEU  | CB-CA-C   | 6.10  | 117.95      | 108.61   |
| 2   | Q     | 439 | PHE  | CA-CB-CG  | 6.10  | 119.90      | 113.80   |
| 2   | P     | 395 | THR  | CA-CB-OG1 | -6.10 | 100.45      | 109.60   |
| 1   | D     | 94  | ARG  | NE-CZ-NH1 | -6.08 | 115.42      | 121.50   |
| 1   | E     | 127 | ASN  | CA-CB-CG  | -6.07 | 106.53      | 112.60   |
| 1   | C     | 138 | HIS  | CA-C-N    | 6.06  | 130.73      | 122.19   |
| 1   | C     | 138 | HIS  | C-N-CA    | 6.06  | 130.73      | 122.19   |
| 2   | P     | 457 | ARG  | CD-NE-CZ  | 6.06  | 132.88      | 124.40   |
| 1   | D     | 5   | LEU  | N-CA-C    | -6.04 | 102.17      | 109.83   |
| 2   | R     | 328 | ILE  | N-CA-C    | 6.03  | 116.15      | 110.30   |
| 1   | F     | 5   | LEU  | N-CA-C    | -6.00 | 102.21      | 109.83   |
| 1   | B     | 176 | GLU  | CB-CG-CD  | 6.00  | 122.79      | 112.60   |
| 1   | B     | 198 | PHE  | CA-CB-CG  | 6.00  | 119.80      | 113.80   |
| 2   | R     | 475 | ILE  | N-CA-CB   | 5.99  | 119.67      | 111.41   |
| 1   | B     | 133 | ARG  | CA-CB-CG  | 5.98  | 126.07      | 114.10   |
| 1   | F     | 23  | LEU  | CB-CA-C   | 5.97  | 120.41      | 110.92   |
| 1   | B     | 94  | ARG  | NE-CZ-NH1 | 5.96  | 127.46      | 121.50   |
| 2   | R     | 496 | ALA  | N-CA-C    | 5.95  | 117.77      | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | R     | 450 | ARG  | CA-C-O     | -5.95 | 115.21      | 122.41   |
| 1   | A     | 167 | ARG  | CD-NE-CZ   | -5.94 | 116.08      | 124.40   |
| 2   | O     | 452 | GLY  | N-CA-C     | -5.94 | 100.22      | 112.34   |
| 1   | F     | 94  | ARG  | CD-NE-CZ   | 5.94  | 132.71      | 124.40   |
| 2   | M     | 353 | HIS  | CA-CB-CG   | -5.92 | 107.88      | 113.80   |
| 2   | N     | 357 | GLY  | CA-C-N     | 5.92  | 128.21      | 120.28   |
| 2   | N     | 357 | GLY  | C-N-CA     | 5.92  | 128.21      | 120.28   |
| 2   | N     | 383 | ARG  | CD-NE-CZ   | -5.92 | 116.11      | 124.40   |
| 2   | Q     | 354 | LEU  | CB-CA-C    | 5.91  | 119.52      | 109.53   |
| 1   | F     | 132 | ALA  | CA-C-O     | 5.91  | 127.62      | 121.06   |
| 2   | Q     | 497 | ASN  | N-CA-C     | 5.91  | 117.45      | 109.24   |
| 2   | N     | 451 | ASN  | N-CA-C     | -5.90 | 99.10       | 108.30   |
| 1   | B     | 53  | GLY  | CA-C-N     | 5.89  | 131.82      | 122.62   |
| 1   | B     | 53  | GLY  | C-N-CA     | 5.89  | 131.82      | 122.62   |
| 1   | B     | 11  | GLN  | CA-C-O     | -5.87 | 114.77      | 121.40   |
| 1   | D     | 100 | ASP  | CA-CB-CG   | -5.87 | 106.73      | 112.60   |
| 2   | O     | 481 | GLU  | CB-CG-CD   | 5.86  | 122.56      | 112.60   |
| 1   | F     | 66  | SER  | N-CA-CB    | 5.84  | 118.72      | 110.36   |
| 1   | C     | 66  | SER  | N-CA-CB    | 5.84  | 119.16      | 110.29   |
| 1   | E     | 162 | GLU  | N-CA-C     | 5.84  | 118.14      | 111.02   |
| 2   | N     | 415 | TYR  | O-C-N      | 5.83  | 130.04      | 122.87   |
| 2   | P     | 333 | ARG  | CB-CA-C    | 5.83  | 119.90      | 109.29   |
| 2   | M     | 313 | ARG  | CB-CA-C    | 5.83  | 121.18      | 110.11   |
| 2   | R     | 330 | ARG  | N-CA-C     | 5.82  | 119.15      | 112.57   |
| 2   | O     | 306 | SER  | N-CA-C     | 5.82  | 119.05      | 109.85   |
| 1   | A     | 94  | ARG  | CG-CD-NE   | 5.82  | 124.80      | 112.00   |
| 1   | C     | 150 | GLN  | N-CA-CB    | 5.79  | 118.36      | 109.91   |
| 1   | F     | 105 | THR  | O-C-N      | 5.78  | 129.86      | 123.33   |
| 2   | O     | 502 | GLN  | OE1-CD-NE2 | 5.78  | 128.38      | 122.60   |
| 2   | Q     | 494 | SER  | N-CA-C     | -5.78 | 105.33      | 112.38   |
| 1   | F     | 181 | THR  | N-CA-CB    | 5.77  | 118.60      | 109.71   |
| 2   | Q     | 383 | ARG  | N-CA-CB    | -5.76 | 100.89      | 111.37   |
| 1   | A     | 133 | ARG  | CA-CB-CG   | 5.75  | 125.61      | 114.10   |
| 2   | R     | 420 | ASP  | CB-CA-C    | 5.73  | 116.53      | 110.17   |
| 2   | P     | 324 | TYR  | CA-C-N     | 5.73  | 129.41      | 120.82   |
| 2   | P     | 324 | TYR  | C-N-CA     | 5.73  | 129.41      | 120.82   |
| 2   | Q     | 420 | ASP  | O-C-N      | 5.73  | 127.65      | 121.12   |
| 2   | Q     | 457 | ARG  | CA-CB-CG   | 5.72  | 125.54      | 114.10   |
| 1   | D     | 108 | THR  | N-CA-CB    | -5.70 | 101.31      | 110.55   |
| 2   | P     | 481 | GLU  | CB-CG-CD   | 5.70  | 122.29      | 112.60   |
| 1   | E     | 94  | ARG  | CG-CD-NE   | 5.70  | 124.54      | 112.00   |
| 2   | O     | 366 | ASN  | N-CA-C     | 5.69  | 120.09      | 113.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | M     | 451 | ASN  | O-C-N      | 5.69  | 125.04      | 120.83   |
| 2   | M     | 339 | ILE  | O-C-N      | 5.68  | 127.58      | 121.10   |
| 2   | M     | 367 | PHE  | CA-C-O     | -5.68 | 111.14      | 120.80   |
| 1   | D     | 86  | GLU  | CG-CD-OE1  | 5.68  | 131.46      | 118.40   |
| 1   | F     | 4   | LEU  | N-CA-CB    | -5.68 | 101.37      | 110.51   |
| 1   | E     | 163 | GLN  | CA-C-O     | 5.67  | 123.52      | 119.32   |
| 1   | D     | 86  | GLU  | CB-CG-CD   | 5.67  | 122.24      | 112.60   |
| 2   | R     | 376 | GLU  | O-C-N      | 5.67  | 130.00      | 123.02   |
| 2   | O     | 314 | ASN  | N-CA-C     | -5.66 | 106.53      | 113.50   |
| 2   | P     | 451 | ASN  | CA-C-O     | -5.65 | 116.55      | 119.77   |
| 2   | Q     | 522 | ARG  | CD-NE-CZ   | -5.64 | 116.50      | 124.40   |
| 2   | O     | 463 | PHE  | CA-C-O     | -5.64 | 114.51      | 121.11   |
| 1   | C     | 7   | GLU  | CB-CG-CD   | 5.64  | 122.18      | 112.60   |
| 1   | D     | 177 | VAL  | CB-CA-C    | 5.62  | 118.01      | 110.42   |
| 1   | E     | 106 | LEU  | N-CA-CB    | -5.62 | 101.06      | 111.13   |
| 2   | N     | 457 | ARG  | CA-CB-CG   | 5.62  | 125.34      | 114.10   |
| 2   | P     | 489 | CYS  | N-CA-C     | 5.62  | 117.74      | 109.42   |
| 1   | F     | 177 | VAL  | CB-CA-C    | 5.62  | 118.01      | 110.42   |
| 2   | P     | 512 | ASN  | OD1-CG-ND2 | 5.62  | 128.22      | 122.60   |
| 1   | D     | 7   | GLU  | CB-CG-CD   | 5.61  | 122.14      | 112.60   |
| 2   | O     | 354 | LEU  | N-CA-C     | -5.60 | 101.35      | 110.20   |
| 1   | F     | 177 | VAL  | O-C-N      | 5.60  | 129.00      | 123.18   |
| 1   | A     | 4   | LEU  | N-CA-CB    | -5.60 | 99.94       | 110.07   |
| 1   | E     | 133 | ARG  | N-CA-C     | -5.59 | 101.77      | 110.10   |
| 2   | M     | 372 | LEU  | N-CA-CB    | -5.57 | 100.85      | 110.10   |
| 1   | D     | 21  | LEU  | N-CA-CB    | -5.56 | 102.05      | 111.27   |
| 1   | A     | 183 | TYR  | N-CA-CB    | 5.54  | 120.12      | 110.81   |
| 1   | B     | 171 | ILE  | N-CA-C     | 5.54  | 116.08      | 107.99   |
| 1   | D     | 133 | ARG  | N-CA-CB    | -5.53 | 101.23      | 109.69   |
| 2   | M     | 516 | MET  | CA-C-O     | -5.52 | 113.80      | 120.32   |
| 2   | R     | 524 | ASP  | CB-CA-C    | 5.52  | 118.95      | 109.51   |
| 2   | M     | 446 | PRO  | N-CA-C     | -5.51 | 103.51      | 111.22   |
| 2   | N     | 533 | THR  | CA-CB-OG1  | -5.51 | 101.34      | 109.60   |
| 2   | R     | 440 | ARG  | NH1-CZ-NH2 | 5.50  | 126.45      | 119.30   |
| 1   | F     | 5   | LEU  | O-C-N      | 5.49  | 127.57      | 121.43   |
| 1   | A     | 177 | VAL  | O-C-N      | 5.48  | 128.88      | 123.18   |
| 1   | F     | 138 | HIS  | CA-C-N     | 5.48  | 129.70      | 122.30   |
| 1   | F     | 138 | HIS  | C-N-CA     | 5.48  | 129.70      | 122.30   |
| 1   | A     | 21  | LEU  | N-CA-CB    | -5.46 | 102.62      | 110.65   |
| 1   | A     | 64  | ARG  | NE-CZ-NH1  | -5.46 | 116.04      | 121.50   |
| 1   | F     | 7   | GLU  | CB-CG-CD   | 5.46  | 121.88      | 112.60   |
| 2   | P     | 489 | CYS  | CA-C-O     | 5.46  | 123.66      | 119.46   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | N     | 331 | SER  | O-C-N      | 5.46  | 126.79      | 121.66   |
| 2   | N     | 394 | ASN  | CA-C-O     | -5.45 | 115.52      | 121.84   |
| 2   | R     | 386 | ASP  | N-CA-C     | -5.45 | 101.94      | 110.17   |
| 2   | M     | 428 | ARG  | CG-CD-NE   | 5.45  | 123.98      | 112.00   |
| 1   | C     | 96  | ALA  | CA-C-O     | -5.44 | 115.61      | 121.38   |
| 2   | N     | 416 | LEU  | CB-CA-C    | 5.44  | 121.27      | 110.17   |
| 1   | B     | 21  | LEU  | N-CA-CB    | -5.43 | 102.02      | 110.98   |
| 1   | B     | 81  | ASP  | CA-CB-CG   | -5.43 | 107.17      | 112.60   |
| 2   | O     | 384 | VAL  | O-C-N      | 5.43  | 129.45      | 123.10   |
| 2   | O     | 492 | VAL  | N-CA-C     | -5.43 | 105.24      | 110.72   |
| 1   | E     | 199 | ASP  | O-C-N      | 5.43  | 129.66      | 123.31   |
| 1   | B     | 94  | ARG  | NE-CZ-NH2  | -5.42 | 114.32      | 119.20   |
| 1   | D     | 23  | LEU  | CB-CA-C    | 5.42  | 119.83      | 110.84   |
| 1   | A     | 94  | ARG  | CD-NE-CZ   | 5.41  | 131.98      | 124.40   |
| 1   | E     | 133 | ARG  | CA-CB-CG   | 5.41  | 124.92      | 114.10   |
| 2   | M     | 447 | TYR  | O-C-N      | 5.41  | 126.05      | 121.83   |
| 2   | R     | 430 | LEU  | CB-CA-C    | 5.40  | 118.67      | 109.75   |
| 1   | C     | 127 | ASN  | CA-CB-CG   | -5.40 | 107.20      | 112.60   |
| 1   | C     | 5   | LEU  | O-C-N      | 5.39  | 127.46      | 121.43   |
| 1   | F     | 165 | GLN  | OE1-CD-NE2 | -5.38 | 117.22      | 122.60   |
| 2   | P     | 514 | ASN  | CB-CA-C    | 5.38  | 115.50      | 110.17   |
| 1   | B     | 38  | ARG  | NE-CZ-NH2  | -5.38 | 114.36      | 119.20   |
| 2   | O     | 533 | THR  | CA-CB-OG1  | -5.37 | 101.54      | 109.60   |
| 2   | M     | 514 | ASN  | O-C-N      | 5.37  | 126.24      | 121.19   |
| 1   | A     | 94  | ARG  | NE-CZ-NH1  | 5.36  | 126.86      | 121.50   |
| 1   | B     | 188 | ARG  | CB-CG-CD   | 5.36  | 123.62      | 111.30   |
| 2   | N     | 386 | ASP  | CA-CB-CG   | 5.36  | 117.96      | 112.60   |
| 1   | A     | 52  | LEU  | CB-CA-C    | 5.36  | 121.35      | 109.94   |
| 2   | P     | 434 | ASP  | O-C-N      | 5.36  | 128.72      | 122.24   |
| 2   | N     | 314 | ASN  | N-CA-C     | -5.35 | 106.92      | 113.50   |
| 1   | E     | 4   | LEU  | CA-C-O     | -5.35 | 115.35      | 121.82   |
| 1   | E     | 48  | HIS  | CA-CB-CG   | -5.35 | 108.45      | 113.80   |
| 2   | N     | 308 | PHE  | CB-CA-C    | 5.35  | 119.00      | 109.38   |
| 2   | M     | 474 | LEU  | N-CA-CB    | -5.34 | 101.58      | 111.52   |
| 2   | M     | 441 | THR  | N-CA-CB    | -5.34 | 102.92      | 110.51   |
| 1   | B     | 61  | HIS  | CA-CB-CG   | -5.34 | 108.46      | 113.80   |
| 2   | R     | 328 | ILE  | N-CA-CB    | 5.34  | 116.44      | 110.62   |
| 2   | R     | 352 | SER  | N-CA-CB    | 5.34  | 118.58      | 110.14   |
| 2   | R     | 481 | GLU  | CB-CG-CD   | 5.34  | 121.68      | 112.60   |
| 2   | O     | 463 | PHE  | O-C-N      | 5.34  | 129.80      | 123.24   |
| 1   | D     | 38  | ARG  | CD-NE-CZ   | -5.34 | 116.93      | 124.40   |
| 1   | A     | 133 | ARG  | NE-CZ-NH1  | 5.33  | 126.83      | 121.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | Q     | 432 | ASP  | CA-CB-CG   | 5.33  | 117.92      | 112.60   |
| 2   | P     | 392 | VAL  | CA-C-O     | -5.32 | 117.26      | 120.88   |
| 1   | B     | 94  | ARG  | CG-CD-NE   | 5.32  | 123.70      | 112.00   |
| 1   | B     | 24  | GLU  | CA-CB-CG   | 5.31  | 124.72      | 114.10   |
| 2   | R     | 458 | PRO  | N-CA-C     | -5.31 | 102.94      | 111.38   |
| 2   | M     | 314 | ASN  | CB-CA-C    | 5.30  | 118.94      | 109.29   |
| 2   | O     | 353 | HIS  | CB-CG-CD2  | -5.30 | 124.31      | 131.20   |
| 2   | N     | 413 | ASP  | CB-CA-C    | 5.30  | 119.07      | 110.22   |
| 2   | O     | 514 | ASN  | OD1-CG-ND2 | -5.30 | 117.30      | 122.60   |
| 2   | Q     | 518 | CYS  | N-CA-C     | 5.30  | 117.13      | 109.07   |
| 2   | N     | 428 | ARG  | CB-CG-CD   | 5.30  | 123.48      | 111.30   |
| 1   | C     | 30  | THR  | CA-CB-OG1  | -5.30 | 101.66      | 109.60   |
| 2   | P     | 489 | CYS  | CA-C-N     | 5.29  | 124.93      | 119.05   |
| 2   | P     | 489 | CYS  | C-N-CA     | 5.29  | 124.93      | 119.05   |
| 1   | B     | 146 | ASP  | CA-C-O     | -5.29 | 112.87      | 119.38   |
| 1   | E     | 5   | LEU  | O-C-N      | 5.28  | 127.35      | 121.43   |
| 1   | F     | 32  | ASP  | CA-CB-CG   | -5.28 | 107.32      | 112.60   |
| 2   | N     | 354 | LEU  | N-CA-C     | -5.28 | 103.06      | 110.50   |
| 2   | R     | 419 | LEU  | N-CA-C     | -5.28 | 103.57      | 110.53   |
| 1   | D     | 131 | PHE  | CA-CB-CG   | 5.27  | 119.07      | 113.80   |
| 2   | N     | 475 | ILE  | N-CA-CB    | 5.27  | 118.68      | 111.41   |
| 2   | N     | 532 | LYS  | N-CA-C     | -5.26 | 102.69      | 110.48   |
| 1   | F     | 163 | GLN  | CB-CG-CD   | 5.26  | 121.55      | 112.60   |
| 2   | P     | 367 | PHE  | CA-C-O     | -5.26 | 111.85      | 120.80   |
| 1   | B     | 57  | ASP  | CA-CB-CG   | 5.25  | 117.85      | 112.60   |
| 1   | B     | 177 | VAL  | O-C-N      | 5.25  | 128.64      | 123.18   |
| 1   | A     | 192 | GLU  | CB-CA-C    | -5.25 | 102.41      | 109.71   |
| 1   | F     | 88  | ALA  | N-CA-C     | -5.25 | 106.38      | 112.89   |
| 2   | O     | 489 | CYS  | CA-C-N     | 5.25  | 125.05      | 119.28   |
| 2   | O     | 489 | CYS  | C-N-CA     | 5.25  | 125.05      | 119.28   |
| 2   | O     | 394 | ASN  | CA-CB-CG   | -5.24 | 107.36      | 112.60   |
| 2   | Q     | 464 | GLY  | N-CA-C     | -5.24 | 100.77      | 113.18   |
| 2   | N     | 514 | ASN  | O-C-N      | 5.24  | 126.38      | 120.83   |
| 1   | E     | 38  | ARG  | CD-NE-CZ   | -5.23 | 117.08      | 124.40   |
| 2   | R     | 415 | TYR  | N-CA-C     | -5.22 | 103.13      | 110.50   |
| 2   | P     | 514 | ASN  | CA-CB-CG   | 5.22  | 117.82      | 112.60   |
| 1   | A     | 138 | HIS  | CA-CB-CG   | -5.22 | 108.58      | 113.80   |
| 1   | A     | 188 | ARG  | NE-CZ-NH2  | -5.21 | 114.52      | 119.20   |
| 2   | N     | 357 | GLY  | N-CA-C     | -5.20 | 104.55      | 112.51   |
| 2   | O     | 440 | ARG  | O-C-N      | 5.20  | 129.49      | 123.30   |
| 2   | Q     | 339 | ILE  | O-C-N      | 5.20  | 124.97      | 121.69   |
| 2   | Q     | 430 | LEU  | N-CA-C     | -5.20 | 101.23      | 109.76   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | R     | 534 | HIS  | CA-CB-CG  | 5.20  | 119.00      | 113.80   |
| 2   | P     | 475 | ILE  | N-CA-CB   | 5.20  | 118.39      | 111.64   |
| 2   | Q     | 391 | PRO  | CA-C-O    | -5.19 | 115.53      | 121.56   |
| 1   | B     | 169 | THR  | CA-CB-CG2 | 5.19  | 119.33      | 110.50   |
| 2   | N     | 481 | GLU  | CB-CG-CD  | 5.19  | 121.43      | 112.60   |
| 1   | E     | 181 | THR  | CB-CA-C   | -5.19 | 101.59      | 109.89   |
| 1   | A     | 187 | ILE  | O-C-N     | 5.19  | 128.63      | 123.18   |
| 2   | O     | 440 | ARG  | NE-CZ-NH2 | -5.18 | 114.53      | 119.20   |
| 2   | N     | 367 | PHE  | CA-C-O    | -5.18 | 111.99      | 120.80   |
| 2   | R     | 417 | ALA  | N-CA-C    | -5.18 | 103.25      | 109.83   |
| 1   | D     | 128 | ILE  | N-CA-C    | 5.18  | 115.93      | 108.48   |
| 2   | Q     | 448 | PRO  | CA-C-O    | -5.18 | 115.55      | 121.86   |
| 1   | F     | 158 | LEU  | CB-CA-C   | 5.18  | 120.21      | 110.63   |
| 2   | Q     | 359 | HIS  | CA-CB-CG  | -5.17 | 108.63      | 113.80   |
| 2   | N     | 522 | ARG  | O-C-N     | 5.16  | 129.38      | 123.29   |
| 2   | O     | 494 | SER  | CA-CB-OG  | 5.16  | 121.41      | 111.10   |
| 2   | P     | 428 | ARG  | CB-CG-CD  | 5.15  | 123.15      | 111.30   |
| 1   | F     | 52  | LEU  | CB-CA-C   | 5.15  | 120.19      | 110.62   |
| 1   | F     | 41  | LYS  | N-CA-C    | -5.14 | 103.19      | 110.29   |
| 2   | R     | 514 | ASN  | O-C-N     | 5.14  | 126.02      | 121.19   |
| 2   | P     | 483 | ASP  | CB-CA-C   | 5.14  | 117.36      | 109.60   |
| 2   | P     | 424 | GLY  | CA-C-N    | 5.13  | 128.55      | 121.26   |
| 2   | P     | 424 | GLY  | C-N-CA    | 5.13  | 128.55      | 121.26   |
| 1   | A     | 97  | THR  | CA-CB-OG1 | -5.13 | 101.91      | 109.60   |
| 1   | A     | 57  | ASP  | CA-CB-CG  | 5.13  | 117.73      | 112.60   |
| 1   | C     | 99  | PHE  | N-CA-C    | -5.12 | 106.13      | 112.38   |
| 2   | O     | 315 | TRP  | CA-C-O    | 5.12  | 126.03      | 120.55   |
| 2   | M     | 328 | ILE  | N-CA-C    | 5.12  | 115.33      | 110.42   |
| 1   | A     | 23  | LEU  | CB-CA-C   | 5.11  | 119.33      | 110.84   |
| 1   | C     | 162 | GLU  | N-CA-CB   | 5.11  | 117.59      | 109.82   |
| 1   | E     | 140 | HIS  | CB-CA-C   | -5.11 | 100.18      | 109.38   |
| 2   | O     | 508 | LEU  | CA-C-O    | -5.11 | 115.57      | 121.19   |
| 2   | M     | 428 | ARG  | CB-CG-CD  | 5.10  | 123.04      | 111.30   |
| 2   | N     | 460 | HIS  | CA-CB-CG  | -5.10 | 108.70      | 113.80   |
| 2   | P     | 372 | LEU  | CB-CA-C   | 5.09  | 115.76      | 108.68   |
| 2   | Q     | 450 | ARG  | CD-NE-CZ  | -5.09 | 117.27      | 124.40   |
| 1   | A     | 103 | GLU  | CG-CD-OE1 | -5.09 | 106.70      | 118.40   |
| 1   | B     | 174 | ARG  | CD-NE-CZ  | -5.09 | 117.28      | 124.40   |
| 2   | N     | 499 | GLU  | CA-CB-CG  | 5.09  | 124.28      | 114.10   |
| 2   | R     | 433 | SER  | CA-CB-OG  | -5.09 | 100.92      | 111.10   |
| 2   | M     | 450 | ARG  | CA-C-N    | 5.09  | 128.66      | 121.79   |
| 2   | M     | 450 | ARG  | C-N-CA    | 5.09  | 128.66      | 121.79   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | R     | 311 | ARG  | NE-CZ-NH2 | -5.09 | 114.62      | 119.20   |
| 2   | N     | 321 | THR  | CA-C-N    | 5.08  | 125.12      | 119.32   |
| 2   | N     | 321 | THR  | C-N-CA    | 5.08  | 125.12      | 119.32   |
| 2   | Q     | 497 | ASN  | N-CA-CB   | -5.08 | 103.57      | 110.23   |
| 1   | D     | 3   | GLU  | CA-C-O    | -5.08 | 114.88      | 120.36   |
| 2   | M     | 386 | ASP  | CA-CB-CG  | 5.07  | 117.67      | 112.60   |
| 1   | A     | 5   | LEU  | O-C-N     | 5.07  | 127.11      | 121.53   |
| 2   | N     | 432 | ASP  | CA-C-N    | 5.07  | 127.78      | 120.38   |
| 2   | N     | 432 | ASP  | C-N-CA    | 5.07  | 127.78      | 120.38   |
| 1   | A     | 14  | GLY  | CA-C-N    | 5.07  | 124.68      | 119.56   |
| 1   | A     | 14  | GLY  | C-N-CA    | 5.07  | 124.68      | 119.56   |
| 2   | Q     | 514 | ASN  | CA-CB-CG  | 5.07  | 117.67      | 112.60   |
| 2   | R     | 447 | TYR  | O-C-N     | 5.07  | 125.78      | 121.83   |
| 2   | P     | 483 | ASP  | CA-CB-CG  | 5.06  | 117.66      | 112.60   |
| 1   | F     | 133 | ARG  | N-CA-C    | -5.06 | 102.55      | 110.10   |
| 2   | N     | 414 | ARG  | CD-NE-CZ  | -5.06 | 117.31      | 124.40   |
| 2   | O     | 441 | THR  | N-CA-CB   | -5.06 | 103.32      | 110.51   |
| 1   | F     | 140 | HIS  | CB-CA-C   | -5.06 | 101.99      | 110.19   |
| 2   | Q     | 522 | ARG  | NE-CZ-NH1 | -5.06 | 116.44      | 121.50   |
| 1   | A     | 95  | THR  | CA-C-O    | -5.06 | 116.04      | 121.45   |
| 2   | Q     | 533 | THR  | N-CA-C    | -5.05 | 103.86      | 110.53   |
| 1   | B     | 52  | LEU  | CB-CA-C   | 5.05  | 120.70      | 109.94   |
| 1   | B     | 138 | HIS  | N-CA-CB   | 5.05  | 117.46      | 110.04   |
| 1   | A     | 4   | LEU  | CA-C-O    | -5.05 | 115.19      | 121.55   |
| 1   | E     | 107 | HIS  | CA-CB-CG  | -5.04 | 108.75      | 113.80   |
| 2   | P     | 376 | GLU  | CB-CG-CD  | 5.04  | 121.17      | 112.60   |
| 2   | N     | 452 | GLY  | CA-C-O    | -5.04 | 117.57      | 122.46   |
| 2   | P     | 401 | GLN  | O-C-N     | 5.04  | 128.33      | 123.29   |
| 1   | E     | 81  | ASP  | CA-CB-CG  | -5.04 | 107.56      | 112.60   |
| 1   | A     | 99  | PHE  | N-CA-C    | -5.04 | 106.39      | 112.54   |
| 2   | P     | 306 | SER  | N-CA-C    | 5.04  | 116.64      | 109.14   |
| 1   | C     | 115 | ASN  | O-C-N     | 5.04  | 128.72      | 123.03   |
| 2   | O     | 514 | ASN  | O-C-N     | 5.04  | 125.92      | 121.19   |
| 2   | M     | 420 | ASP  | O-C-N     | 5.03  | 127.53      | 121.29   |
| 1   | B     | 125 | HIS  | CA-CB-CG  | -5.03 | 108.77      | 113.80   |
| 2   | N     | 417 | ALA  | N-CA-C    | -5.03 | 103.44      | 109.83   |
| 1   | E     | 66  | SER  | N-CA-CB   | 5.03  | 117.93      | 110.29   |
| 1   | D     | 44  | ALA  | N-CA-C    | -5.03 | 103.70      | 109.93   |
| 2   | P     | 496 | ALA  | N-CA-C    | 5.03  | 117.65      | 111.82   |
| 2   | Q     | 423 | PHE  | CB-CA-C   | 5.02  | 117.88      | 110.14   |
| 2   | M     | 395 | THR  | CA-CB-OG1 | -5.02 | 102.07      | 109.60   |
| 1   | D     | 162 | GLU  | CA-CB-CG  | 5.02  | 124.14      | 114.10   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 11  | GLN  | CA-CB-CG | 5.02  | 124.14      | 114.10   |
| 1   | D     | 137 | ILE  | CB-CA-C  | 5.02  | 118.20      | 110.28   |
| 1   | C     | 87  | ASN  | CA-CB-CG | 5.01  | 117.61      | 112.60   |
| 2   | N     | 461 | ILE  | CA-C-O   | -5.01 | 115.13      | 120.39   |
| 1   | A     | 21  | LEU  | N-CA-C   | 5.00  | 120.22      | 113.72   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 184 | ARG  | Sidechain |

## 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   | A     | 1571  | 0        | 1499     | 38      | 0            |
| 1   | B     | 1571  | 0        | 1499     | 45      | 0            |
| 1   | C     | 1571  | 0        | 1499     | 38      | 1            |
| 1   | D     | 1571  | 0        | 1499     | 40      | 1            |
| 1   | E     | 1571  | 0        | 1499     | 48      | 0            |
| 1   | F     | 1571  | 0        | 1499     | 77      | 0            |
| 2   | M     | 1840  | 0        | 1792     | 66      | 0            |
| 2   | N     | 1840  | 0        | 1792     | 38      | 0            |
| 2   | O     | 1840  | 0        | 1792     | 39      | 0            |
| 2   | P     | 1840  | 0        | 1792     | 44      | 0            |
| 2   | Q     | 1840  | 0        | 1792     | 58      | 0            |
| 2   | R     | 1840  | 0        | 1792     | 61      | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 4     | 0        | 5        | 1       | 0            |
| 4   | N     | 4     | 0        | 5        | 0       | 0            |
| 4   | O     | 4     | 0        | 5        | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | P     | 4     | 0        | 5        | 0       | 0            |
| 4   | Q     | 4     | 0        | 5        | 2       | 0            |
| 4   | R     | 4     | 0        | 5        | 0       | 0            |
| 5   | M     | 22    | 0        | 7        | 2       | 0            |
| 5   | N     | 22    | 0        | 6        | 2       | 0            |
| 5   | O     | 22    | 0        | 6        | 2       | 0            |
| 5   | P     | 22    | 0        | 7        | 1       | 0            |
| 5   | Q     | 22    | 0        | 7        | 2       | 0            |
| 5   | R     | 22    | 0        | 7        | 3       | 0            |
| 6   | A     | 82    | 0        | 0        | 0       | 0            |
| 6   | B     | 85    | 0        | 0        | 0       | 0            |
| 6   | C     | 82    | 0        | 0        | 1       | 0            |
| 6   | D     | 81    | 0        | 0        | 0       | 0            |
| 6   | E     | 84    | 0        | 0        | 0       | 0            |
| 6   | F     | 81    | 0        | 0        | 2       | 0            |
| 6   | M     | 163   | 0        | 0        | 6       | 0            |
| 6   | N     | 167   | 0        | 0        | 5       | 0            |
| 6   | O     | 162   | 0        | 0        | 6       | 0            |
| 6   | P     | 157   | 0        | 0        | 4       | 0            |
| 6   | Q     | 165   | 0        | 0        | 8       | 1            |
| 6   | R     | 167   | 0        | 0        | 4       | 0            |
| All | All   | 22104 | 0        | 19816    | 540     | 2            |

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 13.

All (540) 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:M:364:LEU:HD22 | 2:M:440:ARG:HD3  | 1.27                     | 1.17              |
| 1:D:64:ARG:NH1   | 1:D:100:ASP:O    | 1.82                     | 1.12              |
| 1:F:165:GLN:H    | 1:F:165:GLN:NE2  | 1.49                     | 1.10              |
| 1:B:165:GLN:H    | 1:B:165:GLN:NE2  | 1.50                     | 1.10              |
| 2:P:364:LEU:HD22 | 2:P:440:ARG:HD3  | 1.21                     | 1.09              |
| 1:F:64:ARG:NH1   | 1:F:100:ASP:O    | 1.86                     | 1.08              |
| 1:E:165:GLN:H    | 1:E:165:GLN:NE2  | 1.54                     | 1.05              |
| 1:A:165:GLN:H    | 1:A:165:GLN:NE2  | 1.54                     | 1.05              |
| 1:B:165:GLN:H    | 1:B:165:GLN:HE21 | 1.06                     | 1.01              |
| 1:E:176:GLU:OE2  | 1:E:179:GLY:HA2  | 1.60                     | 0.99              |
| 1:D:165:GLN:H    | 1:D:165:GLN:HE21 | 1.05                     | 0.98              |
| 1:C:64:ARG:NH1   | 1:C:100:ASP:O    | 1.97                     | 0.98              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:GLN:HE21 | 1:E:165:GLN:N    | 1.61                     | 0.97              |
| 1:C:165:GLN:H    | 1:C:165:GLN:NE2  | 1.64                     | 0.96              |
| 1:A:165:GLN:H    | 1:A:165:GLN:HE21 | 1.09                     | 0.93              |
| 1:E:67:PHE:HZ    | 1:E:94:ARG:HD2   | 1.34                     | 0.92              |
| 1:C:25:ALA:O     | 2:O:411:LYS:NZ   | 2.03                     | 0.92              |
| 2:R:361:HIS:H    | 2:R:361:HIS:CD2  | 1.88                     | 0.91              |
| 2:P:364:LEU:CD2  | 2:P:440:ARG:HD3  | 1.98                     | 0.91              |
| 1:C:165:GLN:H    | 1:C:165:GLN:HE21 | 1.14                     | 0.91              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:HA2  | 1.71                     | 0.89              |
| 1:C:99:PHE:HE2   | 2:O:411:LYS:HZ3  | 1.20                     | 0.89              |
| 1:F:165:GLN:H    | 1:F:165:GLN:HE21 | 1.17                     | 0.88              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:H    | 1.72                     | 0.87              |
| 2:M:522:ARG:NH1  | 6:M:665:HOH:O    | 2.08                     | 0.87              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:H    | 1.72                     | 0.87              |
| 1:D:176:GLU:OE2  | 1:D:179:GLY:HA2  | 1.73                     | 0.87              |
| 1:A:64:ARG:NH1   | 1:A:100:ASP:O    | 2.07                     | 0.87              |
| 2:N:390:LYS:HD2  | 6:N:649:HOH:O    | 1.74                     | 0.87              |
| 1:D:165:GLN:H    | 1:D:165:GLN:NE2  | 1.73                     | 0.85              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:O    | 1.78                     | 0.84              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:HE21 | 1.24                     | 0.84              |
| 2:P:390:LYS:HD3  | 6:P:650:HOH:O    | 1.78                     | 0.83              |
| 2:M:364:LEU:HD22 | 2:M:440:ARG:CD   | 2.08                     | 0.83              |
| 1:F:165:GLN:HE21 | 1:F:165:GLN:N    | 1.76                     | 0.82              |
| 1:B:25:ALA:O     | 2:N:411:LYS:NZ   | 2.13                     | 0.82              |
| 2:M:390:LYS:HD2  | 6:M:642:HOH:O    | 1.79                     | 0.81              |
| 2:R:497:ASN:HD22 | 2:R:499:GLU:H    | 1.27                     | 0.81              |
| 2:P:497:ASN:C    | 2:P:497:ASN:HD22 | 1.88                     | 0.81              |
| 1:F:41:LYS:HD2   | 1:F:88:ALA:HA    | 1.61                     | 0.81              |
| 1:A:67:PHE:HZ    | 1:A:94:ARG:HD2   | 1.45                     | 0.80              |
| 1:E:168:GLU:HA   | 1:E:171:ILE:HD12 | 1.64                     | 0.80              |
| 2:Q:361:HIS:CD2  | 2:Q:361:HIS:H    | 1.97                     | 0.80              |
| 1:F:165:GLN:NE2  | 1:F:165:GLN:N    | 2.29                     | 0.79              |
| 2:N:364:LEU:HD22 | 2:N:440:ARG:HD3  | 1.64                     | 0.78              |
| 1:B:165:GLN:HE21 | 1:B:165:GLN:N    | 1.79                     | 0.78              |
| 1:F:25:ALA:O     | 2:R:411:LYS:NZ   | 2.13                     | 0.78              |
| 2:O:390:LYS:HD2  | 6:O:653:HOH:O    | 1.83                     | 0.77              |
| 2:M:497:ASN:HD22 | 2:M:499:GLU:H    | 1.29                     | 0.77              |
| 1:E:67:PHE:CZ    | 1:E:94:ARG:HD2   | 2.19                     | 0.76              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:O    | 1.84                     | 0.76              |
| 2:P:497:ASN:ND2  | 2:P:499:GLU:H    | 1.83                     | 0.76              |
| 2:R:361:HIS:H    | 2:R:361:HIS:HD2  | 1.31                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:GLN:HE21 | 1:A:165:GLN:N    | 1.83                     | 0.76              |
| 2:O:497:ASN:ND2  | 2:O:499:GLU:H    | 1.84                     | 0.75              |
| 2:P:361:HIS:H    | 2:P:361:HIS:CD2  | 2.04                     | 0.74              |
| 2:M:305:ASN:O    | 2:M:533:THR:HG23 | 1.86                     | 0.74              |
| 1:A:176:GLU:OE2  | 1:A:179:GLY:HA2  | 1.87                     | 0.74              |
| 1:C:165:GLN:HE21 | 1:C:165:GLN:N    | 1.85                     | 0.73              |
| 5:Q:550:IHB:H2   | 6:Q:1225:HOH:O   | 1.87                     | 0.73              |
| 2:P:360:ASP:OD2  | 2:P:428:ARG:HD2  | 1.87                     | 0.73              |
| 1:F:26:ALA:C     | 2:R:411:LYS:HZ2  | 1.96                     | 0.73              |
| 1:B:67:PHE:HZ    | 1:B:94:ARG:HD2   | 1.52                     | 0.73              |
| 2:N:522:ARG:NH1  | 6:N:671:HOH:O    | 2.22                     | 0.73              |
| 2:P:307:ARG:HG2  | 2:P:533:THR:HG22 | 1.70                     | 0.73              |
| 1:F:35:ILE:HG22  | 1:F:94:ARG:HG3   | 1.70                     | 0.72              |
| 1:F:165:GLN:H    | 1:F:165:GLN:CD   | 1.94                     | 0.72              |
| 1:E:64:ARG:NH1   | 1:E:100:ASP:O    | 2.22                     | 0.72              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:HE21 | 1.35                     | 0.72              |
| 1:A:98:THR:OG1   | 1:A:102:GLY:N    | 2.22                     | 0.72              |
| 1:A:67:PHE:CZ    | 1:A:94:ARG:HD2   | 2.24                     | 0.72              |
| 2:Q:497:ASN:C    | 2:Q:497:ASN:HD22 | 1.97                     | 0.71              |
| 1:F:50:LEU:HD12  | 1:F:51:LEU:N     | 2.05                     | 0.71              |
| 2:M:356:PHE:HD1  | 2:M:428:ARG:HD3  | 1.56                     | 0.70              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:NE2  | 1.90                     | 0.69              |
| 1:C:98:THR:OG1   | 1:C:102:GLY:N    | 2.24                     | 0.69              |
| 1:E:51:LEU:HD12  | 1:E:106:LEU:HD23 | 1.73                     | 0.69              |
| 2:O:361:HIS:H    | 2:O:361:HIS:CD2  | 2.11                     | 0.68              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:HE21 | 1.40                     | 0.68              |
| 1:B:65:ASP:OD2   | 1:B:133:ARG:HD3  | 1.93                     | 0.68              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:C    | 2.17                     | 0.68              |
| 2:M:361:HIS:H    | 2:M:361:HIS:CD2  | 2.10                     | 0.68              |
| 1:F:98:THR:OG1   | 1:F:102:GLY:N    | 2.24                     | 0.68              |
| 2:P:390:LYS:HE2  | 6:P:726:HOH:O    | 1.93                     | 0.68              |
| 1:E:134:GLY:HA3  | 2:Q:326:THR:HG22 | 1.75                     | 0.67              |
| 1:F:163:GLN:HB3  | 1:F:165:GLN:NE2  | 2.10                     | 0.67              |
| 2:M:364:LEU:CD2  | 2:M:440:ARG:HD3  | 2.17                     | 0.67              |
| 1:C:41:LYS:HD2   | 1:C:88:ALA:HA    | 1.77                     | 0.67              |
| 2:N:416:LEU:HD23 | 2:N:416:LEU:C    | 2.18                     | 0.67              |
| 2:N:326:THR:HG22 | 2:N:330:ARG:HD2  | 1.77                     | 0.66              |
| 2:O:497:ASN:C    | 2:O:497:ASN:HD22 | 2.02                     | 0.66              |
| 1:E:98:THR:OG1   | 1:E:102:GLY:N    | 2.29                     | 0.66              |
| 1:E:99:PHE:HE2   | 2:Q:411:LYS:NZ   | 1.93                     | 0.66              |
| 2:N:361:HIS:CD2  | 2:N:361:HIS:H    | 2.12                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:165:GLN:HE21 | 1:D:165:GLN:N    | 1.87                     | 0.66              |
| 1:F:188:ARG:HG3  | 1:F:188:ARG:HH11 | 1.60                     | 0.66              |
| 2:Q:497:ASN:HD22 | 2:Q:498:PRO:N    | 1.93                     | 0.65              |
| 2:M:377:ARG:CZ   | 2:P:416:LEU:HD21 | 2.26                     | 0.65              |
| 2:Q:376:GLU:OE1  | 6:Q:1049:HOH:O   | 2.13                     | 0.65              |
| 2:R:522:ARG:NH1  | 6:R:1345:HOH:O   | 2.23                     | 0.65              |
| 1:D:100:ASP:OD1  | 1:D:100:ASP:N    | 2.28                     | 0.65              |
| 2:Q:361:HIS:H    | 2:Q:361:HIS:HD2  | 1.45                     | 0.65              |
| 2:O:416:LEU:C    | 2:O:416:LEU:HD23 | 2.21                     | 0.65              |
| 2:M:356:PHE:CD1  | 2:M:428:ARG:HD3  | 2.32                     | 0.65              |
| 1:F:100:ASP:N    | 1:F:100:ASP:OD1  | 2.29                     | 0.65              |
| 1:C:18:HIS:NE2   | 6:C:222:HOH:O    | 2.30                     | 0.64              |
| 2:O:497:ASN:HD22 | 2:O:498:PRO:N    | 1.95                     | 0.64              |
| 1:B:99:PHE:HE2   | 2:N:411:LYS:NZ   | 1.94                     | 0.64              |
| 2:O:363:LEU:HD23 | 2:O:425:GLY:HA2  | 1.80                     | 0.64              |
| 2:R:364:LEU:HD22 | 2:R:440:ARG:HD3  | 1.79                     | 0.64              |
| 1:A:98:THR:HB    | 1:A:100:ASP:OD1  | 1.96                     | 0.64              |
| 2:Q:450:ARG:NE   | 6:Q:1470:HOH:O   | 2.16                     | 0.64              |
| 2:N:307:ARG:HG2  | 2:N:533:THR:HG22 | 1.78                     | 0.64              |
| 1:F:99:PHE:HE2   | 2:R:411:LYS:HZ3  | 1.46                     | 0.64              |
| 2:Q:536:GLU:HB2  | 6:Q:1142:HOH:O   | 1.98                     | 0.64              |
| 2:R:400:TRP:HA   | 2:R:425:GLY:O    | 1.98                     | 0.63              |
| 1:B:114:VAL:HG23 | 1:B:122:MET:HE3  | 1.79                     | 0.63              |
| 1:F:114:VAL:HG23 | 1:F:122:MET:HE3  | 1.80                     | 0.63              |
| 2:R:304:ASP:HB2  | 2:R:343:ILE:HB   | 1.80                     | 0.63              |
| 1:C:114:VAL:HG23 | 1:C:122:MET:HE3  | 1.81                     | 0.63              |
| 2:P:497:ASN:HD22 | 2:P:499:GLU:H    | 1.47                     | 0.63              |
| 1:E:39:LEU:HD11  | 1:E:93:GLY:HA3   | 1.81                     | 0.62              |
| 1:E:110:LYS:NZ   | 1:E:147:ASP:OD1  | 2.31                     | 0.62              |
| 2:N:315:TRP:HZ2  | 2:N:503:GLN:HE21 | 1.45                     | 0.62              |
| 1:D:84:ASN:OD1   | 1:D:86:GLU:HB2   | 2.00                     | 0.62              |
| 2:M:360:ASP:OD2  | 2:M:428:ARG:HD2  | 1.99                     | 0.62              |
| 2:Q:307:ARG:HG2  | 2:Q:533:THR:HG22 | 1.81                     | 0.62              |
| 2:R:350:ASN:OD1  | 2:R:352:SER:HB2  | 2.00                     | 0.62              |
| 1:A:19:ILE:HG21  | 2:M:410:HIS:HB2  | 1.82                     | 0.62              |
| 1:E:165:GLN:H    | 1:E:165:GLN:HE21 | 0.76                     | 0.62              |
| 1:F:67:PHE:HZ    | 1:F:94:ARG:HD2   | 1.65                     | 0.61              |
| 1:B:165:GLN:NE2  | 1:B:165:GLN:N    | 2.35                     | 0.61              |
| 2:M:315:TRP:CZ2  | 2:M:503:GLN:NE2  | 2.68                     | 0.61              |
| 2:P:497:ASN:HD22 | 2:P:498:PRO:N    | 1.98                     | 0.61              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:H    | 1.98                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:143:LEU:HD23 | 1:E:143:LEU:C    | 2.25                     | 0.61              |
| 1:E:41:LYS:HD2   | 1:E:88:ALA:HA    | 1.81                     | 0.61              |
| 1:E:19:ILE:HG22  | 1:E:26:ALA:HB1   | 1.82                     | 0.61              |
| 1:E:25:ALA:O     | 2:Q:411:LYS:NZ   | 2.34                     | 0.60              |
| 1:D:25:ALA:O     | 2:P:411:LYS:NZ   | 2.34                     | 0.60              |
| 2:Q:376:GLU:O    | 2:Q:442:ILE:HA   | 2.02                     | 0.60              |
| 1:E:28:ASN:HB3   | 1:E:29:PRO:HD2   | 1.83                     | 0.60              |
| 1:B:15:PRO:HB3   | 1:B:133:ARG:HD2  | 1.84                     | 0.60              |
| 1:F:110:LYS:NZ   | 1:F:148:GLU:OE2  | 2.27                     | 0.60              |
| 2:O:376:GLU:O    | 2:O:442:ILE:HA   | 2.01                     | 0.60              |
| 1:D:28:ASN:HB3   | 1:D:29:PRO:HD2   | 1.84                     | 0.60              |
| 1:F:143:LEU:C    | 1:F:143:LEU:HD23 | 2.27                     | 0.59              |
| 1:F:121:PRO:O    | 6:F:1400:HOH:O   | 2.17                     | 0.59              |
| 2:R:447:TYR:OH   | 5:R:550:IHB:O4   | 2.20                     | 0.59              |
| 1:B:99:PHE:HE2   | 2:N:411:LYS:HZ3  | 1.48                     | 0.59              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:NE2  | 2.18                     | 0.59              |
| 2:N:478:LEU:C    | 2:N:478:LEU:HD23 | 2.28                     | 0.59              |
| 2:Q:488:MET:HE2  | 1:F:1:PRO:HG3    | 1.84                     | 0.59              |
| 2:O:497:ASN:HD22 | 2:O:499:GLU:H    | 1.49                     | 0.58              |
| 1:F:188:ARG:HG3  | 1:F:188:ARG:NH1  | 2.18                     | 0.58              |
| 2:R:413:ASP:C    | 2:R:414:ARG:HD2  | 2.28                     | 0.58              |
| 1:A:110:LYS:NZ   | 1:A:147:ASP:OD1  | 2.36                     | 0.58              |
| 1:B:67:PHE:CZ    | 1:B:94:ARG:HD2   | 2.37                     | 0.58              |
| 1:F:67:PHE:CZ    | 1:F:94:ARG:HD2   | 2.37                     | 0.58              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:CA   | 2.48                     | 0.58              |
| 1:A:144:TYR:CE1  | 1:A:158:LEU:HD13 | 2.38                     | 0.58              |
| 1:B:19:ILE:O     | 2:N:426:VAL:HG21 | 2.03                     | 0.58              |
| 1:A:176:GLU:HA   | 1:A:180:LYS:O    | 2.03                     | 0.58              |
| 1:F:24:GLU:O     | 1:F:27:GLY:N     | 2.35                     | 0.58              |
| 1:B:98:THR:OG1   | 1:B:102:GLY:N    | 2.36                     | 0.58              |
| 2:M:416:LEU:C    | 2:M:416:LEU:HD23 | 2.28                     | 0.58              |
| 1:B:180:LYS:HG2  | 1:B:181:THR:N    | 2.19                     | 0.58              |
| 1:E:61:HIS:ND1   | 1:F:163:GLN:HG3  | 2.18                     | 0.58              |
| 1:F:131:PHE:CD2  | 2:R:475:ILE:HD12 | 2.39                     | 0.58              |
| 1:A:50:LEU:O     | 1:A:182:ALA:HA   | 2.03                     | 0.57              |
| 1:C:176:GLU:HG3  | 1:C:180:LYS:O    | 2.04                     | 0.57              |
| 2:Q:361:HIS:CG   | 4:Q:601:BME:H21  | 2.39                     | 0.57              |
| 2:P:416:LEU:C    | 2:P:416:LEU:HD23 | 2.29                     | 0.57              |
| 5:M:550:IHB:H2   | 6:M:742:HOH:O    | 2.05                     | 0.57              |
| 1:D:176:GLU:HG3  | 1:D:180:LYS:O    | 2.05                     | 0.57              |
| 1:F:36:TRP:CG    | 1:F:37:ASN:H     | 2.23                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:383:ARG:HG3  | 2:Q:436:TYR:CE1  | 2.39                     | 0.57              |
| 1:F:41:LYS:HE3   | 1:F:87:ASN:O     | 2.05                     | 0.57              |
| 1:E:99:PHE:HE2   | 2:Q:411:LYS:HZ3  | 1.43                     | 0.57              |
| 1:A:19:ILE:HG22  | 1:A:26:ALA:HB1   | 1.86                     | 0.57              |
| 2:P:400:TRP:HA   | 2:P:425:GLY:O    | 2.05                     | 0.57              |
| 2:Q:416:LEU:HD23 | 2:Q:416:LEU:C    | 2.30                     | 0.57              |
| 2:M:400:TRP:HA   | 2:M:425:GLY:O    | 2.05                     | 0.56              |
| 1:C:35:ILE:HG21  | 1:C:92:PHE:HE2   | 1.70                     | 0.56              |
| 2:M:307:ARG:HG2  | 2:M:533:THR:HG22 | 1.86                     | 0.56              |
| 1:D:98:THR:OG1   | 1:D:102:GLY:N    | 2.39                     | 0.56              |
| 1:F:54:GLN:HG2   | 1:F:102:GLY:O    | 2.05                     | 0.56              |
| 1:F:147:ASP:OD2  | 1:F:174:ARG:HD2  | 2.06                     | 0.56              |
| 2:P:416:LEU:C    | 2:P:416:LEU:CD2  | 2.78                     | 0.56              |
| 2:R:383:ARG:HD2  | 2:R:436:TYR:CZ   | 2.41                     | 0.56              |
| 2:Q:465:ILE:HD12 | 2:Q:465:ILE:N    | 2.21                     | 0.56              |
| 1:A:132:ALA:HB3  | 1:A:135:ILE:HD12 | 1.87                     | 0.56              |
| 1:E:98:THR:O     | 1:E:102:GLY:HA2  | 2.06                     | 0.56              |
| 1:C:176:GLU:OE2  | 1:C:179:GLY:HA2  | 2.05                     | 0.55              |
| 1:E:168:GLU:HA   | 1:E:171:ILE:CD1  | 2.34                     | 0.55              |
| 2:N:416:LEU:C    | 2:N:416:LEU:CD2  | 2.80                     | 0.55              |
| 1:F:50:LEU:HD12  | 1:F:50:LEU:C     | 2.31                     | 0.55              |
| 1:C:100:ASP:N    | 1:C:100:ASP:OD1  | 2.39                     | 0.55              |
| 1:B:131:PHE:CD2  | 1:B:138:HIS:HB3  | 2.40                     | 0.55              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:H    | 2.03                     | 0.55              |
| 1:A:176:GLU:HG3  | 1:A:180:LYS:O    | 2.06                     | 0.55              |
| 1:F:98:THR:O     | 1:F:102:GLY:HA2  | 2.06                     | 0.55              |
| 2:M:497:ASN:HD22 | 2:M:497:ASN:C    | 2.15                     | 0.55              |
| 1:B:51:LEU:HD12  | 1:B:106:LEU:HD22 | 1.89                     | 0.54              |
| 1:B:64:ARG:NH1   | 1:B:100:ASP:O    | 2.40                     | 0.54              |
| 1:F:50:LEU:O     | 1:F:182:ALA:HA   | 2.07                     | 0.54              |
| 1:A:26:ALA:C     | 2:M:411:LYS:NZ   | 2.65                     | 0.54              |
| 1:E:176:GLU:OE2  | 1:E:179:GLY:CA   | 2.46                     | 0.54              |
| 2:P:361:HIS:H    | 2:P:361:HIS:HD2  | 1.51                     | 0.54              |
| 2:M:361:HIS:H    | 2:M:361:HIS:HD2  | 1.55                     | 0.54              |
| 1:D:100:ASP:CG   | 1:D:101:ALA:H    | 2.14                     | 0.54              |
| 2:R:407:ARG:NH1  | 2:R:417:ALA:O    | 2.34                     | 0.54              |
| 1:B:33:GLN:HG2   | 1:B:85:LEU:HD12  | 1.90                     | 0.54              |
| 2:R:364:LEU:HD11 | 2:R:442:ILE:HG23 | 1.90                     | 0.54              |
| 1:A:26:ALA:C     | 2:M:411:LYS:HZ2  | 2.15                     | 0.54              |
| 2:Q:432:ASP:OD1  | 2:Q:434:ASP:N    | 2.36                     | 0.54              |
| 1:B:165:GLN:H    | 1:B:165:GLN:CD   | 2.15                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:376:GLU:O    | 2:N:442:ILE:HA   | 2.07                     | 0.53              |
| 2:O:315:TRP:HE1  | 2:O:503:GLN:HE22 | 1.56                     | 0.53              |
| 2:R:390:LYS:HD3  | 6:R:1425:HOH:O   | 2.08                     | 0.53              |
| 1:E:176:GLU:HG3  | 1:E:180:LYS:O    | 2.07                     | 0.53              |
| 1:E:184:ARG:NH1  | 1:E:184:ARG:HG3  | 2.23                     | 0.53              |
| 2:M:536:GLU:HB2  | 6:M:697:HOH:O    | 2.08                     | 0.53              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:NE2  | 1.99                     | 0.53              |
| 2:Q:478:LEU:C    | 2:Q:478:LEU:HD23 | 2.34                     | 0.53              |
| 2:P:356:PHE:CD1  | 2:P:428:ARG:HD3  | 2.44                     | 0.53              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:NE2  | 2.05                     | 0.53              |
| 2:N:359:HIS:O    | 2:N:366:ASN:HB3  | 2.09                     | 0.53              |
| 2:M:434:ASP:HB3  | 2:M:436:TYR:CE2  | 2.43                     | 0.52              |
| 1:C:24:GLU:O     | 1:C:27:GLY:N     | 2.40                     | 0.52              |
| 1:D:143:LEU:C    | 1:D:143:LEU:HD23 | 2.34                     | 0.52              |
| 1:B:6:PRO:HB2    | 2:N:503:GLN:HE22 | 1.74                     | 0.52              |
| 1:F:78:GLU:OE2   | 2:R:301:PRO:HG3  | 2.09                     | 0.52              |
| 2:M:497:ASN:HD22 | 2:M:498:PRO:N    | 2.07                     | 0.52              |
| 1:D:78:GLU:HG2   | 2:P:301:PRO:HG2  | 1.91                     | 0.52              |
| 2:R:371:GLY:N    | 2:R:422:ASN:ND2  | 2.58                     | 0.52              |
| 1:D:65:ASP:OD2   | 1:D:133:ARG:HD3  | 2.09                     | 0.52              |
| 2:R:497:ASN:HD22 | 2:R:498:PRO:N    | 2.08                     | 0.52              |
| 1:B:51:LEU:HD12  | 1:B:106:LEU:CD2  | 2.40                     | 0.52              |
| 1:B:98:THR:O     | 1:B:102:GLY:HA2  | 2.10                     | 0.52              |
| 2:Q:390:LYS:HE2  | 6:Q:1179:HOH:O   | 2.09                     | 0.51              |
| 1:F:131:PHE:O    | 1:F:132:ALA:HB2  | 2.10                     | 0.51              |
| 2:R:497:ASN:HD22 | 2:R:497:ASN:C    | 2.18                     | 0.51              |
| 1:B:131:PHE:CE2  | 1:B:138:HIS:HB3  | 2.45                     | 0.51              |
| 2:Q:522:ARG:NH1  | 6:Q:1099:HOH:O   | 2.44                     | 0.51              |
| 1:A:41:LYS:HD2   | 1:A:88:ALA:HA    | 1.93                     | 0.51              |
| 2:R:326:THR:HG22 | 2:R:330:ARG:HD2  | 1.90                     | 0.51              |
| 2:R:447:TYR:OH   | 5:R:550:IHB:C4   | 2.58                     | 0.51              |
| 2:M:376:GLU:OE1  | 6:M:637:HOH:O    | 2.19                     | 0.51              |
| 1:F:36:TRP:CD1   | 1:F:37:ASN:H     | 2.28                     | 0.51              |
| 1:A:19:ILE:CG2   | 2:M:410:HIS:HB2  | 2.41                     | 0.51              |
| 2:N:364:LEU:HD22 | 2:N:440:ARG:CD   | 2.38                     | 0.51              |
| 2:M:377:ARG:NH1  | 2:P:416:LEU:HD21 | 2.26                     | 0.51              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:HB2  | 2.26                     | 0.51              |
| 2:Q:416:LEU:HD23 | 2:Q:417:ALA:N    | 2.26                     | 0.51              |
| 1:F:3:GLU:OE1    | 1:F:3:GLU:HA     | 2.11                     | 0.51              |
| 1:C:16:TYR:O     | 1:C:19:ILE:HG23  | 2.11                     | 0.51              |
| 2:Q:408:TYR:HE1  | 2:Q:447:TYR:CZ   | 2.29                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:50:LEU:O     | 1:D:182:ALA:HA   | 2.11                     | 0.50              |
| 2:M:434:ASP:HB3  | 2:M:436:TYR:CD2  | 2.46                     | 0.50              |
| 1:C:26:ALA:C     | 2:O:411:LYS:HZ2  | 2.18                     | 0.50              |
| 1:F:44:ALA:O     | 1:F:48:HIS:NE2   | 2.31                     | 0.50              |
| 2:N:400:TRP:HA   | 2:N:425:GLY:O    | 2.11                     | 0.50              |
| 2:N:410:HIS:CE1  | 2:N:411:LYS:HG3  | 2.47                     | 0.50              |
| 2:P:497:ASN:ND2  | 2:P:499:GLU:N    | 2.58                     | 0.50              |
| 1:A:78:GLU:CD    | 2:M:301:PRO:HG3  | 2.36                     | 0.50              |
| 1:F:26:ALA:C     | 2:R:411:LYS:NZ   | 2.68                     | 0.50              |
| 1:F:52:LEU:CD2   | 1:F:184:ARG:NH1  | 2.75                     | 0.50              |
| 1:F:115:ASN:HA   | 1:F:121:PRO:HA   | 1.94                     | 0.50              |
| 1:F:78:GLU:CD    | 2:R:301:PRO:HG3  | 2.37                     | 0.50              |
| 2:R:307:ARG:HG2  | 2:R:533:THR:HG22 | 1.94                     | 0.50              |
| 2:O:522:ARG:NH1  | 6:O:676:HOH:O    | 2.44                     | 0.50              |
| 2:R:385:VAL:O    | 2:R:526:VAL:HA   | 2.12                     | 0.49              |
| 2:N:497:ASN:HD22 | 2:N:499:GLU:H    | 1.59                     | 0.49              |
| 1:C:44:ALA:O     | 1:C:48:HIS:NE2   | 2.33                     | 0.49              |
| 2:Q:447:TYR:CE1  | 5:Q:550:IHB:C5   | 2.95                     | 0.49              |
| 2:M:413:ASP:C    | 2:M:414:ARG:HD2  | 2.37                     | 0.49              |
| 2:N:447:TYR:OH   | 5:N:550:IHB:C5   | 2.59                     | 0.49              |
| 1:E:99:PHE:CE2   | 2:Q:411:LYS:NZ   | 2.71                     | 0.49              |
| 1:E:168:GLU:CA   | 1:E:171:ILE:HD12 | 2.41                     | 0.49              |
| 2:N:364:LEU:CD2  | 2:N:440:ARG:HD3  | 2.39                     | 0.49              |
| 2:O:447:TYR:OH   | 5:O:550:IHB:C5   | 2.60                     | 0.49              |
| 2:Q:359:HIS:O    | 2:Q:366:ASN:HB3  | 2.12                     | 0.49              |
| 1:B:100:ASP:CG   | 1:B:101:ALA:H    | 2.21                     | 0.49              |
| 1:C:36:TRP:CG    | 1:C:37:ASN:H     | 2.30                     | 0.49              |
| 2:M:376:GLU:O    | 2:M:442:ILE:HA   | 2.13                     | 0.49              |
| 1:B:19:ILE:HG22  | 1:B:26:ALA:HB1   | 1.95                     | 0.49              |
| 1:D:24:GLU:O     | 1:D:27:GLY:HA2   | 2.13                     | 0.49              |
| 1:F:52:LEU:HD21  | 1:F:184:ARG:NH1  | 2.27                     | 0.49              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:N    | 2.53                     | 0.48              |
| 1:B:168:GLU:HA   | 1:B:171:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:133:ARG:HG2  | 2:M:326:THR:HG21 | 1.96                     | 0.48              |
| 1:D:98:THR:O     | 1:D:102:GLY:HA2  | 2.13                     | 0.48              |
| 1:D:176:GLU:OE2  | 1:D:179:GLY:CA   | 2.54                     | 0.48              |
| 2:P:497:ASN:C    | 2:P:497:ASN:ND2  | 2.61                     | 0.48              |
| 2:P:376:GLU:O    | 2:P:442:ILE:HA   | 2.13                     | 0.48              |
| 1:F:116:ASN:OD1  | 1:F:116:ASN:C    | 2.56                     | 0.48              |
| 1:D:70:VAL:HG21  | 1:D:106:LEU:HD21 | 1.94                     | 0.48              |
| 1:E:184:ARG:HG3  | 1:E:184:ARG:HH11 | 1.78                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:16:TYR:O     | 1:F:19:ILE:HG12  | 2.14                     | 0.48              |
| 1:F:94:ARG:NH2   | 2:R:398:GLU:OE2  | 2.37                     | 0.48              |
| 2:P:326:THR:HG22 | 2:P:330:ARG:HD2  | 1.96                     | 0.48              |
| 2:O:497:ASN:ND2  | 2:O:497:ASN:C    | 2.71                     | 0.48              |
| 1:D:132:ALA:HB3  | 1:D:135:ILE:HD12 | 1.94                     | 0.48              |
| 2:Q:486:ILE:HB   | 2:Q:487:PRO:HD3  | 1.94                     | 0.48              |
| 5:R:550:IHB:H2   | 6:R:1471:HOH:O   | 2.14                     | 0.48              |
| 1:A:163:GLN:HG3  | 1:C:61:HIS:ND1   | 2.28                     | 0.48              |
| 1:D:39:LEU:HB3   | 1:D:90:ASN:O     | 2.14                     | 0.48              |
| 2:P:434:ASP:HB3  | 2:P:436:TYR:CE2  | 2.49                     | 0.48              |
| 1:F:52:LEU:O     | 1:F:184:ARG:HA   | 2.13                     | 0.48              |
| 2:M:359:HIS:O    | 2:M:366:ASN:HB3  | 2.13                     | 0.47              |
| 1:C:50:LEU:O     | 1:C:182:ALA:HA   | 2.14                     | 0.47              |
| 5:O:550:IHB:H2   | 6:O:760:HOH:O    | 2.13                     | 0.47              |
| 1:F:15:PRO:HB3   | 1:F:133:ARG:HD2  | 1.95                     | 0.47              |
| 2:M:488:MET:HE1  | 2:P:508:LEU:HD23 | 1.96                     | 0.47              |
| 1:C:98:THR:OG1   | 1:C:101:ALA:HB3  | 2.14                     | 0.47              |
| 2:O:400:TRP:HA   | 2:O:425:GLY:O    | 2.15                     | 0.47              |
| 1:C:99:PHE:HE2   | 2:O:411:LYS:NZ   | 2.01                     | 0.47              |
| 2:O:410:HIS:CE1  | 2:O:412:ASN:H    | 2.30                     | 0.47              |
| 2:Q:399:MET:HA   | 2:Q:462:HIS:O    | 2.14                     | 0.47              |
| 2:P:364:LEU:HD11 | 2:P:442:ILE:HG23 | 1.96                     | 0.47              |
| 1:F:163:GLN:HB3  | 1:F:165:GLN:HE22 | 1.79                     | 0.47              |
| 1:A:4:LEU:HB3    | 2:M:387:GLN:HB3  | 1.95                     | 0.47              |
| 2:P:360:ASP:HB3  | 2:P:428:ARG:HG3  | 1.97                     | 0.47              |
| 2:R:486:ILE:HB   | 2:R:487:PRO:HD3  | 1.95                     | 0.47              |
| 2:P:489:CYS:HA   | 2:P:490:PRO:HD3  | 1.64                     | 0.47              |
| 2:Q:385:VAL:O    | 2:Q:526:VAL:HA   | 2.15                     | 0.47              |
| 1:B:61:HIS:ND1   | 1:C:163:GLN:HG3  | 2.29                     | 0.47              |
| 2:Q:522:ARG:HE   | 2:Q:524:ASP:CG   | 2.23                     | 0.47              |
| 2:R:390:LYS:HD2  | 6:R:1307:HOH:O   | 2.13                     | 0.47              |
| 1:C:52:LEU:CD2   | 1:C:184:ARG:NH1  | 2.77                     | 0.47              |
| 2:P:372:LEU:HA   | 2:P:373:PRO:HD3  | 1.77                     | 0.47              |
| 2:R:410:HIS:CE1  | 2:R:411:LYS:HG3  | 2.50                     | 0.47              |
| 2:O:489:CYS:HA   | 2:O:490:PRO:HD3  | 1.71                     | 0.46              |
| 2:M:416:LEU:C    | 2:M:416:LEU:CD2  | 2.87                     | 0.46              |
| 1:F:176:GLU:HA   | 1:F:180:LYS:O    | 2.15                     | 0.46              |
| 2:R:315:TRP:CZ2  | 2:R:503:GLN:NE2  | 2.78                     | 0.46              |
| 2:M:360:ASP:HB3  | 2:M:428:ARG:HG3  | 1.97                     | 0.46              |
| 2:O:361:HIS:CG   | 4:O:601:BME:H21  | 2.50                     | 0.46              |
| 2:O:465:ILE:HD12 | 2:O:465:ILE:N    | 2.31                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:497:ASN:ND2  | 2:R:499:GLU:N    | 2.54                     | 0.46              |
| 2:O:410:HIS:ND1  | 2:O:412:ASN:N    | 2.50                     | 0.46              |
| 1:F:19:ILE:HD11  | 2:R:408:TYR:HD1  | 1.80                     | 0.46              |
| 2:N:497:ASN:HD22 | 2:N:497:ASN:C    | 2.23                     | 0.46              |
| 1:E:100:ASP:OD1  | 1:E:100:ASP:N    | 2.48                     | 0.46              |
| 2:R:356:PHE:CD1  | 2:R:428:ARG:HD3  | 2.50                     | 0.46              |
| 2:Q:450:ARG:NH2  | 6:Q:1470:HOH:O   | 2.42                     | 0.46              |
| 1:B:143:LEU:C    | 1:B:143:LEU:HD23 | 2.41                     | 0.46              |
| 1:B:176:GLU:OE2  | 1:B:179:GLY:C    | 2.58                     | 0.45              |
| 2:N:536:GLU:HB2  | 6:N:704:HOH:O    | 2.16                     | 0.45              |
| 1:E:177:VAL:O    | 1:E:180:LYS:HB3  | 2.16                     | 0.45              |
| 1:A:19:ILE:HG21  | 1:A:19:ILE:HD13  | 1.75                     | 0.45              |
| 1:C:98:THR:HG1   | 1:C:101:ALA:HB3  | 1.82                     | 0.45              |
| 1:C:52:LEU:HD21  | 1:C:184:ARG:NH1  | 2.32                     | 0.45              |
| 2:R:448:PRO:HD3  | 2:R:456:TRP:CZ3  | 2.52                     | 0.45              |
| 1:A:36:TRP:CG    | 1:A:37:ASN:H     | 2.34                     | 0.45              |
| 2:O:364:LEU:HD11 | 2:O:442:ILE:HG23 | 1.99                     | 0.45              |
| 1:E:70:VAL:HG12  | 1:E:128:ILE:HG12 | 1.98                     | 0.45              |
| 2:R:383:ARG:NH2  | 2:R:391:PRO:HG3  | 2.32                     | 0.45              |
| 2:M:403:ASN:HB2  | 6:M:610:HOH:O    | 2.16                     | 0.45              |
| 2:Q:360:ASP:OD2  | 2:Q:428:ARG:HD2  | 2.17                     | 0.45              |
| 2:Q:497:ASN:HD22 | 2:Q:499:GLU:H    | 1.65                     | 0.45              |
| 1:F:17:VAL:CG2   | 1:F:21:LEU:HD12  | 2.47                     | 0.45              |
| 2:R:415:TYR:CE1  | 2:R:416:LEU:HD22 | 2.52                     | 0.45              |
| 1:B:23:LEU:N     | 1:B:23:LEU:HD12  | 2.32                     | 0.45              |
| 2:Q:438:SER:O    | 4:Q:601:BME:H22  | 2.16                     | 0.45              |
| 1:F:94:ARG:HH22  | 2:R:398:GLU:CD   | 2.22                     | 0.45              |
| 2:R:414:ARG:HD2  | 2:R:414:ARG:N    | 2.32                     | 0.45              |
| 1:A:35:ILE:HD13  | 2:M:351:PHE:CE1  | 2.52                     | 0.45              |
| 2:M:489:CYS:HA   | 2:M:490:PRO:HD3  | 1.81                     | 0.45              |
| 2:Q:522:ARG:HH11 | 2:Q:522:ARG:HD3  | 1.50                     | 0.45              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:C    | 2.41                     | 0.45              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:NE2  | 2.32                     | 0.45              |
| 1:C:155:CYS:HB3  | 1:C:158:LEU:HB2  | 1.98                     | 0.45              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:HB2  | 2.32                     | 0.45              |
| 2:M:517:ASP:C    | 2:M:517:ASP:OD1  | 2.60                     | 0.44              |
| 2:R:491:ILE:O    | 2:R:494:SER:OG   | 2.29                     | 0.44              |
| 1:D:36:TRP:CG    | 1:D:37:ASN:H     | 2.34                     | 0.44              |
| 1:A:39:LEU:HD11  | 1:A:93:GLY:HA3   | 1.99                     | 0.44              |
| 2:M:497:ASN:HD21 | 2:M:499:GLU:HB2  | 1.83                     | 0.44              |
| 1:D:24:GLU:O     | 1:D:27:GLY:N     | 2.47                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:131:PHE:CD2 | 1:D:138:HIS:HB3  | 2.53                     | 0.44              |
| 1:A:165:GLN:NE2 | 1:A:165:GLN:N    | 2.39                     | 0.44              |
| 2:M:362:ASP:OD1 | 2:M:440:ARG:HD2  | 2.17                     | 0.44              |
| 2:M:383:ARG:HG3 | 2:M:436:TYR:CE1  | 2.51                     | 0.44              |
| 1:E:165:GLN:NE2 | 1:E:165:GLN:N    | 2.39                     | 0.44              |
| 1:F:19:ILE:HG22 | 1:F:26:ALA:HB1   | 2.00                     | 0.44              |
| 2:R:416:LEU:C   | 2:R:416:LEU:HD23 | 2.42                     | 0.44              |
| 2:R:489:CYS:O   | 2:R:493:LYS:HE3  | 2.16                     | 0.44              |
| 2:N:497:ASN:HA  | 2:N:498:PRO:HD2  | 1.85                     | 0.44              |
| 1:D:176:GLU:HA  | 1:D:180:LYS:O    | 2.18                     | 0.44              |
| 1:E:9:PRO:HD2   | 2:Q:504:LEU:HD21 | 2.00                     | 0.44              |
| 2:M:497:ASN:HA  | 2:M:498:PRO:HD2  | 1.76                     | 0.44              |
| 2:N:315:TRP:HZ2 | 2:N:503:GLN:NE2  | 2.15                     | 0.44              |
| 1:C:52:LEU:C    | 1:C:52:LEU:HD22  | 2.42                     | 0.44              |
| 1:F:65:ASP:OD2  | 1:F:133:ARG:HD3  | 2.18                     | 0.44              |
| 1:E:176:GLU:HA  | 1:E:180:LYS:O    | 2.17                     | 0.44              |
| 1:F:68:LEU:N    | 1:F:68:LEU:HD12  | 2.32                     | 0.44              |
| 1:C:168:GLU:HA  | 1:C:171:ILE:HD12 | 1.99                     | 0.44              |
| 2:Q:450:ARG:CZ  | 6:Q:1470:HOH:O   | 2.63                     | 0.44              |
| 2:Q:522:ARG:NE  | 2:Q:524:ASP:OD1  | 2.51                     | 0.44              |
| 2:R:331:SER:HA  | 2:R:332:PRO:HD3  | 1.92                     | 0.44              |
| 2:R:497:ASN:HA  | 2:R:498:PRO:HD3  | 1.80                     | 0.44              |
| 2:M:448:PRO:CB  | 2:P:516:MET:HA   | 2.48                     | 0.43              |
| 2:N:483:ASP:HB3 | 2:N:486:ILE:HG13 | 2.00                     | 0.43              |
| 1:C:98:THR:O    | 1:C:102:GLY:HA2  | 2.18                     | 0.43              |
| 1:D:133:ARG:NH2 | 1:E:162:GLU:OE2  | 2.51                     | 0.43              |
| 1:E:24:GLU:O    | 1:E:27:GLY:N     | 2.48                     | 0.43              |
| 1:B:74:ASP:OD2  | 1:B:80:GLN:NE2   | 2.51                     | 0.43              |
| 1:B:3:GLU:HA    | 1:B:3:GLU:OE1    | 2.18                     | 0.43              |
| 1:D:35:ILE:HD13 | 2:P:351:PHE:CE1  | 2.53                     | 0.43              |
| 2:P:420:ASP:HA  | 2:P:421:PRO:HD2  | 1.83                     | 0.43              |
| 2:P:443:LYS:HE2 | 2:P:480:PHE:CG   | 2.53                     | 0.43              |
| 2:Q:343:ILE:O   | 2:Q:343:ILE:HG12 | 2.18                     | 0.43              |
| 2:Q:420:ASP:HA  | 2:Q:421:PRO:HD2  | 1.83                     | 0.43              |
| 2:P:308:PHE:HA  | 2:P:529:GLY:O    | 2.18                     | 0.43              |
| 2:Q:315:TRP:CZ2 | 2:Q:503:GLN:NE2  | 2.85                     | 0.43              |
| 2:Q:489:CYS:HA  | 2:Q:490:PRO:HD3  | 1.75                     | 0.43              |
| 1:F:36:TRP:CG   | 1:F:37:ASN:N     | 2.86                     | 0.43              |
| 2:M:335:ALA:HB2 | 2:O:328:ILE:HD12 | 1.99                     | 0.43              |
| 1:C:120:VAL:HA  | 1:C:121:PRO:HD3  | 1.69                     | 0.43              |
| 2:R:410:HIS:ND1 | 2:R:410:HIS:C    | 2.76                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:361:HIS:CD2  | 2:Q:361:HIS:N    | 2.72                     | 0.43              |
| 1:A:191:GLY:O    | 1:A:194:GLU:HB2  | 2.19                     | 0.43              |
| 1:B:36:TRP:CG    | 1:B:37:ASN:H     | 2.37                     | 0.43              |
| 2:N:489:CYS:HA   | 2:N:490:PRO:HD3  | 1.77                     | 0.43              |
| 1:E:8:THR:HA     | 1:E:9:PRO:HD3    | 1.83                     | 0.43              |
| 1:F:132:ALA:HB3  | 1:F:135:ILE:HD12 | 2.00                     | 0.43              |
| 2:R:341:GLN:HB3  | 2:R:346:THR:CG2  | 2.49                     | 0.43              |
| 1:B:50:LEU:O     | 1:B:182:ALA:HA   | 2.19                     | 0.43              |
| 1:C:116:ASN:OD1  | 1:C:116:ASN:C    | 2.62                     | 0.43              |
| 2:O:383:ARG:HA   | 2:O:435:GLY:O    | 2.19                     | 0.43              |
| 1:D:54:GLN:HG3   | 1:D:184:ARG:HH22 | 1.84                     | 0.43              |
| 2:M:390:LYS:HA   | 2:M:391:PRO:HD3  | 1.89                     | 0.43              |
| 5:N:550:IHB:H2   | 6:N:758:HOH:O    | 2.19                     | 0.43              |
| 1:F:131:PHE:CE2  | 1:F:138:HIS:HB3  | 2.54                     | 0.43              |
| 2:O:361:HIS:CD2  | 2:O:361:HIS:N    | 2.85                     | 0.42              |
| 2:M:486:ILE:HB   | 2:M:487:PRO:HD3  | 2.02                     | 0.42              |
| 2:M:515:PRO:HB3  | 2:P:453:PRO:O    | 2.20                     | 0.42              |
| 2:O:437:TYR:CD1  | 2:O:437:TYR:C    | 2.96                     | 0.42              |
| 2:Q:325:LYS:HG2  | 2:R:335:ALA:HB1  | 2.01                     | 0.42              |
| 1:F:47:GLU:O     | 1:F:49:ILE:HG23  | 2.19                     | 0.42              |
| 2:N:390:LYS:HA   | 2:N:391:PRO:HD3  | 1.79                     | 0.42              |
| 1:F:31:ARG:NH1   | 2:R:428:ARG:HG2  | 2.34                     | 0.42              |
| 2:O:318:LYS:HA   | 2:O:318:LYS:HD3  | 1.90                     | 0.42              |
| 2:O:416:LEU:C    | 2:O:416:LEU:CD2  | 2.90                     | 0.42              |
| 1:E:131:PHE:CE2  | 1:E:138:HIS:HB3  | 2.54                     | 0.42              |
| 1:F:18:HIS:CE1   | 6:F:1278:HOH:O   | 2.72                     | 0.42              |
| 1:D:162:GLU:OE2  | 1:F:133:ARG:NH2  | 2.51                     | 0.42              |
| 1:E:100:ASP:CG   | 1:E:101:ALA:H    | 2.26                     | 0.42              |
| 2:Q:392:VAL:HG12 | 2:Q:395:THR:HB   | 2.02                     | 0.42              |
| 1:F:85:LEU:HD23  | 1:F:85:LEU:HA    | 1.77                     | 0.42              |
| 2:M:372:LEU:HA   | 2:M:373:PRO:HD3  | 1.92                     | 0.42              |
| 2:M:399:MET:HA   | 2:M:462:HIS:O    | 2.19                     | 0.42              |
| 2:N:373:PRO:HB3  | 2:N:423:PHE:HB2  | 2.00                     | 0.42              |
| 2:P:478:LEU:C    | 2:P:478:LEU:HD23 | 2.45                     | 0.42              |
| 2:O:410:HIS:CE1  | 2:O:412:ASN:HB2  | 2.55                     | 0.42              |
| 2:P:405:GLY:HA3  | 6:P:653:HOH:O    | 2.19                     | 0.42              |
| 2:P:497:ASN:HD22 | 2:P:499:GLU:N    | 2.13                     | 0.42              |
| 1:B:123:ALA:HB3  | 1:B:144:TYR:CE2  | 2.55                     | 0.42              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:HB2  | 2.35                     | 0.42              |
| 2:Q:410:HIS:CE1  | 2:Q:412:ASN:H    | 2.37                     | 0.42              |
| 1:F:99:PHE:HE2   | 2:R:411:LYS:NZ   | 2.14                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:ASP:OD2  | 1:A:174:ARG:HD2  | 2.20                     | 0.42              |
| 2:O:450:ARG:HG3  | 6:O:642:HOH:O    | 2.19                     | 0.42              |
| 1:D:25:ALA:C     | 1:D:27:GLY:N     | 2.77                     | 0.42              |
| 1:F:8:THR:HA     | 1:F:9:PRO:HD3    | 1.89                     | 0.42              |
| 2:N:348:GLY:HA3  | 6:N:648:HOH:O    | 2.20                     | 0.41              |
| 1:C:28:ASN:HB3   | 1:C:29:PRO:HD2   | 2.01                     | 0.41              |
| 1:D:158:LEU:HD12 | 1:D:158:LEU:HA   | 1.88                     | 0.41              |
| 2:R:361:HIS:CD2  | 2:R:361:HIS:N    | 2.62                     | 0.41              |
| 1:A:165:GLN:H    | 1:A:165:GLN:CD   | 2.20                     | 0.41              |
| 2:M:361:HIS:CG   | 4:M:601:BME:H21  | 2.55                     | 0.41              |
| 1:B:19:ILE:O     | 2:N:426:VAL:CG2  | 2.68                     | 0.41              |
| 1:E:131:PHE:O    | 1:E:132:ALA:HB2  | 2.20                     | 0.41              |
| 2:Q:413:ASP:C    | 2:Q:414:ARG:HD2  | 2.45                     | 0.41              |
| 2:R:478:LEU:HD12 | 2:R:523:PHE:CD2  | 2.55                     | 0.41              |
| 2:O:361:HIS:HD2  | 6:O:711:HOH:O    | 2.03                     | 0.41              |
| 2:Q:400:TRP:HA   | 2:Q:425:GLY:O    | 2.20                     | 0.41              |
| 2:Q:497:ASN:C    | 2:Q:497:ASN:ND2  | 2.69                     | 0.41              |
| 1:B:39:LEU:HD11  | 1:B:93:GLY:HA3   | 2.01                     | 0.41              |
| 1:D:41:LYS:HD2   | 1:D:87:ASN:O     | 2.19                     | 0.41              |
| 1:D:51:LEU:HD12  | 1:D:106:LEU:HD23 | 2.03                     | 0.41              |
| 1:D:131:PHE:CE2  | 1:D:138:HIS:HB3  | 2.55                     | 0.41              |
| 1:E:158:LEU:HD12 | 1:E:161:ILE:HD12 | 2.02                     | 0.41              |
| 1:F:19:ILE:HD13  | 1:F:19:ILE:HG21  | 1.79                     | 0.41              |
| 1:D:100:ASP:CG   | 1:D:101:ALA:N    | 2.79                     | 0.41              |
| 1:E:157:VAL:O    | 1:E:160:LEU:HB2  | 2.21                     | 0.41              |
| 2:Q:356:PHE:HD1  | 2:Q:428:ARG:HD3  | 1.86                     | 0.41              |
| 2:R:497:ASN:HD21 | 2:R:499:GLU:HB2  | 1.85                     | 0.41              |
| 1:C:5:LEU:O      | 2:O:387:GLN:HG2  | 2.20                     | 0.41              |
| 2:M:447:TYR:HB2  | 2:M:448:PRO:HD2  | 2.03                     | 0.41              |
| 2:M:447:TYR:OH   | 5:M:550:IHB:C5   | 2.68                     | 0.41              |
| 2:O:304:ASP:HB2  | 2:O:343:ILE:HB   | 2.03                     | 0.41              |
| 1:D:64:ARG:HD3   | 1:D:99:PHE:O     | 2.20                     | 0.41              |
| 1:D:123:ALA:O    | 1:D:124:PRO:C    | 2.64                     | 0.41              |
| 2:M:451:ASN:HB3  | 2:M:455:ASP:OD2  | 2.21                     | 0.41              |
| 2:M:478:LEU:HD23 | 2:M:478:LEU:C    | 2.46                     | 0.41              |
| 1:B:3:GLU:OE1    | 1:B:3:GLU:CA     | 2.69                     | 0.41              |
| 2:N:516:MET:HE3  | 2:N:516:MET:HB3  | 1.62                     | 0.41              |
| 1:D:24:GLU:O     | 1:D:27:GLY:CA    | 2.69                     | 0.41              |
| 5:P:550:IHB:H2   | 6:P:749:HOH:O    | 2.19                     | 0.41              |
| 1:E:19:ILE:HD13  | 1:E:19:ILE:HG21  | 1.80                     | 0.41              |
| 1:E:36:TRP:HA    | 1:E:36:TRP:CE3   | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:65:ASP:OD2   | 1:E:133:ARG:HD3  | 2.21                     | 0.41              |
| 2:Q:495:ILE:CG2  | 2:Q:500:ALA:HB3  | 2.50                     | 0.41              |
| 2:O:372:LEU:HA   | 2:O:373:PRO:HD3  | 1.91                     | 0.41              |
| 1:F:25:ALA:C     | 1:F:27:GLY:N     | 2.79                     | 0.41              |
| 2:M:519:LEU:HD11 | 2:P:485:LEU:HD11 | 2.03                     | 0.40              |
| 1:B:58:GLY:CA    | 1:B:190:GLN:HB3  | 2.51                     | 0.40              |
| 2:N:356:PHE:CD1  | 2:N:428:ARG:HD3  | 2.55                     | 0.40              |
| 1:C:35:ILE:HG21  | 1:C:92:PHE:CE2   | 2.54                     | 0.40              |
| 1:E:50:LEU:O     | 1:E:182:ALA:HA   | 2.21                     | 0.40              |
| 2:M:316:HIS:HB3  | 2:M:317:PRO:HD2  | 2.03                     | 0.40              |
| 2:M:448:PRO:HB2  | 2:P:516:MET:HA   | 2.03                     | 0.40              |
| 1:B:25:ALA:C     | 1:B:27:GLY:N     | 2.77                     | 0.40              |
| 2:N:497:ASN:HD22 | 2:N:498:PRO:N    | 2.19                     | 0.40              |
| 1:E:19:ILE:HG21  | 2:Q:410:HIS:HB2  | 2.03                     | 0.40              |
| 2:Q:408:TYR:HE1  | 2:Q:447:TYR:CE2  | 2.38                     | 0.40              |
| 1:F:131:PHE:CD2  | 1:F:138:HIS:HB3  | 2.56                     | 0.40              |
| 2:R:306:SER:CB   | 2:R:530:GLN:HE21 | 2.34                     | 0.40              |
| 1:A:157:VAL:O    | 1:A:160:LEU:HB2  | 2.22                     | 0.40              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:HE22 | 1.83                     | 0.40              |
| 1:F:52:LEU:C     | 1:F:52:LEU:HD22  | 2.47                     | 0.40              |
| 1:A:78:GLU:HG2   | 2:M:301:PRO:HG2  | 2.03                     | 0.40              |
| 1:A:98:THR:HB    | 1:A:100:ASP:CG   | 2.46                     | 0.40              |
| 1:C:41:LYS:NZ    | 1:C:86:GLU:O     | 2.42                     | 0.40              |
| 2:O:390:LYS:HD3  | 6:O:732:HOH:O    | 2.20                     | 0.40              |
| 2:O:486:ILE:HB   | 2:O:487:PRO:HD3  | 2.03                     | 0.40              |
| 1:D:19:ILE:O     | 2:P:426:VAL:HG21 | 2.21                     | 0.40              |
| 2:P:314:ASN:OD1  | 2:P:318:LYS:HE2  | 2.22                     | 0.40              |
| 2:Q:495:ILE:HG21 | 2:Q:500:ALA:HB3  | 2.02                     | 0.40              |
| 1:F:177:VAL:O    | 1:F:180:LYS:HB3  | 2.21                     | 0.40              |
| 2:R:359:HIS:O    | 2:R:366:ASN:HB3  | 2.21                     | 0.40              |
| 1:A:98:THR:O     | 1:A:102:GLY:HA2  | 2.22                     | 0.40              |
| 1:C:98:THR:C     | 1:C:100:ASP:N    | 2.77                     | 0.40              |
| 2:O:484:PRO:O    | 2:O:488:MET:HE3  | 2.22                     | 0.40              |
| 2:P:350:ASN:OD1  | 2:P:352:SER:HB2  | 2.22                     | 0.40              |
| 1:F:35:ILE:HG21  | 1:F:92:PHE:HE2   | 1.85                     | 0.40              |
| 2:R:356:PHE:HD1  | 2:R:428:ARG:HD3  | 1.86                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:C:46:GLY:O   | 1:D:150:GLN:OE1[3_554] | 1.84                     | 0.36              |
| 6:Q:1200:HOH:O | 6:Q:1200:HOH:O[2_555]  | 2.10                     | 0.10              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 198/200 (99%)   | 192 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | B     | 198/200 (99%)   | 191 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | C     | 198/200 (99%)   | 191 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | D     | 198/200 (99%)   | 188 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 1   | E     | 198/200 (99%)   | 193 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | F     | 198/200 (99%)   | 192 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 2   | M     | 229/238 (96%)   | 222 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 2   | N     | 229/238 (96%)   | 220 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 2   | O     | 229/238 (96%)   | 220 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 2   | P     | 229/238 (96%)   | 221 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 2   | Q     | 229/238 (96%)   | 218 (95%)  | 11 (5%) | 0        | 100         | 100 |
| 2   | R     | 229/238 (96%)   | 221 (96%)  | 7 (3%)  | 1 (0%)   | 30          | 33  |
| All | All   | 2562/2628 (98%) | 2469 (96%) | 92 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 535 | PHE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 162/163 (99%)   | 154 (95%)  | 8 (5%)   | 22          | 27 |
| 1   | B     | 162/163 (99%)   | 156 (96%)  | 6 (4%)   | 30          | 39 |
| 1   | C     | 162/163 (99%)   | 152 (94%)  | 10 (6%)  | 16          | 18 |
| 1   | D     | 162/163 (99%)   | 155 (96%)  | 7 (4%)   | 26          | 33 |
| 1   | E     | 162/163 (99%)   | 154 (95%)  | 8 (5%)   | 22          | 27 |
| 1   | F     | 162/163 (99%)   | 154 (95%)  | 8 (5%)   | 22          | 27 |
| 2   | M     | 196/202 (97%)   | 187 (95%)  | 9 (5%)   | 24          | 30 |
| 2   | N     | 196/202 (97%)   | 185 (94%)  | 11 (6%)  | 19          | 22 |
| 2   | O     | 196/202 (97%)   | 187 (95%)  | 9 (5%)   | 24          | 30 |
| 2   | P     | 196/202 (97%)   | 187 (95%)  | 9 (5%)   | 24          | 30 |
| 2   | Q     | 196/202 (97%)   | 188 (96%)  | 8 (4%)   | 27          | 35 |
| 2   | R     | 196/202 (97%)   | 188 (96%)  | 8 (4%)   | 27          | 35 |
| All | All   | 2148/2190 (98%) | 2047 (95%) | 101 (5%) | 23          | 29 |

All (101) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 91  | SER  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 114 | VAL  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 192 | GLU  |
| 2   | M     | 344 | SER  |
| 2   | M     | 395 | THR  |
| 2   | M     | 416 | LEU  |
| 2   | M     | 433 | SER  |
| 2   | M     | 434 | ASP  |
| 2   | M     | 440 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 478 | LEU  |
| 2   | M     | 507 | LYS  |
| 2   | M     | 534 | HIS  |
| 1   | B     | 4   | LEU  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 52  | LEU  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 165 | GLN  |
| 2   | N     | 364 | LEU  |
| 2   | N     | 372 | LEU  |
| 2   | N     | 395 | THR  |
| 2   | N     | 399 | MET  |
| 2   | N     | 411 | LYS  |
| 2   | N     | 416 | LEU  |
| 2   | N     | 433 | SER  |
| 2   | N     | 440 | ARG  |
| 2   | N     | 442 | ILE  |
| 2   | N     | 478 | LEU  |
| 2   | N     | 507 | LYS  |
| 1   | C     | 4   | LEU  |
| 1   | C     | 19  | ILE  |
| 1   | C     | 38  | ARG  |
| 1   | C     | 50  | LEU  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 66  | SER  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 106 | LEU  |
| 1   | C     | 158 | LEU  |
| 1   | C     | 165 | GLN  |
| 2   | O     | 372 | LEU  |
| 2   | O     | 395 | THR  |
| 2   | O     | 411 | LYS  |
| 2   | O     | 416 | LEU  |
| 2   | O     | 434 | ASP  |
| 2   | O     | 465 | ILE  |
| 2   | O     | 473 | LYS  |
| 2   | O     | 507 | LYS  |
| 2   | O     | 534 | HIS  |
| 1   | D     | 4   | LEU  |
| 1   | D     | 19  | ILE  |
| 1   | D     | 42  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 52  | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 114 | VAL  |
| 1   | D     | 165 | GLN  |
| 2   | P     | 364 | LEU  |
| 2   | P     | 395 | THR  |
| 2   | P     | 411 | LYS  |
| 2   | P     | 416 | LEU  |
| 2   | P     | 433 | SER  |
| 2   | P     | 440 | ARG  |
| 2   | P     | 478 | LEU  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 534 | HIS  |
| 1   | E     | 4   | LEU  |
| 1   | E     | 38  | ARG  |
| 1   | E     | 49  | ILE  |
| 1   | E     | 52  | LEU  |
| 1   | E     | 66  | SER  |
| 1   | E     | 143 | LEU  |
| 1   | E     | 165 | GLN  |
| 1   | E     | 181 | THR  |
| 2   | Q     | 343 | ILE  |
| 2   | Q     | 372 | LEU  |
| 2   | Q     | 395 | THR  |
| 2   | Q     | 411 | LYS  |
| 2   | Q     | 416 | LEU  |
| 2   | Q     | 442 | ILE  |
| 2   | Q     | 478 | LEU  |
| 2   | Q     | 507 | LYS  |
| 1   | F     | 4   | LEU  |
| 1   | F     | 30  | THR  |
| 1   | F     | 49  | ILE  |
| 1   | F     | 50  | LEU  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 66  | SER  |
| 1   | F     | 100 | ASP  |
| 1   | F     | 165 | GLN  |
| 2   | R     | 352 | SER  |
| 2   | R     | 372 | LEU  |
| 2   | R     | 395 | THR  |
| 2   | R     | 411 | LYS  |
| 2   | R     | 416 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 428 | ARG  |
| 2   | R     | 442 | ILE  |
| 2   | R     | 465 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 136 | ASN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 165 | GLN  |
| 2   | M     | 359 | HIS  |
| 2   | M     | 361 | HIS  |
| 2   | M     | 412 | ASN  |
| 2   | M     | 497 | ASN  |
| 2   | M     | 503 | GLN  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 165 | GLN  |
| 2   | N     | 361 | HIS  |
| 2   | N     | 497 | ASN  |
| 2   | N     | 503 | GLN  |
| 1   | C     | 11  | GLN  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 165 | GLN  |
| 2   | O     | 361 | HIS  |
| 2   | O     | 412 | ASN  |
| 2   | O     | 497 | ASN  |
| 2   | O     | 503 | GLN  |
| 2   | O     | 514 | ASN  |
| 2   | O     | 530 | GLN  |
| 1   | D     | 59  | ASN  |
| 1   | D     | 163 | GLN  |
| 1   | D     | 165 | GLN  |
| 2   | P     | 305 | ASN  |
| 2   | P     | 361 | HIS  |
| 2   | P     | 394 | ASN  |
| 2   | P     | 412 | ASN  |
| 2   | P     | 422 | ASN  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 514 | ASN  |
| 1   | E     | 11  | GLN  |
| 1   | E     | 107 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 163 | GLN  |
| 1   | E     | 165 | GLN  |
| 2   | Q     | 334 | GLN  |
| 2   | Q     | 361 | HIS  |
| 2   | Q     | 412 | ASN  |
| 2   | Q     | 497 | ASN  |
| 2   | Q     | 503 | GLN  |
| 1   | F     | 11  | GLN  |
| 1   | F     | 163 | GLN  |
| 1   | F     | 165 | GLN  |
| 2   | R     | 359 | HIS  |
| 2   | R     | 361 | HIS  |
| 2   | R     | 412 | ASN  |
| 2   | R     | 422 | ASN  |
| 2   | R     | 497 | ASN  |
| 2   | R     | 503 | GLN  |
| 2   | R     | 530 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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 |
| 5   | IHB  | N     | 550 | 3    | 11,11,11     | 1.75 | 2 (18%)  | 15,15,15    | 0.94 | 1 (6%)   |
| 4   | BME  | N     | 601 | 2    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.08 | 0        |
| 4   | BME  | M     | 601 | 2    | 3,3,3        | 0.31 | 0        | 2,2,2       | 0.28 | 0        |
| 5   | IHB  | O     | 551 | -    | 11,11,11     | 1.67 | 2 (18%)  | 15,15,15    | 1.08 | 2 (13%)  |
| 5   | IHB  | M     | 550 | 3    | 11,11,11     | 1.67 | 3 (27%)  | 15,15,15    | 0.63 | 0        |
| 5   | IHB  | M     | 551 | -    | 11,11,11     | 1.51 | 3 (27%)  | 15,15,15    | 1.04 | 1 (6%)   |
| 5   | IHB  | O     | 550 | 3    | 11,11,11     | 1.64 | 3 (27%)  | 15,15,15    | 0.88 | 0        |
| 5   | IHB  | P     | 550 | 3    | 11,11,11     | 1.81 | 2 (18%)  | 15,15,15    | 0.79 | 0        |
| 5   | IHB  | R     | 550 | 3    | 11,11,11     | 1.44 | 2 (18%)  | 15,15,15    | 0.77 | 0        |
| 4   | BME  | Q     | 601 | 2    | 3,3,3        | 0.50 | 0        | 2,2,2       | 0.29 | 0        |
| 4   | BME  | O     | 601 | 2    | 3,3,3        | 0.45 | 0        | 2,2,2       | 0.35 | 0        |
| 4   | BME  | P     | 601 | 2    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.49 | 0        |
| 5   | IHB  | P     | 551 | -    | 11,11,11     | 1.92 | 4 (36%)  | 15,15,15    | 1.23 | 3 (20%)  |
| 5   | IHB  | Q     | 551 | -    | 11,11,11     | 1.73 | 4 (36%)  | 15,15,15    | 1.06 | 1 (6%)   |
| 4   | BME  | R     | 601 | 2    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.18 | 0        |
| 5   | IHB  | Q     | 550 | 3    | 11,11,11     | 1.88 | 2 (18%)  | 15,15,15    | 0.67 | 0        |
| 5   | IHB  | R     | 551 | -    | 11,11,11     | 1.57 | 2 (18%)  | 15,15,15    | 1.23 | 3 (20%)  |
| 5   | IHB  | N     | 551 | -    | 11,11,11     | 1.38 | 1 (9%)   | 15,15,15    | 1.25 | 3 (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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 5   | IHB  | N     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | N     | 601 | 2    | -       | 0/1/1/1  | -       |
| 4   | BME  | M     | 601 | 2    | -       | 1/1/1/1  | -       |
| 5   | IHB  | O     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | M     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | M     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | O     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | P     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | R     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | Q     | 601 | 2    | -       | 1/1/1/1  | -       |
| 4   | BME  | O     | 601 | 2    | -       | 0/1/1/1  | -       |
| 4   | BME  | P     | 601 | 2    | -       | 1/1/1/1  | -       |
| 5   | IHB  | P     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | Q     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | R     | 601 | 2    | -       | 0/1/1/1  | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 5   | IHB  | Q     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | R     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | IHB  | N     | 551 | -    | -       | 0/4/4/4  | 0/1/1/1 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | P     | 550 | IHB  | C3-I3 | -4.63 | 2.00        | 2.10     |
| 5   | O     | 551 | IHB  | C3-I3 | -4.24 | 2.01        | 2.10     |
| 5   | Q     | 550 | IHB  | C3-I3 | -4.08 | 2.01        | 2.10     |
| 5   | N     | 550 | IHB  | C1-C7 | 3.81  | 1.57        | 1.49     |
| 5   | O     | 550 | IHB  | C3-I3 | -3.61 | 2.02        | 2.10     |
| 5   | P     | 551 | IHB  | C3-I3 | -3.61 | 2.02        | 2.10     |
| 5   | M     | 551 | IHB  | C3-I3 | -3.56 | 2.02        | 2.10     |
| 5   | M     | 550 | IHB  | C3-I3 | -3.47 | 2.02        | 2.10     |
| 5   | R     | 551 | IHB  | C3-I3 | -3.47 | 2.02        | 2.10     |
| 5   | Q     | 550 | IHB  | C1-C7 | 3.36  | 1.56        | 1.49     |
| 5   | N     | 550 | IHB  | C3-I3 | -3.34 | 2.03        | 2.10     |
| 5   | Q     | 551 | IHB  | C1-C7 | 3.14  | 1.56        | 1.49     |
| 5   | P     | 551 | IHB  | C1-C7 | 2.99  | 1.55        | 1.49     |
| 5   | R     | 550 | IHB  | C3-I3 | -2.98 | 2.03        | 2.10     |
| 5   | P     | 551 | IHB  | C6-C1 | 2.82  | 1.43        | 1.39     |
| 5   | M     | 550 | IHB  | C1-C7 | 2.79  | 1.55        | 1.49     |
| 5   | Q     | 551 | IHB  | C3-I3 | -2.69 | 2.04        | 2.10     |
| 5   | P     | 550 | IHB  | C1-C7 | 2.52  | 1.54        | 1.49     |
| 5   | O     | 550 | IHB  | C1-C7 | 2.50  | 1.54        | 1.49     |
| 5   | O     | 550 | IHB  | C6-C1 | 2.41  | 1.43        | 1.39     |
| 5   | P     | 551 | IHB  | O2-C7 | -2.36 | 1.23        | 1.30     |
| 5   | N     | 551 | IHB  | O2-C7 | -2.33 | 1.23        | 1.30     |
| 5   | Q     | 551 | IHB  | O2-C7 | -2.32 | 1.23        | 1.30     |
| 5   | R     | 550 | IHB  | C1-C7 | 2.29  | 1.54        | 1.49     |
| 5   | R     | 551 | IHB  | C1-C7 | 2.29  | 1.54        | 1.49     |
| 5   | M     | 550 | IHB  | C6-C1 | 2.24  | 1.42        | 1.39     |
| 5   | M     | 551 | IHB  | O2-C7 | -2.16 | 1.24        | 1.30     |
| 5   | M     | 551 | IHB  | C1-C7 | 2.12  | 1.54        | 1.49     |
| 5   | O     | 551 | IHB  | O2-C7 | -2.07 | 1.24        | 1.30     |
| 5   | Q     | 551 | IHB  | C6-C5 | 2.05  | 1.42        | 1.38     |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | Q     | 551 | IHB  | O2-C7-O1 | -2.79 | 117.35      | 123.35   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | N     | 550 | IHB  | C4-C3-I3 | -2.73 | 117.12      | 119.76   |
| 5   | P     | 551 | IHB  | O2-C7-O1 | -2.66 | 117.63      | 123.35   |
| 5   | M     | 551 | IHB  | O2-C7-C1 | 2.60  | 121.52      | 114.84   |
| 5   | P     | 551 | IHB  | O4-C4-C3 | 2.57  | 122.13      | 119.16   |
| 5   | R     | 551 | IHB  | O2-C7-C1 | 2.48  | 121.20      | 114.84   |
| 5   | N     | 551 | IHB  | C4-C3-I3 | 2.38  | 122.05      | 119.76   |
| 5   | R     | 551 | IHB  | O2-C7-O1 | -2.33 | 118.34      | 123.35   |
| 5   | P     | 551 | IHB  | O2-C7-C1 | 2.29  | 120.72      | 114.84   |
| 5   | N     | 551 | IHB  | C5-C4-C3 | 2.23  | 121.38      | 119.27   |
| 5   | N     | 551 | IHB  | O2-C7-O1 | -2.18 | 118.67      | 123.35   |
| 5   | O     | 551 | IHB  | O2-C7-O1 | -2.18 | 118.67      | 123.35   |
| 5   | R     | 551 | IHB  | O4-C4-C3 | 2.11  | 121.60      | 119.16   |
| 5   | O     | 551 | IHB  | O2-C7-C1 | 2.10  | 120.22      | 114.84   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | M     | 601 | BME  | O1-C1-C2-S2 |
| 4   | P     | 601 | BME  | O1-C1-C2-S2 |
| 4   | Q     | 601 | BME  | O1-C1-C2-S2 |

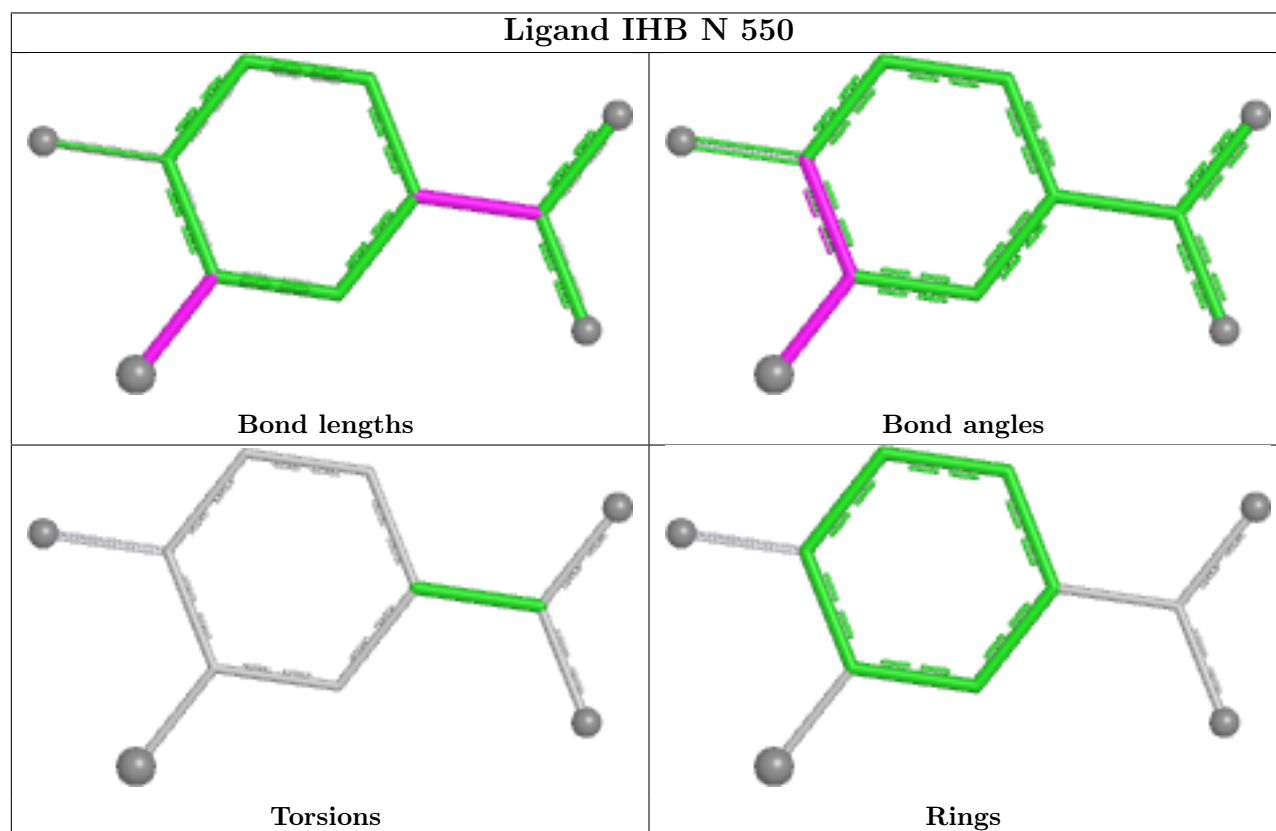
There are no ring outliers.

9 monomers are involved in 16 short contacts:

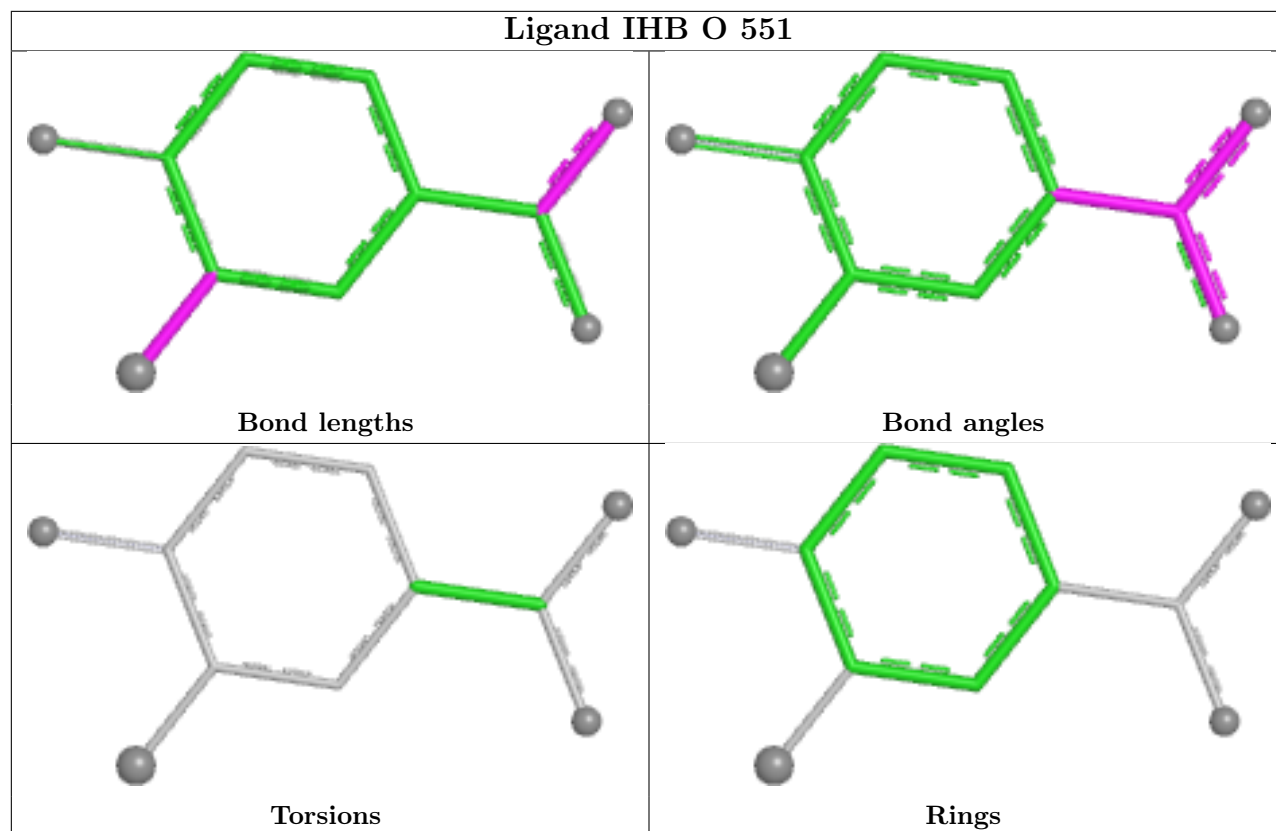
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | N     | 550 | IHB  | 2       | 0            |
| 4   | M     | 601 | BME  | 1       | 0            |
| 5   | M     | 550 | IHB  | 2       | 0            |
| 5   | O     | 550 | IHB  | 2       | 0            |
| 5   | P     | 550 | IHB  | 1       | 0            |
| 5   | R     | 550 | IHB  | 3       | 0            |
| 4   | Q     | 601 | BME  | 2       | 0            |
| 4   | O     | 601 | BME  | 1       | 0            |
| 5   | Q     | 550 | IHB  | 2       | 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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

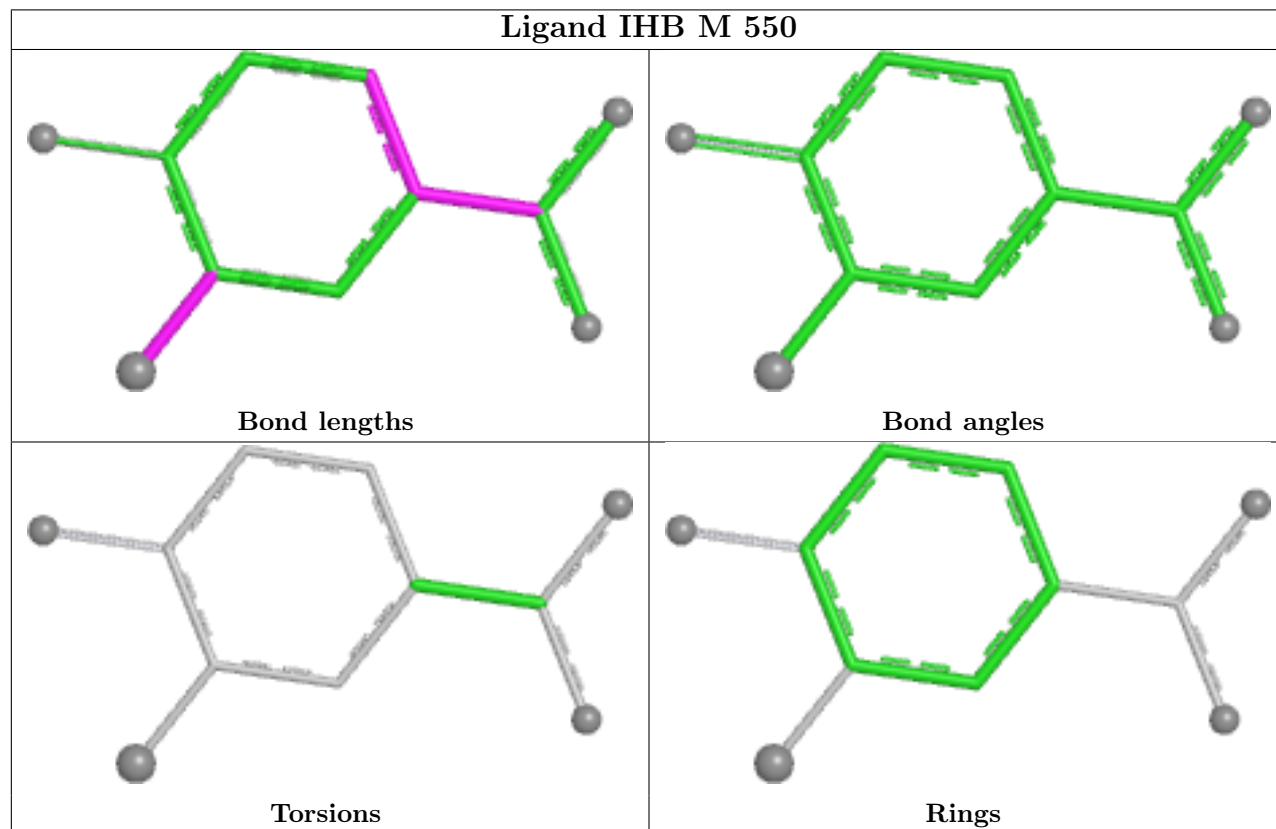
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



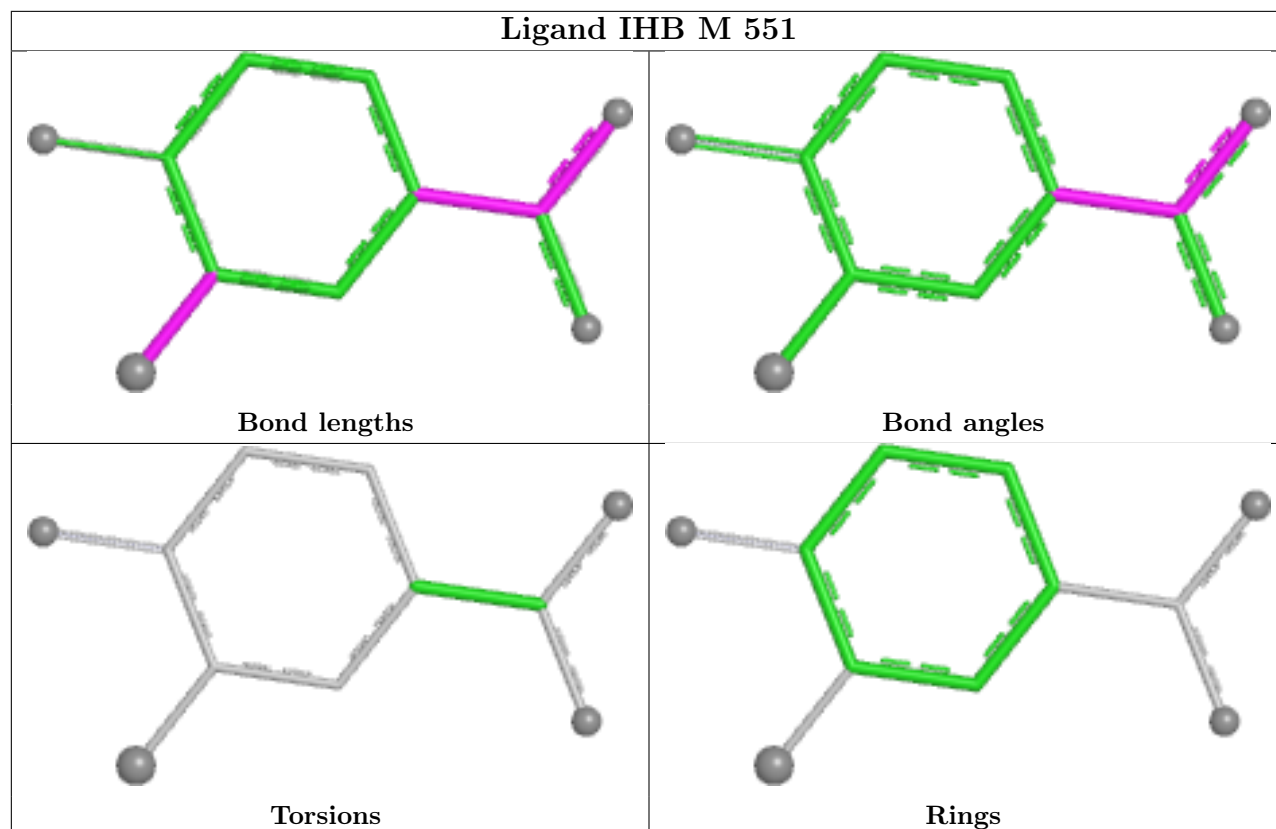
## Ligand IHB O 551



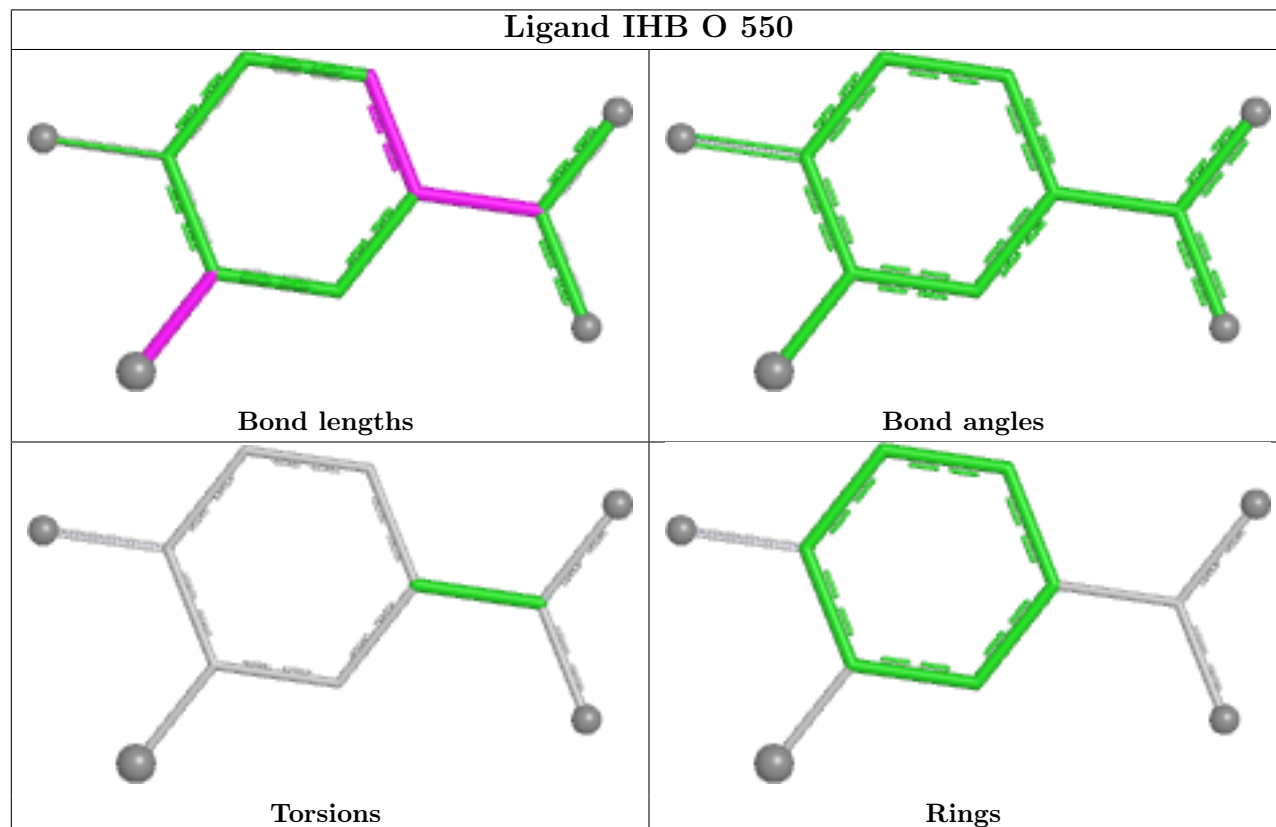
## Ligand IHB M 550



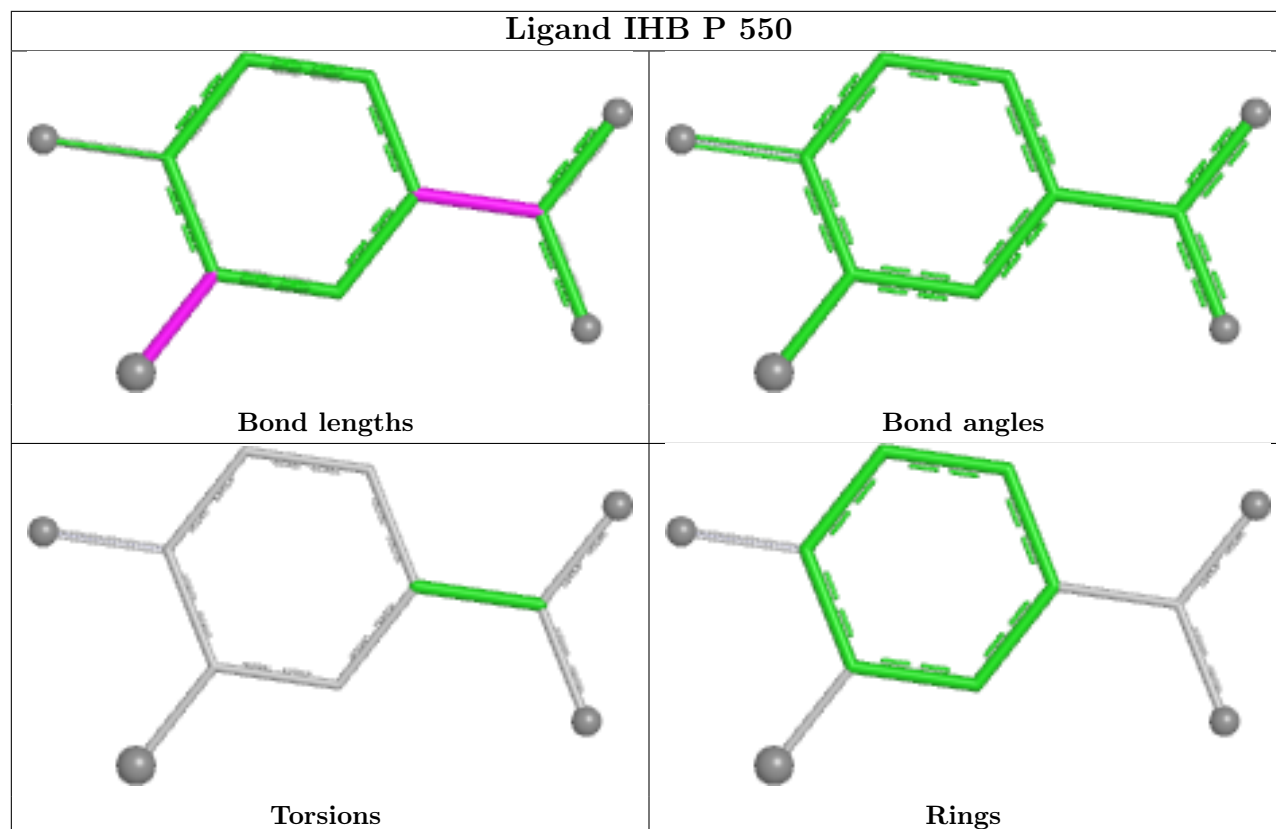
## Ligand IHB M 551



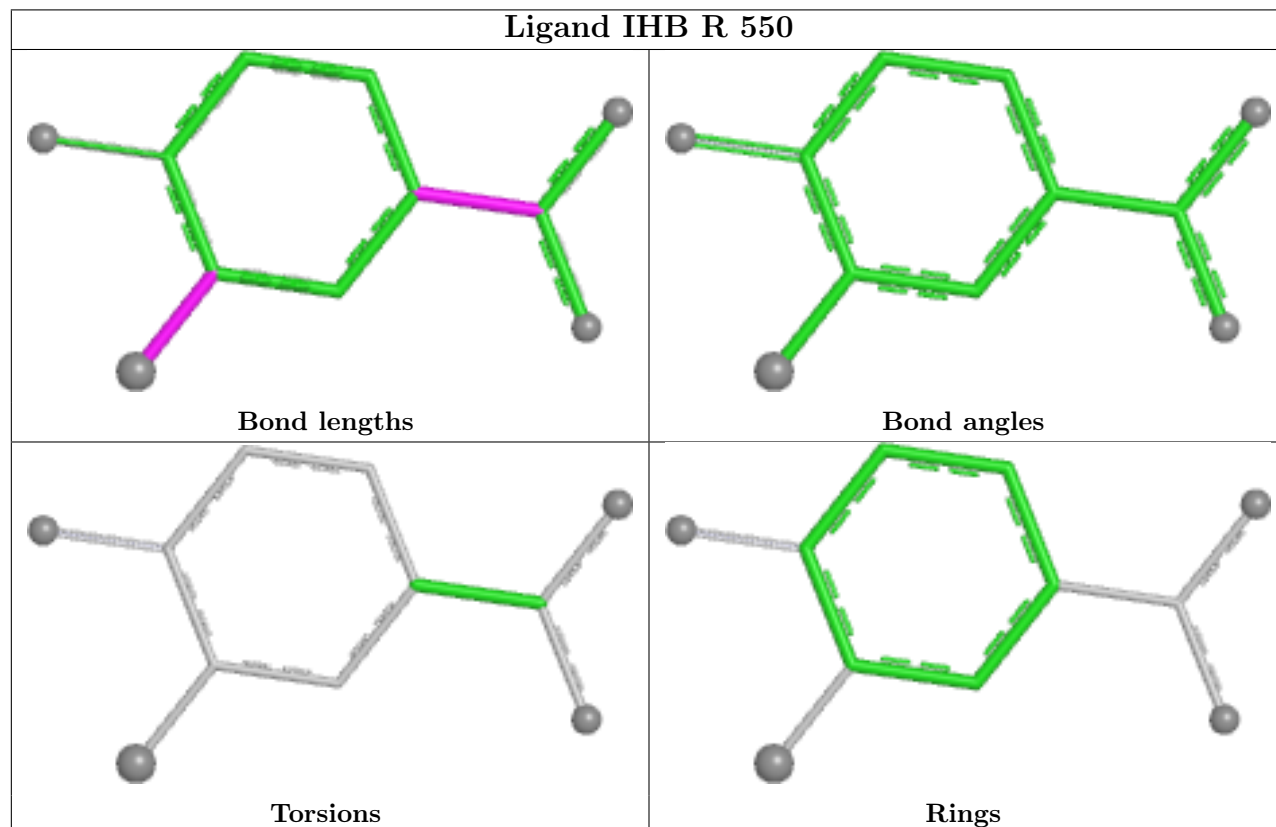
## Ligand IHB O 550



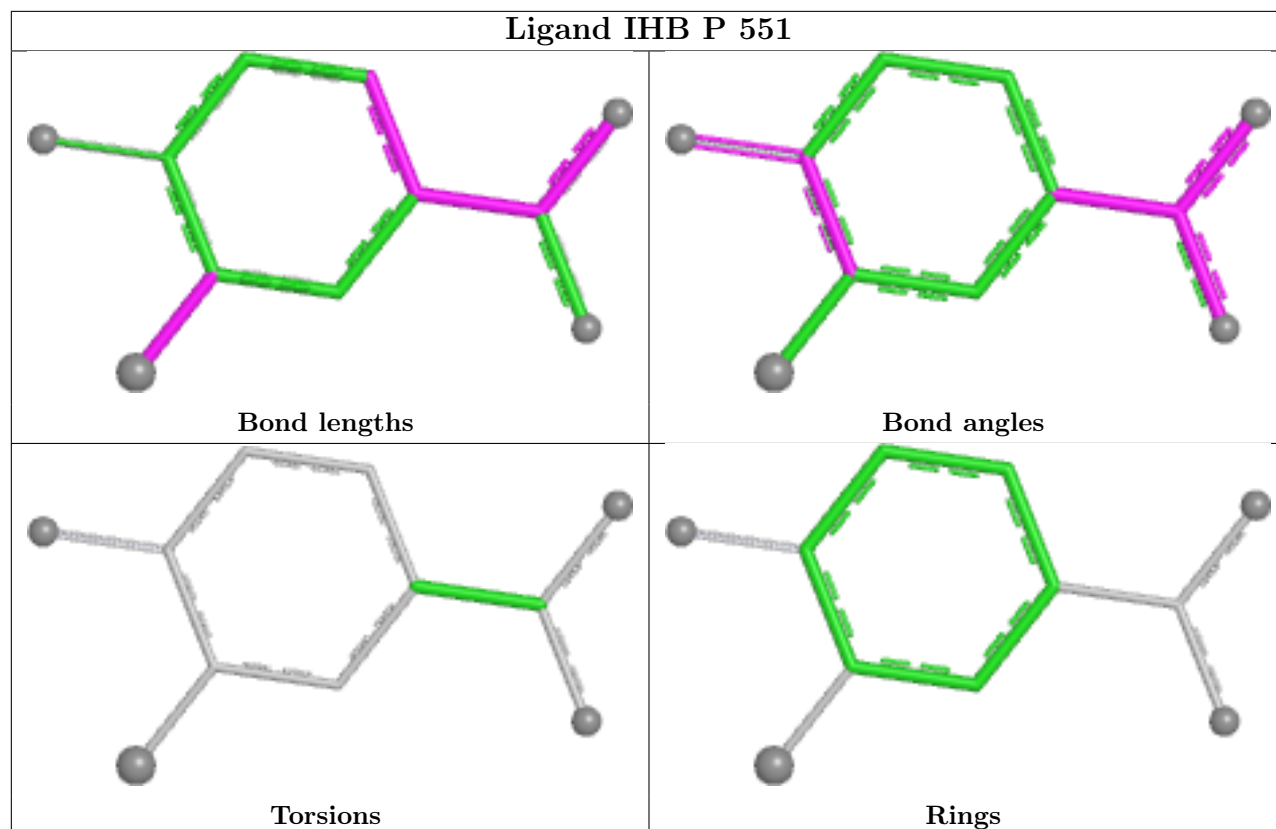
## Ligand IHB P 550



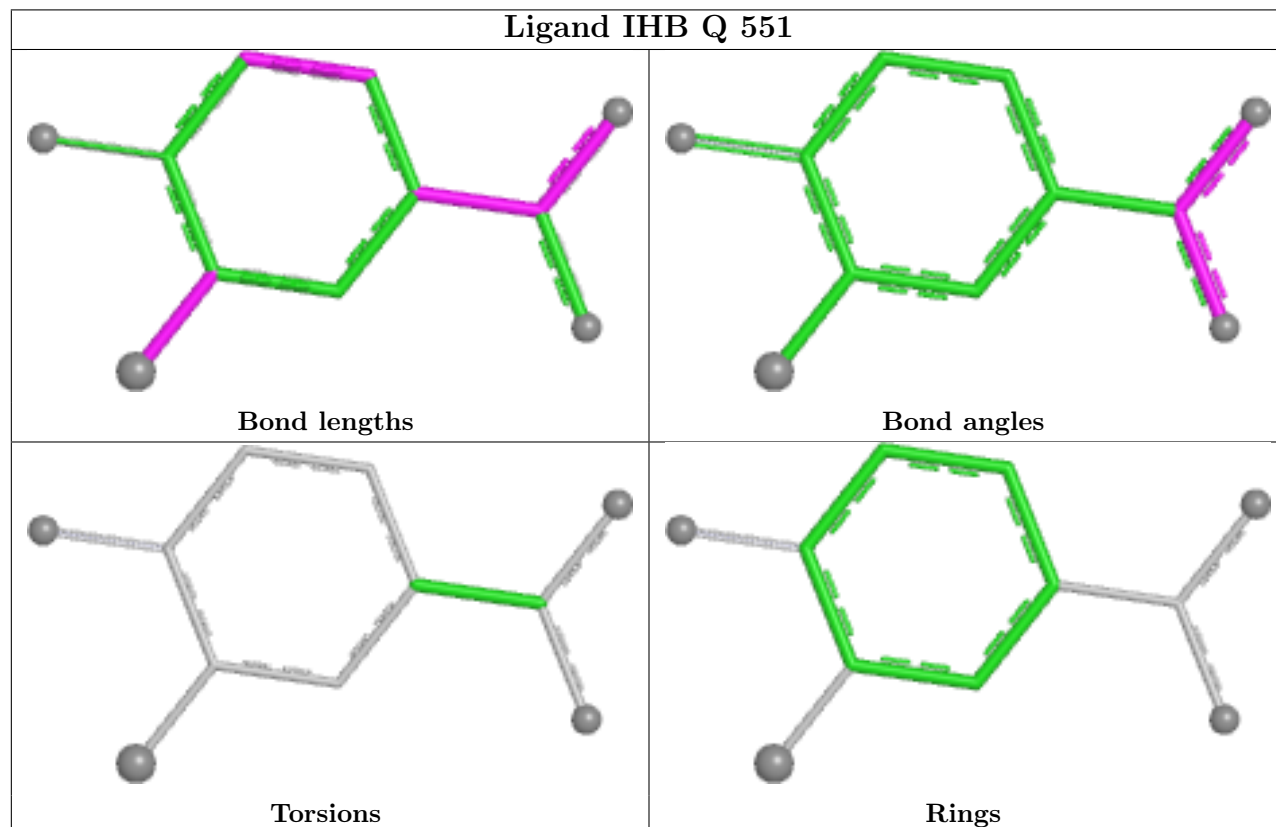
## Ligand IHB R 550



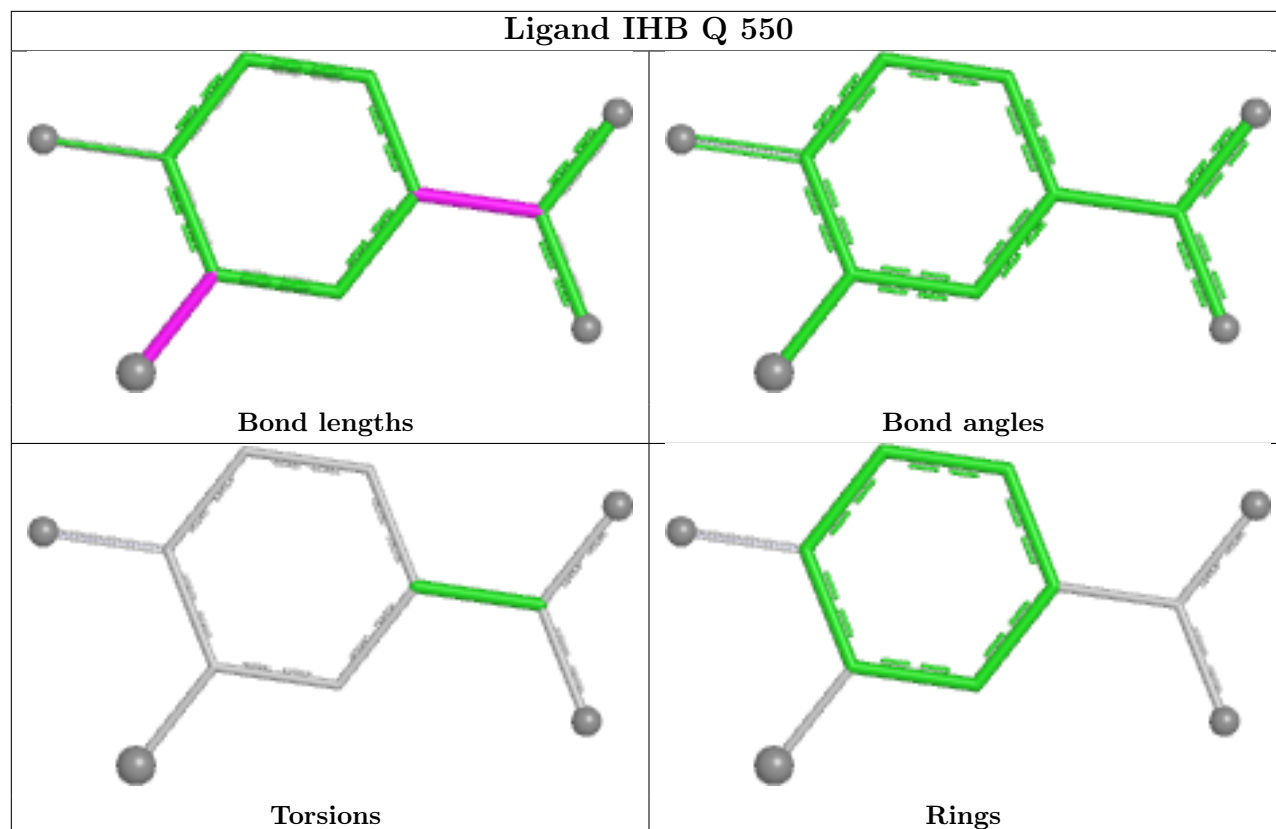
## Ligand IHB P 551



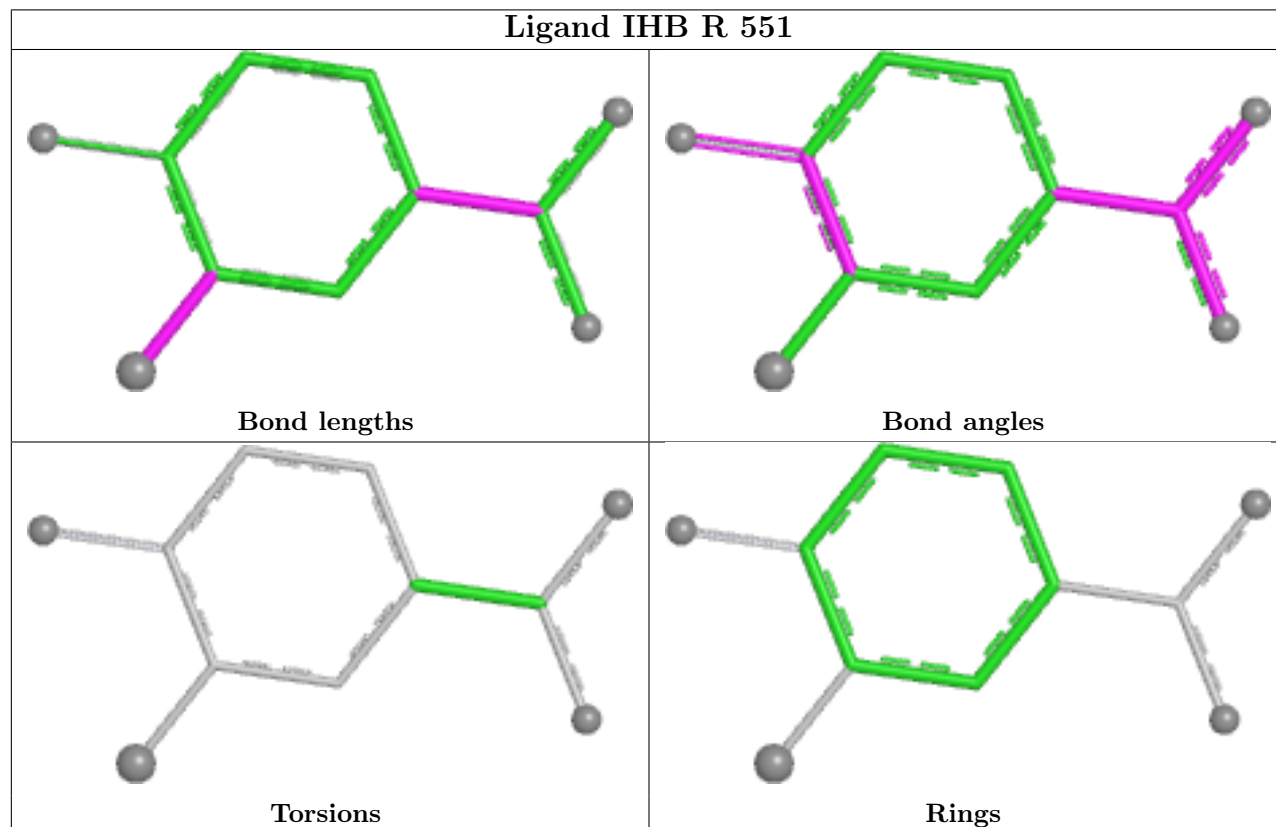
## Ligand IHB Q 551

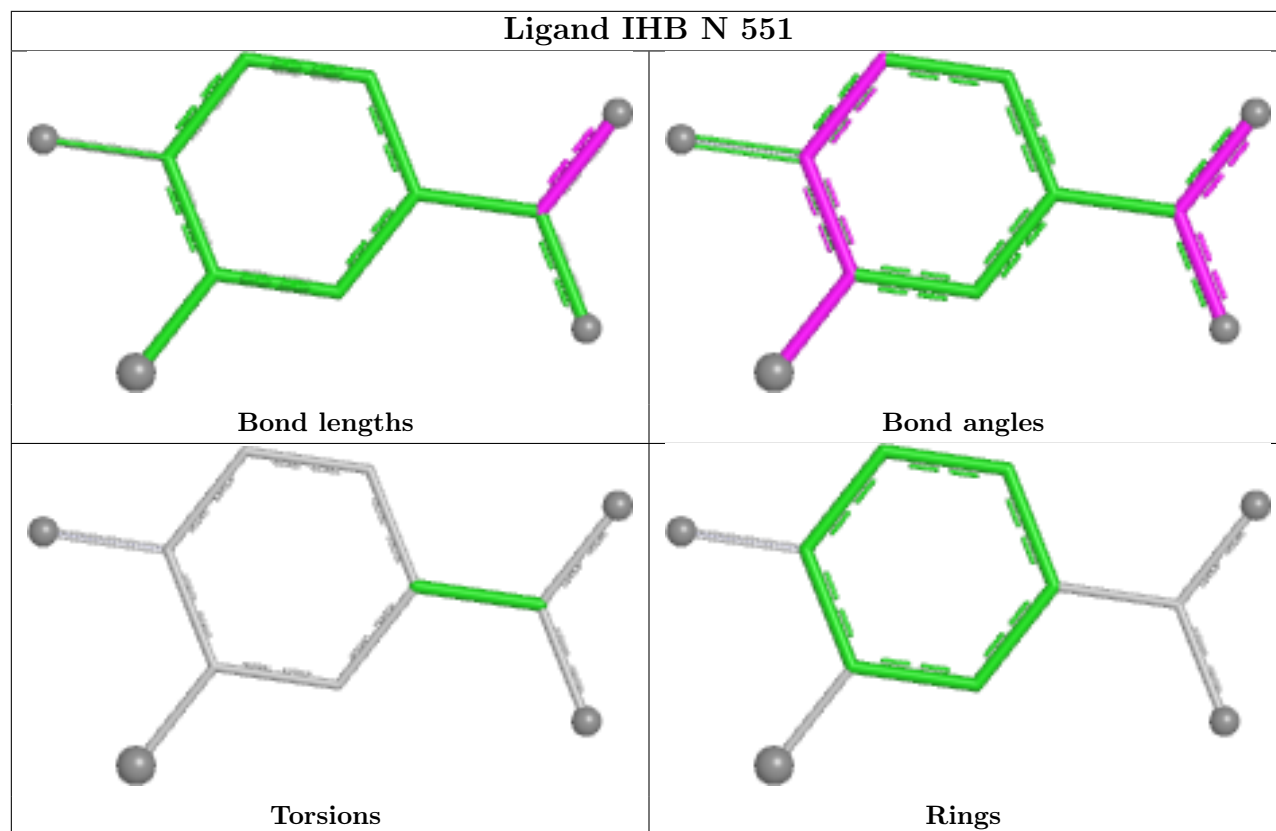


## Ligand IHB Q 550



## Ligand IHB R 551





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.