# Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 08:48 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2BRU |
| Title | : | Complex of the domain I and domain III of Escherichia coli transhydrogenase |
| Authors | : | Johansson, T.; Pedersen, A.; Leckner, J.; Karlsson, B.G. |
| Deposited on | : | 2005-05-11 |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

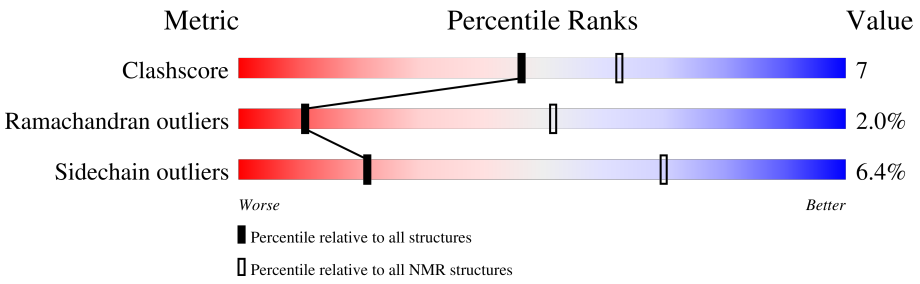
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 401 | 79% 12% 8% |
| 1 | B | 401 | 78% 13% 9% |
| 2 | C | 186 | 68% 20% • 10% |

# 2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:1000-A:1216, A:1224-A:1373, B:998-B:1215, B:1230-B:1376, C:20-C:186 (899) | 1.24 | 3 |

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

# 3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8268 atoms, of which 1440 are hydrogens and 0 are deuteriums.

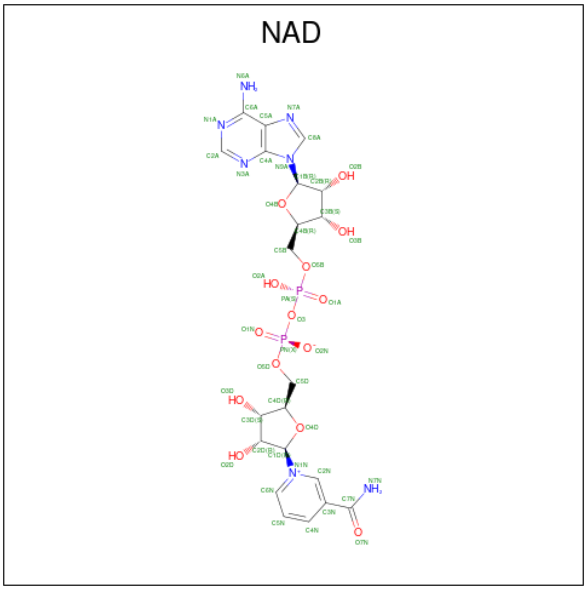
- Molecule 1 is a protein called NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 367 | 3314 | 1734 | 579 | 464 | 525 | 12 | 1 |
| 1 | B | 365 | 3311 | 1729 | 582 | 467 | 521 | 12 | 1 |

- Molecule 2 is a protein called NAD(P) TRANSHYDROGENASE SUBUNIT BETA.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 2 | C | 167 | 1536 | 809 | 264 | 215 | 242 | 6 | 0 |

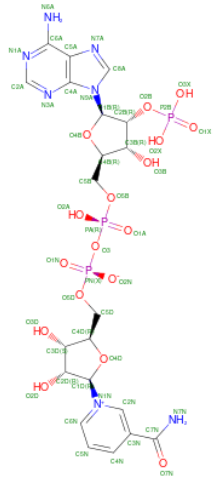
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).




| Mol | Chain | Residues | Atoms | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P |
| 3 | B | 1 | 52 | 21 | 8 | 7 | 14 | 2 |

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP



| Mol | Chain | Residues | Atoms | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P |
| 4 | C | 1 | 55 | 21 | 7 | 7 | 17 | 3 |

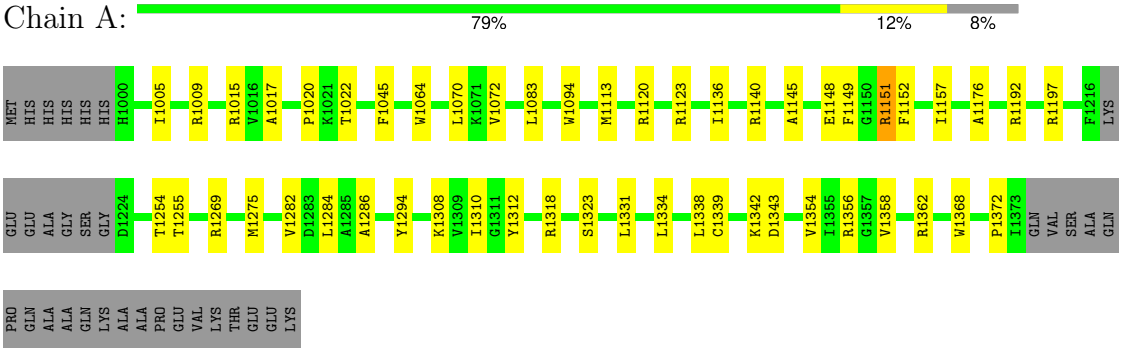
# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

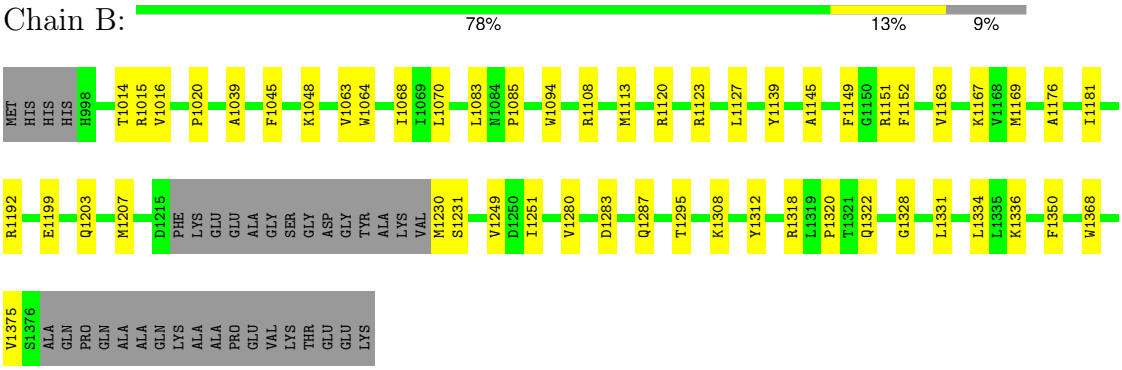
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



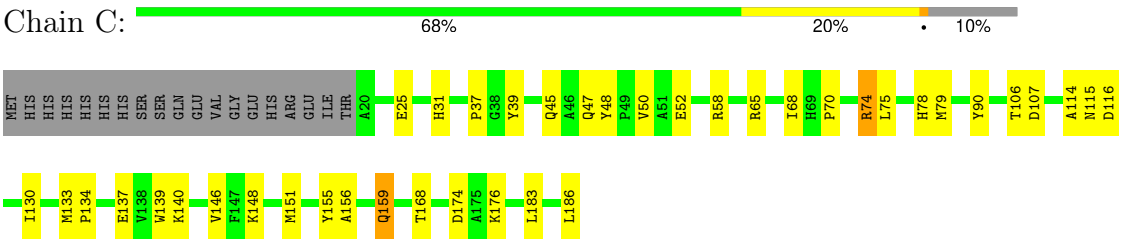

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:




• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:



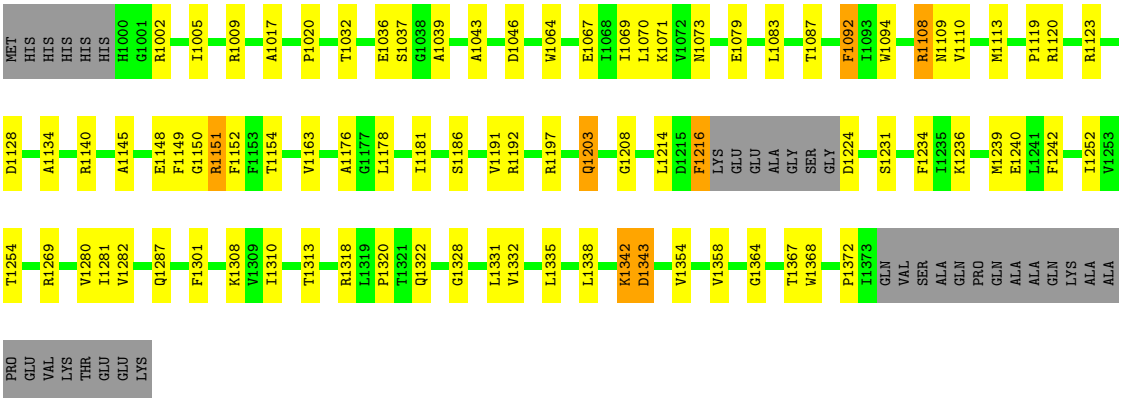
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 70% 19% • 8%

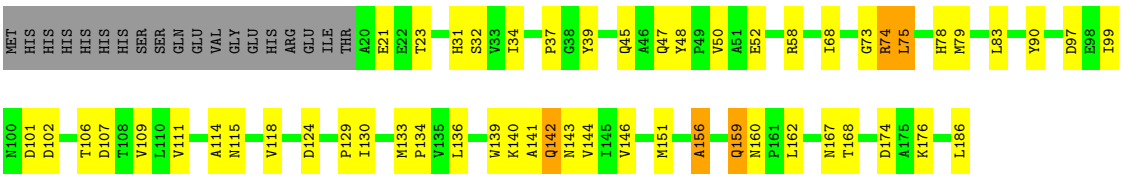



• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 68% 22% • 9%

• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

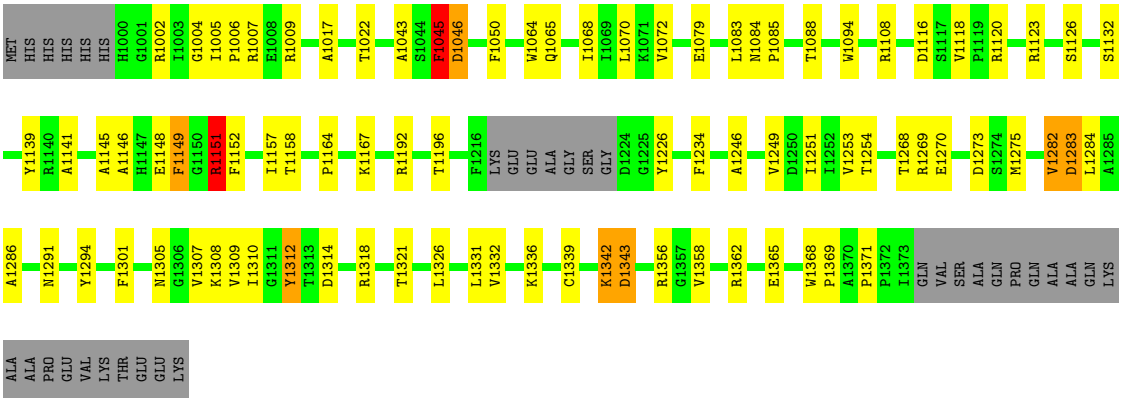
Chain C: 60% 27% • 10%



### 4.2.2 Score per residue for model 2

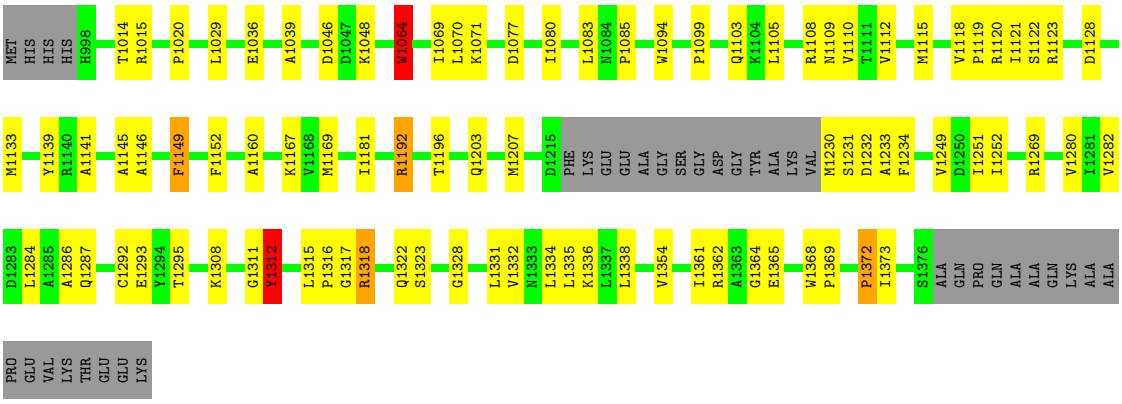
- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 70% 19% • 8%



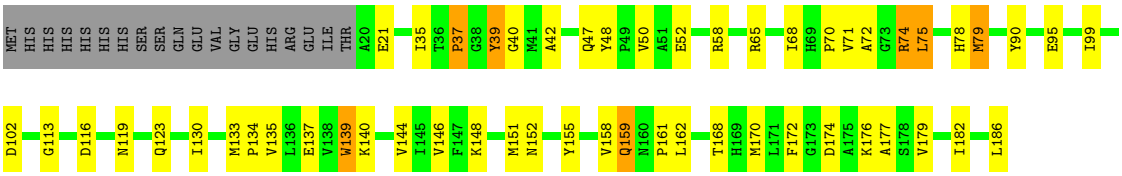

- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 69% 21% • 9%




- Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

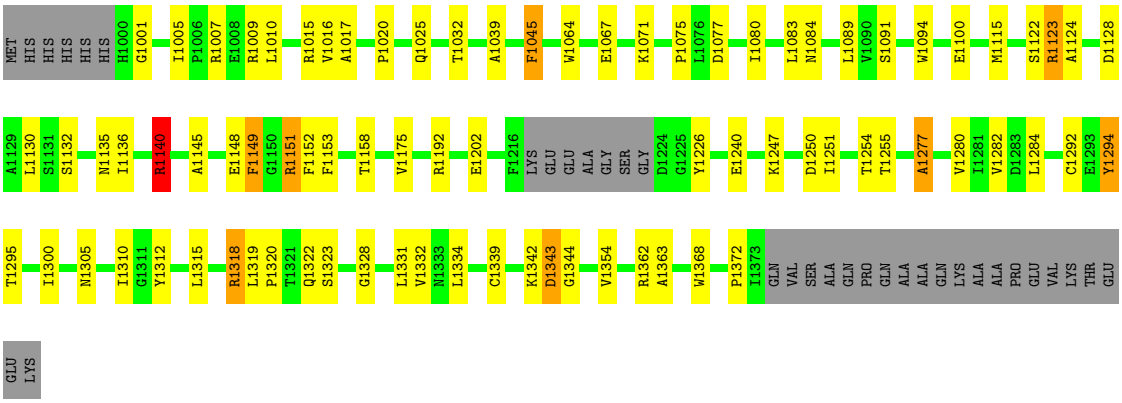
Chain C: 61% 25% • 10%




### 4.2.3 Score per residue for model 3 (medoid)

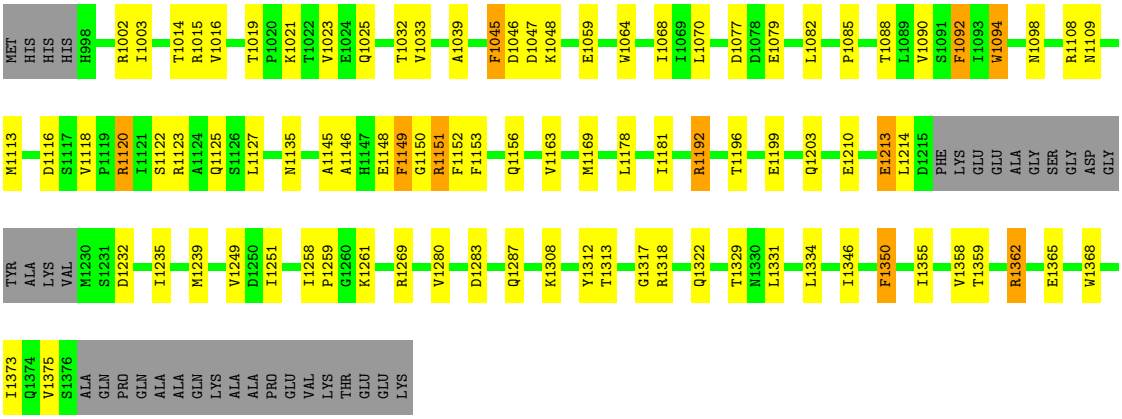
- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



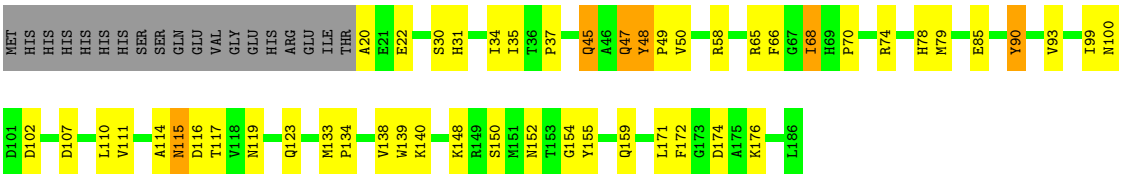

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:




• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

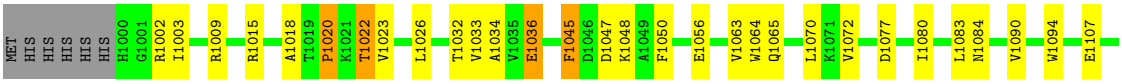
Chain C:




### 4.2.4 Score per residue for model 4

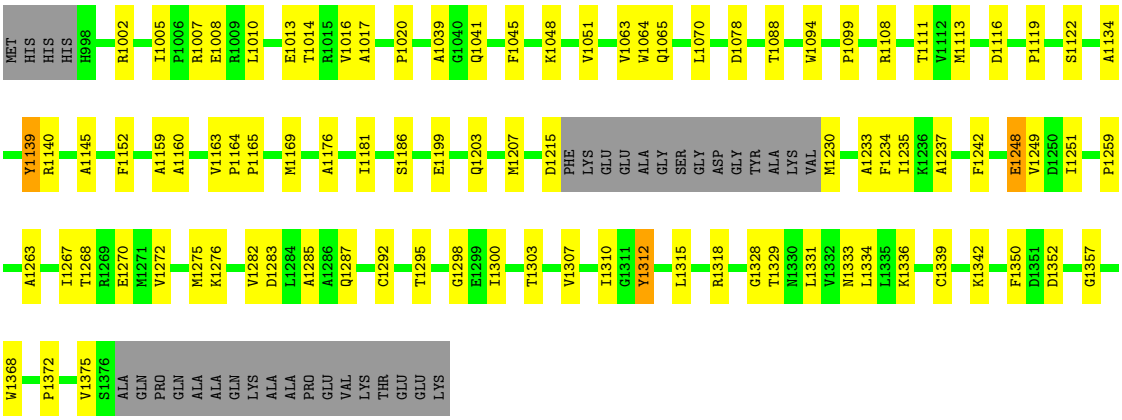
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



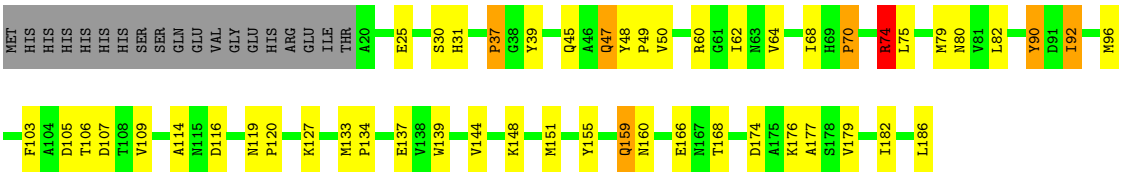
- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:




- Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

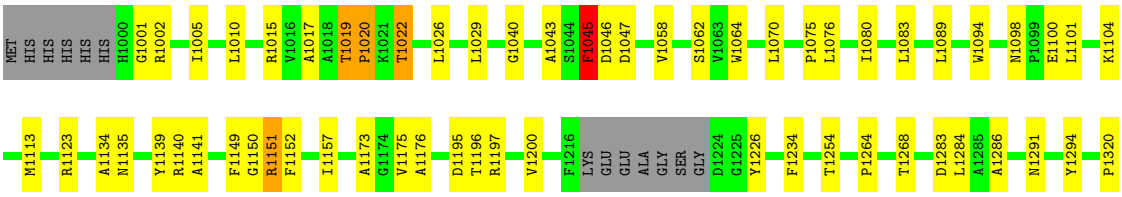
Chain C:

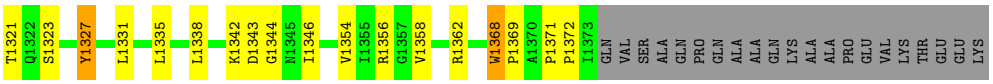



### 4.2.5 Score per residue for model 5

- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

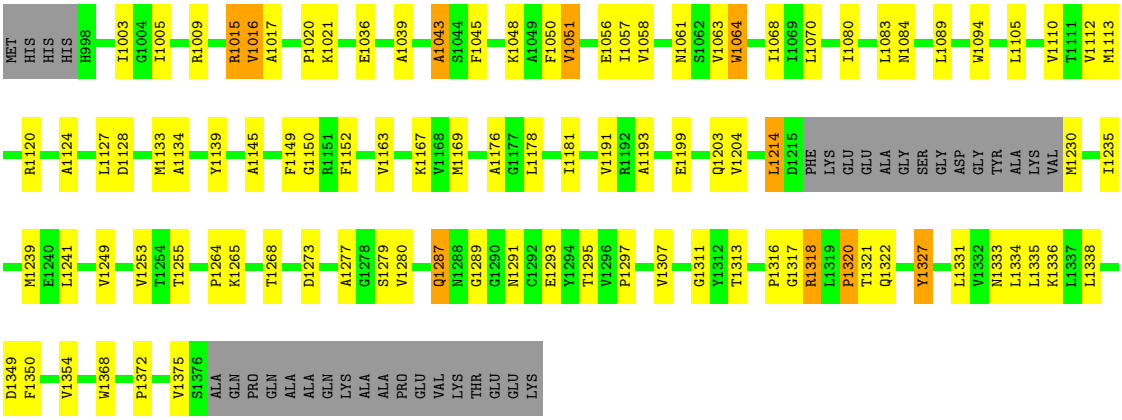
Chain A:






• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:




• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:

### 4.2.6 Score per residue for model 6

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 70% 19% • 9%

MET HIS HIS HIS H998 R1002 R1007 L1010 T1011 N1012 E1013 T1014 R1015 V1016 E1024 K1028 L1029 T1032 E1036 A1039 G1040 Q1041 F1045 K1048 V1063 W1064 Q1065 S1066 E1067 L1070 I1080 P1085 F1092 I1093 W1094 E1100 K1104 R1108 M1113 R1123

S1132 M1133 A1134 N1135 I1136 Y1139 A1145 F1149 G1150 R1151 F1152 T1158 V1163 M1169 V1175 A1176 S1186 R1192 D1195 P1198 E1199 V1200 Q1203 E1213 L1214 D1215 PHE LYS GLU GLU ALA GLY SER GLY ASP GLY TYR ALA LYS VAL M1230 A1233 F1234 I1235

V1249 D1250 I1251 K1265 T1268 M1271 M1275 S1279 V1280 I1281 Q1287 N1288 G1289 E1293 K1308 Y1312 T1313 D1314 L1315 P1316 G1317 R1318 L1319 P1320 T1321 Q1322 L1326 Y1327 G1328 L1331 K1336 R1356 T1367 W1368 S1376 ALA GLN PRO GLN ALA ALA GLN LYS ALA ALA

PRO GLU VAL LYS THR GLU GLU LYS

• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C: 62% 24% • 10%

MET HIS HIS HIS HIS HIS HIS SER SER GLN GLU VAL GLY GLU HIS ARG GLU ILE THR A20 H31 S32 V33 I34 I35 T36 P37 M41 Q45 A46 Q47 Y48 P49 V50 A51 E52 R58 N63 V64 R65 V71 R74 L75 P76 M79 L83 Y90 E95 M96

D102 T106 D107 T108 V109 D116 T117 P120 Q123 P134 V135 L136 E137 V138 W139 Q142 N143 V144 I145 V146 F147 K148 M151 Q159 F163 E166 N167 T168 H169 M170 L171 F172 G173 D174 A175 K176 A177 L183 L186

### 4.2.7 Score per residue for model 7

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 70% 20% • 8%

MET HIS HIS HIS HIS HIS H1000 I1003 G1004 I1005 P1006 T1014 R1015 V1016 A1017 A1018 T1019 T1022 F1031 A1043 S1044 F1045 W1064 E1067 I1068 I1069 L1070 K1071 V1072 P1075 L1083 L1089 I1093 W1094 Q1097 E1100 V1112 M1113 A1114 S1117 R1120 R1123

L1127 I1136 Y1139 A1145 F1149 G1150 R1151 F1152 I1157 V1163 P1164 P1165 A1166 K1167 G1174 N1185 S1186 L1187 T1196 R1197 P1198 E1199 V1200 G1208 F1216 LYS GLU GLU ALA GLY SER GLY D1224 D1232 A1233 F1234 I1251 I1252 T1255 A1256 G1260 T1268 R1269

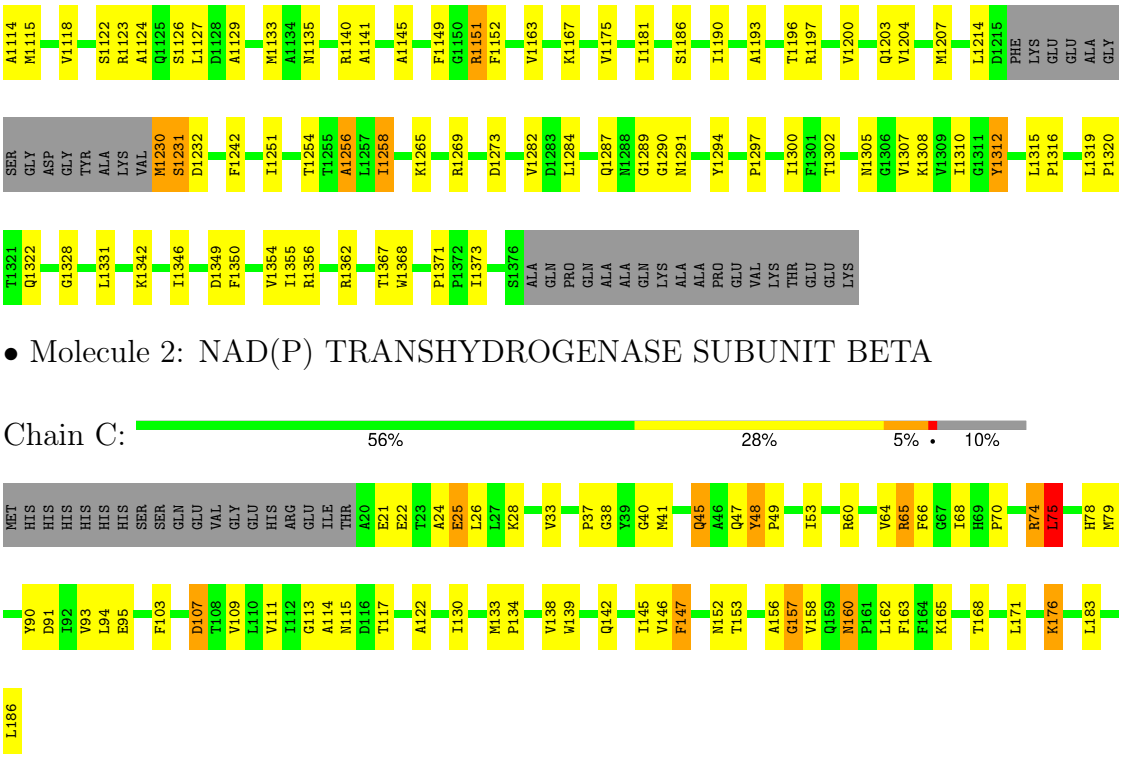
V1272 M1275 K1276 A1277 G1278 S1279 V1280 I1281 V1282 D1283 L1284 A1285 A1286 C1292 E1293 P1297 V1307 K1308 V1309 R1318 Q1322 S1323 L1326 Y1327 G1328 L1331 L1334 L1338 C1339 K1342 D1343 G1344 R1356 W1368 P1372 I1373 GLN VAL SER ALA GLN PRO GLN ALA ALA GLN

LYS ALA ALA PRO GLU VAL LYS THR GLU GLU LYS

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 64% 25% • 9%

MET HIS HIS HIS H998 I1003 E1008 R1009 N1012 E1013 T1014 T1019 P1020 K1021 T1022 G1030 V1035 Q1041 F1045 D1046 I1057 W1064 I1068 I1069 L1070 K1071 V1072 D1077 P1085 T1088 S1091 W1094 Q1097 E1100 L1105 R1108 T1111 V1112 M1113




• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:



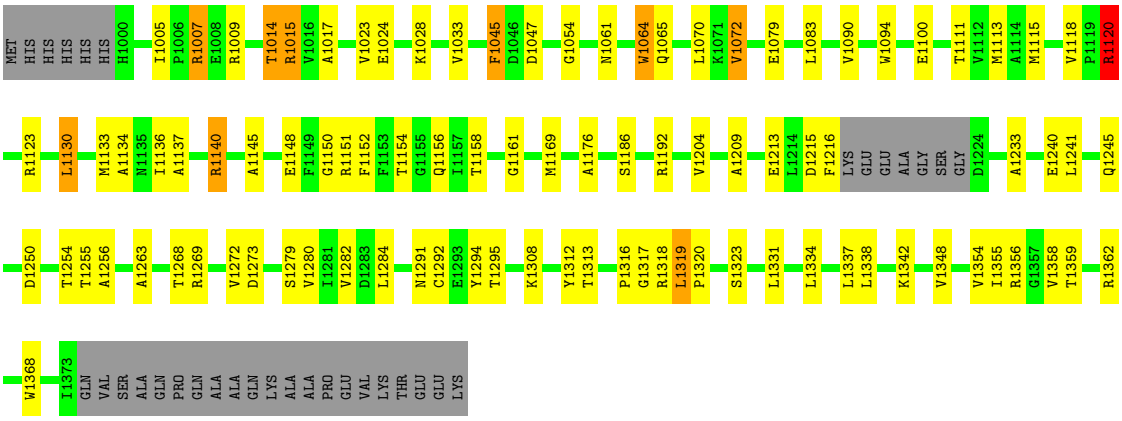




### 4.2.8 Score per residue for model 8

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:

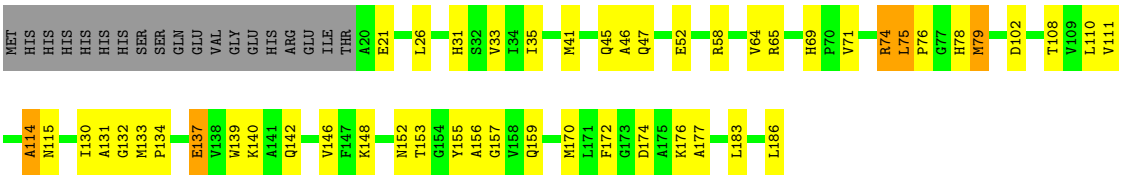



• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:

• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

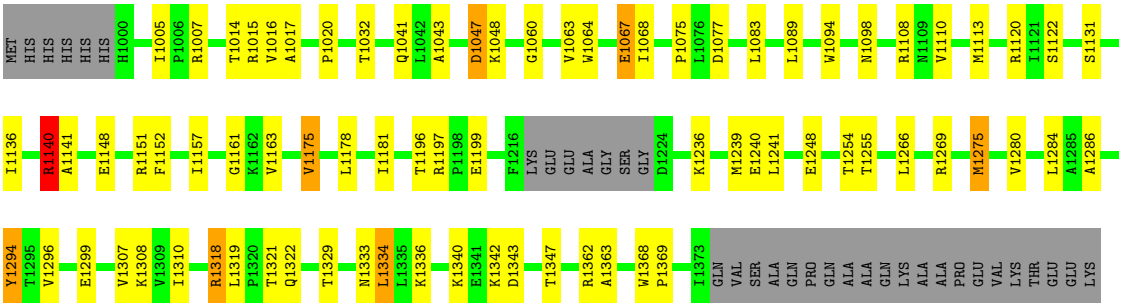
Chain C:




### 4.2.9 Score per residue for model 9

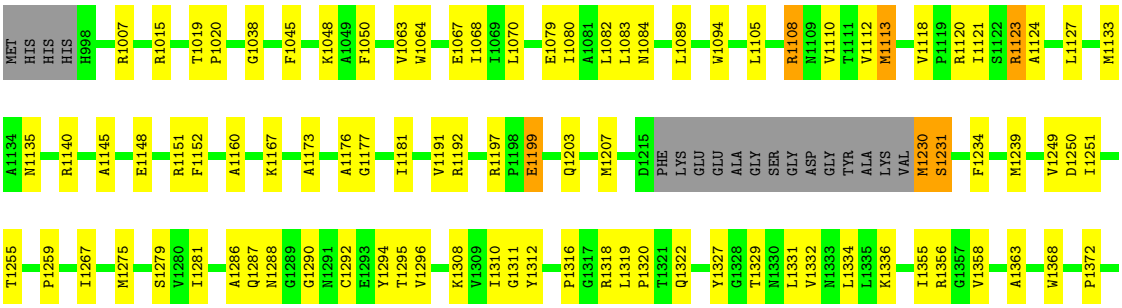
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

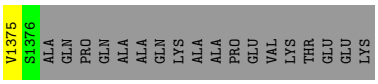
Chain A:




• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

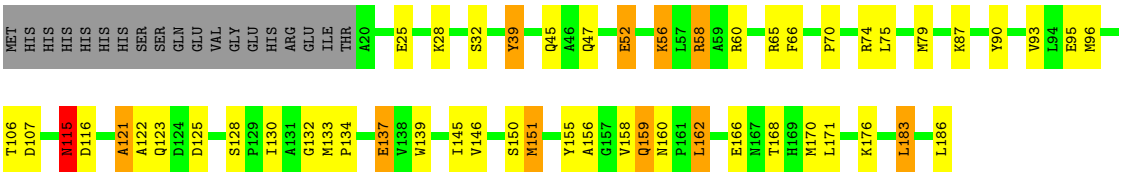
Chain B:






• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:



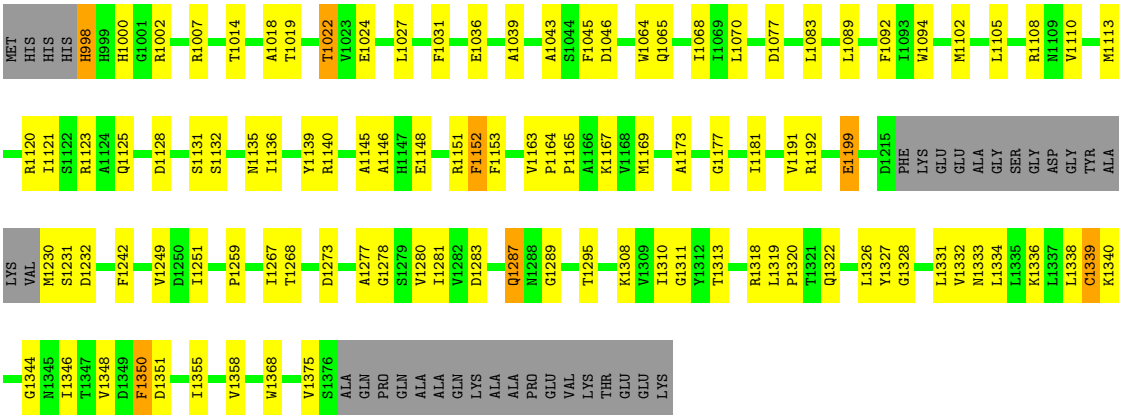

### 4.2.10 Score per residue for model 10

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

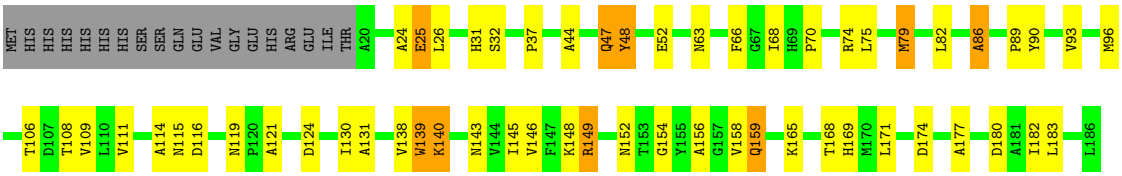
Chain B:




• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:

59%
26%
5%
10%


MET HIS HIS HIS HIS HIS HIS SER SER GLN GLU VAL GLY GLU HIS ARG GLU ILE THR A20 A24 E25 L26 H31 S32 P37 A44 Q47 Y48 E52 N63 F66 G67 I68 H69 P70 R74 L75 M79 L82 A86 P89 Y90 V93 M96
T106 D107 T108 V109 L110 V111 A114 N115 D116 N119 P120 A121 D124 I130 A131 V138 W139 K140 N143 V144 I145 V146 F147 K148 R149 N152 T153 G154 Y155 A156 G157 V158 Q159 K165 T168 H169 M170 L171 D174 A177 D180 A181 I182 L183 L186

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *RIGID BODY MINIMIZATION, MOLECULAR DYNAMICS SIMULATION*.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *?*.

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

| Software name | Classification | Version |
|---|---|---|
| X-PLOR | refinement | |
| X-PLOR | structure solution | |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.82±0.01 | 1±1/2779 ( 0.0± 0.0%) | 1.38±0.02 | 27±6/3776 ( 0.7± 0.2%) |
| 1 | B | 0.83±0.01 | 0±1/2773 ( 0.0± 0.0%) | 1.36±0.02 | 24±3/3768 ( 0.6± 0.1%) |
| 2 | C | 0.83±0.01 | 0±0/1297 ( 0.0± 0.0%) | 1.41±0.03 | 10±2/1764 ( 0.6± 0.1%) |
| All | All | 0.83 | 17/68490 ( 0.0%) | 1.38 | 605/93080 ( 0.6%) |

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

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0.0±0.0 | 2.2±1.9 |
| 1 | B | 0.0±0.0 | 1.2±0.9 |
| 2 | C | 0.0±0.0 | 0.9±0.7 |
| All | All | 0 | 43 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | C | 139 | TRP | NE1-CE2 | -5.80 | 1.30 | 1.37 | 3 | 1 |
| 1 | A | 1064 | TRP | CD1-NE1 | -5.78 | 1.28 | 1.38 | 10 | 1 |
| 1 | B | 1375 | VAL | C-N | -5.64 | 1.21 | 1.34 | 9 | 3 |
| 2 | C | 139 | TRP | CD1-NE1 | -5.48 | 1.28 | 1.38 | 7 | 1 |
| 2 | C | 52 | GLU | CD-OE1 | -5.40 | 1.19 | 1.25 | 1 | 1 |
| 1 | A | 1094 | TRP | CD1-NE1 | -5.34 | 1.28 | 1.38 | 5 | 1 |
| 1 | A | 1372 | PRO | C-N | -5.31 | 1.21 | 1.34 | 10 | 4 |
| 1 | A | 1240 | GLU | CD-OE2 | -5.30 | 1.19 | 1.25 | 8 | 1 |
| 1 | B | 1008 | GLU | CD-OE2 | -5.16 | 1.20 | 1.25 | 4 | 1 |
| 2 | C | 25 | GLU | CD-OE1 | -5.09 | 1.20 | 1.25 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 1199 | GLU | CD-OE2 | -5.04 | 1.20 | 1.25 | 7 | 1 |
| 1 | A | 1368 | TRP | CG-CD2 | -5.03 | 1.35 | 1.43 | 2 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 1064 | TRP | CD1-CG-CD2 | 11.34 | 115.37 | 106.30 | 10 | 10 |
| 1 | B | 1356 | ARG | NE-CZ-NH1 | 10.98 | 125.79 | 120.30 | 9 | 4 |
| 1 | B | 1356 | ARG | NE-CZ-NH2 | -10.97 | 114.81 | 120.30 | 1 | 2 |
| 2 | C | 139 | TRP | CD1-CG-CD2 | 10.54 | 114.73 | 106.30 | 8 | 10 |
| 1 | A | 1064 | TRP | CE2-CD2-CG | -10.46 | 98.93 | 107.30 | 10 | 10 |
| 1 | B | 1108 | ARG | NE-CZ-NH1 | 10.12 | 125.36 | 120.30 | 4 | 3 |
| 1 | A | 1192 | ARG | NE-CZ-NH2 | -10.10 | 115.25 | 120.30 | 2 | 3 |
| 1 | B | 1094 | TRP | CD1-CG-CD2 | 10.07 | 114.36 | 106.30 | 9 | 10 |
| 1 | A | 1123 | ARG | NE-CZ-NH2 | -10.06 | 115.27 | 120.30 | 5 | 5 |
| 1 | B | 1368 | TRP | CE2-CD2-CG | -10.02 | 99.28 | 107.30 | 2 | 8 |
| 1 | A | 1318 | ARG | NE-CZ-NH1 | 10.00 | 125.30 | 120.30 | 7 | 4 |
| 1 | B | 1312 | TYR | CB-CG-CD2 | -9.86 | 115.08 | 121.00 | 8 | 5 |
| 1 | B | 1108 | ARG | NE-CZ-NH2 | -9.85 | 115.38 | 120.30 | 2 | 3 |
| 1 | A | 1362 | ARG | NE-CZ-NH2 | -9.75 | 115.42 | 120.30 | 2 | 4 |
| 1 | A | 1094 | TRP | CE2-CD2-CG | -9.72 | 99.52 | 107.30 | 5 | 10 |
| 1 | A | 1094 | TRP | CD1-CG-CD2 | 9.57 | 113.96 | 106.30 | 4 | 10 |
| 1 | A | 1368 | TRP | CD1-CG-CD2 | 9.46 | 113.86 | 106.30 | 3 | 10 |
| 1 | A | 1151 | ARG | NE-CZ-NH2 | -9.26 | 115.67 | 120.30 | 5 | 4 |
| 2 | C | 139 | TRP | CE2-CD2-CG | -9.24 | 99.90 | 107.30 | 7 | 10 |
| 2 | C | 139 | TRP | CG-CD2-CE3 | 9.14 | 142.13 | 133.90 | 10 | 4 |
| 1 | B | 1197 | ARG | NE-CZ-NH2 | -9.14 | 115.73 | 120.30 | 9 | 3 |
| 1 | B | 1094 | TRP | CE2-CD2-CG | -9.00 | 100.10 | 107.30 | 9 | 10 |
| 1 | A | 1368 | TRP | CE2-CD2-CG | -8.95 | 100.14 | 107.30 | 8 | 10 |
| 1 | B | 1064 | TRP | CD1-CG-CD2 | 8.92 | 113.44 | 106.30 | 7 | 10 |
| 1 | A | 1197 | ARG | NE-CZ-NH1 | 8.90 | 124.75 | 120.30 | 4 | 3 |
| 1 | A | 1368 | TRP | CG-CD2-CE3 | 8.81 | 141.83 | 133.90 | 8 | 4 |
| 2 | C | 65 | ARG | NE-CZ-NH1 | 8.81 | 124.70 | 120.30 | 7 | 4 |
| 1 | A | 1151 | ARG | NE-CZ-NH1 | 8.76 | 124.68 | 120.30 | 7 | 5 |
| 1 | A | 1356 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 | 6 | 4 |
| 1 | B | 1269 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 | 3 | 4 |
| 2 | C | 74 | ARG | NE-CZ-NH1 | 8.59 | 124.59 | 120.30 | 7 | 5 |
| 1 | A | 1318 | ARG | NE-CZ-NH2 | -8.58 | 116.01 | 120.30 | 1 | 5 |
| 1 | B | 1368 | TRP | CD1-CG-CD2 | 8.40 | 113.02 | 106.30 | 2 | 10 |
| 1 | B | 1123 | ARG | NE-CZ-NH1 | 8.37 | 124.48 | 120.30 | 6 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1009 | ARG | NE-CZ-NH2 | -8.36 | 116.12 | 120.30 | 1 | 2 |
| 1 | B | 1140 | ARG | NE-CZ-NH1 | 8.35 | 124.47 | 120.30 | 4 | 3 |
| 1 | B | 1192 | ARG | NE-CZ-NH2 | -8.33 | 116.14 | 120.30 | 1 | 5 |
| 1 | A | 1002 | ARG | NE-CZ-NH1 | 8.28 | 124.44 | 120.30 | 1 | 3 |
| 1 | A | 1294 | TYR | CB-CG-CD2 | -8.21 | 116.08 | 121.00 | 3 | 4 |
| 2 | C | 60 | ARG | NE-CZ-NH2 | -8.19 | 116.21 | 120.30 | 7 | 3 |
| 1 | A | 1140 | ARG | NE-CZ-NH1 | 8.15 | 124.38 | 120.30 | 1 | 3 |
| 2 | C | 90 | TYR | CB-CG-CD2 | -8.14 | 116.12 | 121.00 | 6 | 4 |
| 1 | A | 1094 | TRP | CG-CD2-CE3 | 8.04 | 141.13 | 133.90 | 5 | 4 |
| 1 | B | 1002 | ARG | NE-CZ-NH1 | 8.01 | 124.30 | 120.30 | 3 | 1 |
| 1 | B | 1269 | ARG | NE-CZ-NH1 | 7.95 | 124.27 | 120.30 | 1 | 2 |
| 2 | C | 74 | ARG | NE-CZ-NH2 | -7.95 | 116.33 | 120.30 | 6 | 4 |
| 1 | A | 1015 | ARG | NE-CZ-NH1 | 7.94 | 124.27 | 120.30 | 5 | 5 |
| 1 | A | 1153 | PHE | CB-CG-CD2 | -7.86 | 115.30 | 120.80 | 3 | 1 |
| 1 | B | 1242 | PHE | CB-CG-CD2 | -7.85 | 115.30 | 120.80 | 4 | 4 |
| 1 | B | 1242 | PHE | CB-CG-CD1 | 7.82 | 126.27 | 120.80 | 4 | 1 |
| 2 | C | 155 | TYR | CB-CG-CD2 | -7.79 | 116.33 | 121.00 | 4 | 1 |
| 1 | B | 1123 | ARG | NE-CZ-NH2 | -7.74 | 116.43 | 120.30 | 6 | 4 |
| 1 | A | 1002 | ARG | NE-CZ-NH2 | -7.72 | 116.44 | 120.30 | 1 | 2 |
| 1 | B | 1064 | TRP | CE2-CD2-CG | -7.71 | 101.13 | 107.30 | 1 | 10 |
| 1 | A | 1064 | TRP | CG-CD1-NE1 | -7.71 | 102.39 | 110.10 | 10 | 5 |
| 1 | A | 1197 | ARG | NE-CZ-NH2 | -7.70 | 116.45 | 120.30 | 4 | 3 |
| 1 | A | 1312 | TYR | CB-CG-CD2 | -7.67 | 116.40 | 121.00 | 10 | 3 |
| 1 | A | 1123 | ARG | NE-CZ-NH1 | 7.65 | 124.12 | 120.30 | 10 | 5 |
| 1 | A | 1009 | ARG | NE-CZ-NH2 | -7.63 | 116.48 | 120.30 | 3 | 4 |
| 1 | A | 1192 | ARG | NE-CZ-NH1 | 7.61 | 124.11 | 120.30 | 2 | 2 |
| 1 | A | 1108 | ARG | NE-CZ-NH2 | -7.58 | 116.51 | 120.30 | 2 | 2 |
| 1 | A | 1009 | ARG | NE-CZ-NH1 | 7.50 | 124.05 | 120.30 | 4 | 1 |
| 1 | B | 1283 | ASP | CB-CG-OD1 | 7.49 | 125.04 | 118.30 | 4 | 5 |
| 1 | A | 1120 | ARG | NE-CZ-NH1 | 7.49 | 124.05 | 120.30 | 4 | 4 |
| 2 | C | 48 | TYR | CB-CG-CD2 | -7.43 | 116.54 | 121.00 | 6 | 6 |
| 1 | A | 1342 | LYS | O-C-N | -7.37 | 110.92 | 122.70 | 9 | 9 |
| 1 | B | 1230 | MET | O-C-N | -7.36 | 110.92 | 122.70 | 7 | 7 |
| 1 | A | 1120 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 | 1 | 3 |
| 1 | A | 1007 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 | 3 | 3 |
| 1 | A | 1269 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 | 1 | 2 |
| 1 | A | 1064 | TRP | CB-CG-CD1 | -7.26 | 117.57 | 127.00 | 5 | 3 |
| 2 | C | 39 | TYR | CB-CG-CD2 | -7.25 | 116.65 | 121.00 | 1 | 3 |
| 1 | B | 1092 | PHE | CB-CG-CD2 | -7.20 | 115.76 | 120.80 | 3 | 2 |
| 2 | C | 149 | ARG | NE-CZ-NH1 | 7.15 | 123.88 | 120.30 | 10 | 1 |
| 1 | A | 1064 | TRP | CG-CD2-CE3 | 7.08 | 140.27 | 133.90 | 10 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1009 | ARG | NE-CZ-NH1 | 7.06 | 123.83 | 120.30 | 7 | 3 |
| 2 | C | 139 | TRP | CB-CG-CD1 | -7.02 | 117.88 | 127.00 | 2 | 6 |
| 1 | A | 1140 | ARG | NE-CZ-NH2 | -7.01 | 116.79 | 120.30 | 9 | 4 |
| 1 | A | 1015 | ARG | NE-CZ-NH2 | -6.96 | 116.82 | 120.30 | 5 | 1 |
| 1 | B | 1094 | TRP | CG-CD2-CE3 | 6.96 | 140.16 | 133.90 | 10 | 6 |
| 2 | C | 139 | TRP | CG-CD1-NE1 | -6.94 | 103.16 | 110.10 | 2 | 6 |
| 1 | B | 1151 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 | 7 | 2 |
| 1 | A | 1149 | PHE | CB-CG-CD2 | -6.91 | 115.96 | 120.80 | 6 | 3 |
| 1 | A | 1269 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 | 8 | 5 |
| 1 | A | 1356 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 | 4 | 3 |
| 1 | B | 1094 | TRP | CG-CD1-NE1 | -6.73 | 103.37 | 110.10 | 7 | 5 |
| 1 | A | 1362 | ARG | NE-CZ-NH1 | 6.71 | 123.65 | 120.30 | 3 | 3 |
| 1 | B | 1230 | MET | CA-C-N | 6.70 | 131.93 | 117.20 | 7 | 6 |
| 1 | B | 1094 | TRP | CB-CG-CD1 | -6.63 | 118.38 | 127.00 | 4 | 8 |
| 1 | B | 1139 | TYR | CB-CG-CD2 | -6.62 | 117.03 | 121.00 | 10 | 4 |
| 1 | B | 1151 | ARG | NE-CZ-NH2 | -6.60 | 117.00 | 120.30 | 7 | 1 |
| 1 | B | 1349 | ASP | CB-CG-OD1 | 6.56 | 124.20 | 118.30 | 5 | 1 |
| 1 | A | 1077 | ASP | CB-CG-OD1 | 6.53 | 124.17 | 118.30 | 4 | 1 |
| 1 | B | 1318 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 | 2 | 3 |
| 1 | B | 1368 | TRP | CG-CD1-NE1 | -6.49 | 103.61 | 110.10 | 3 | 3 |
| 1 | B | 1050 | PHE | CB-CG-CD2 | -6.48 | 116.26 | 120.80 | 9 | 1 |
| 1 | A | 1273 | ASP | CB-CG-OD1 | 6.47 | 124.13 | 118.30 | 2 | 1 |
| 1 | A | 1094 | TRP | CG-CD1-NE1 | -6.46 | 103.64 | 110.10 | 3 | 5 |
| 1 | B | 1002 | ARG | NE-CZ-NH2 | -6.46 | 117.07 | 120.30 | 6 | 2 |
| 2 | C | 91 | ASP | CB-CG-OD1 | 6.45 | 124.11 | 118.30 | 7 | 1 |
| 2 | C | 58 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 | 9 | 1 |
| 1 | B | 1031 | PHE | CB-CG-CD2 | -6.40 | 116.32 | 120.80 | 10 | 1 |
| 1 | B | 1064 | TRP | CG-CD1-NE1 | -6.39 | 103.71 | 110.10 | 8 | 4 |
| 1 | A | 1046 | ASP | CB-CG-OD1 | 6.38 | 124.05 | 118.30 | 2 | 1 |
| 2 | C | 137 | GLU | N-CA-C | 6.38 | 128.21 | 111.00 | 8 | 1 |
| 1 | B | 1140 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 | 10 | 1 |
| 1 | B | 1368 | TRP | NE1-CE2-CD2 | 6.37 | 113.67 | 107.30 | 2 | 1 |
| 1 | A | 1007 | ARG | NE-CZ-NH2 | -6.37 | 117.11 | 120.30 | 2 | 3 |
| 1 | A | 1094 | TRP | CB-CG-CD1 | -6.34 | 118.76 | 127.00 | 2 | 3 |
| 2 | C | 124 | ASP | CB-CG-OD1 | 6.32 | 123.99 | 118.30 | 1 | 1 |
| 1 | A | 1368 | TRP | CG-CD1-NE1 | -6.29 | 103.81 | 110.10 | 4 | 6 |
| 1 | B | 1064 | TRP | CB-CG-CD1 | -6.23 | 118.90 | 127.00 | 8 | 3 |
| 2 | C | 147 | PHE | CB-CG-CD2 | -6.22 | 116.44 | 120.80 | 7 | 1 |
| 2 | C | 97 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 | 1 | 1 |
| 1 | B | 1008 | GLU | OE1-CD-OE2 | -6.22 | 115.84 | 123.30 | 1 | 2 |
| 1 | A | 1050 | PHE | CB-CG-CD2 | -6.22 | 116.45 | 120.80 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1120 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 | 3 | 1 |
| 1 | B | 1192 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 | 2 | 2 |
| 1 | A | 1139 | TYR | CB-CG-CD2 | -6.20 | 117.28 | 121.00 | 10 | 3 |
| 2 | C | 65 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 | 2 | 3 |
| 1 | A | 1314 | ASP | CB-CG-OD1 | 6.16 | 123.85 | 118.30 | 2 | 2 |
| 1 | B | 1234 | PHE | CB-CG-CD1 | -6.13 | 116.51 | 120.80 | 9 | 1 |
| 1 | B | 1368 | TRP | CB-CG-CD1 | -6.07 | 119.11 | 127.00 | 8 | 2 |
| 2 | C | 186 | LEU | CA-CB-CG | 6.06 | 129.23 | 115.30 | 9 | 3 |
| 1 | B | 1007 | ARG | NE-CZ-NH2 | -6.03 | 117.28 | 120.30 | 6 | 1 |
| 1 | A | 1139 | TYR | CB-CG-CD1 | -6.03 | 117.38 | 121.00 | 5 | 1 |
| 1 | A | 1342 | LYS | CA-C-N | 6.00 | 130.41 | 117.20 | 4 | 8 |
| 1 | B | 1312 | TYR | CB-CG-CD1 | 5.98 | 124.59 | 121.00 | 8 | 2 |
| 1 | B | 1045 | PHE | CB-CG-CD2 | -5.97 | 116.62 | 120.80 | 3 | 1 |
| 1 | B | 1015 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 | 6 | 1 |
| 1 | B | 1318 | ARG | NE-CZ-NH1 | 5.95 | 123.27 | 120.30 | 2 | 1 |
| 1 | A | 1294 | TYR | CB-CG-CD1 | -5.94 | 117.44 | 121.00 | 4 | 2 |
| 1 | A | 1128 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 | 1 | 3 |
| 1 | A | 1327 | TYR | CB-CG-CD2 | -5.92 | 117.45 | 121.00 | 5 | 1 |
| 1 | B | 1273 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 | 7 | 1 |
| 1 | A | 1240 | GLU | OE1-CD-OE2 | -5.88 | 116.24 | 123.30 | 3 | 1 |
| 1 | A | 1226 | TYR | CB-CG-CD2 | -5.87 | 117.48 | 121.00 | 5 | 1 |
| 2 | C | 103 | PHE | CB-CG-CD2 | -5.86 | 116.70 | 120.80 | 4 | 1 |
| 1 | A | 1368 | TRP | CB-CG-CD1 | -5.85 | 119.39 | 127.00 | 1 | 2 |
| 1 | A | 1226 | TYR | CB-CG-CD1 | -5.83 | 117.50 | 121.00 | 3 | 1 |
| 2 | C | 58 | ARG | NE-CZ-NH2 | 5.81 | 123.20 | 120.30 | 8 | 3 |
| 1 | A | 1108 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 | 9 | 1 |
| 1 | A | 1286 | ALA | CB-CA-C | -5.76 | 101.46 | 110.10 | 5 | 1 |
| 2 | C | 163 | PHE | CB-CG-CD2 | -5.74 | 116.79 | 120.80 | 6 | 2 |
| 1 | B | 1350 | PHE | CB-CG-CD2 | -5.71 | 116.81 | 120.80 | 10 | 2 |
| 2 | C | 172 | PHE | CB-CG-CD2 | -5.69 | 116.82 | 120.80 | 6 | 1 |
| 2 | C | 114 | ALA | N-CA-C | 5.68 | 126.34 | 111.00 | 8 | 1 |
| 1 | A | 1275 | MET | CA-CB-CG | 5.67 | 122.95 | 113.30 | 4 | 1 |
| 2 | C | 149 | ARG | NE-CZ-NH2 | -5.67 | 117.47 | 120.30 | 10 | 1 |
| 1 | B | 1051 | VAL | CG1-CB-CG2 | -5.66 | 101.84 | 110.90 | 5 | 1 |
| 1 | B | 1319 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 | 10 | 2 |
| 2 | C | 107 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 | 7 | 1 |
| 1 | B | 1362 | ARG | NE-CZ-NH1 | 5.63 | 123.11 | 120.30 | 2 | 2 |
| 2 | C | 137 | GLU | OE1-CD-OE2 | -5.60 | 116.58 | 123.30 | 9 | 1 |
| 1 | B | 1152 | PHE | CB-CG-CD2 | -5.60 | 116.88 | 120.80 | 10 | 3 |
| 1 | B | 1149 | PHE | CB-CG-CD2 | -5.59 | 116.89 | 120.80 | 3 | 3 |
| 2 | C | 166 | GLU | OE1-CD-OE2 | -5.59 | 116.60 | 123.30 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1213 | GLU | OE1-CD-OE2 | -5.56 | 116.62 | 123.30 | 3 | 1 |
| 1 | B | 1197 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 | 1 | 1 |
| 1 | B | 1327 | TYR | CB-CG-CD1 | -5.50 | 117.70 | 121.00 | 6 | 3 |
| 2 | C | 174 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 | 3 | 1 |
| 1 | A | 1283 | ASP | CB-CG-OD1 | 5.47 | 123.23 | 118.30 | 2 | 1 |
| 1 | B | 1327 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 | 10 | 1 |
| 1 | A | 1047 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 | 5 | 1 |
| 1 | B | 1293 | GLU | OE1-CD-OE2 | -5.43 | 116.78 | 123.30 | 2 | 1 |
| 1 | B | 1120 | ARG | NE-CZ-NH1 | 5.43 | 123.01 | 120.30 | 5 | 1 |
| 1 | A | 1241 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 | 9 | 1 |
| 2 | C | 106 | THR | CA-CB-CG2 | 5.40 | 119.96 | 112.40 | 6 | 2 |
| 1 | A | 1368 | TRP | NE1-CE2-CZ2 | -5.35 | 124.51 | 130.40 | 8 | 1 |
| 1 | B | 1064 | TRP | CG-CD2-CE3 | 5.35 | 138.72 | 133.90 | 8 | 1 |
| 1 | B | 1056 | GLU | OE1-CD-OE2 | -5.34 | 116.89 | 123.30 | 5 | 1 |
| 1 | A | 1234 | PHE | CB-CG-CD2 | -5.33 | 117.07 | 120.80 | 7 | 2 |
| 1 | B | 1296 | VAL | N-CA-C | -5.32 | 96.65 | 111.00 | 9 | 1 |
| 1 | A | 1277 | ALA | N-CA-CB | -5.29 | 102.70 | 110.10 | 3 | 1 |
| 1 | A | 1358 | VAL | CG1-CB-CG2 | -5.28 | 102.44 | 110.90 | 6 | 1 |
| 1 | A | 1043 | ALA | CB-CA-C | -5.28 | 102.18 | 110.10 | 2 | 2 |
| 1 | A | 1152 | PHE | CB-CG-CD1 | 5.28 | 124.50 | 120.80 | 6 | 1 |
| 1 | B | 1116 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 | 4 | 1 |
| 1 | A | 1059 | GLU | OE1-CD-OE2 | -5.26 | 116.98 | 123.30 | 6 | 1 |
| 1 | B | 1318 | ARG | N-CA-C | 5.26 | 125.20 | 111.00 | 2 | 2 |
| 1 | A | 1045 | PHE | CB-CG-CD2 | -5.24 | 117.14 | 120.80 | 3 | 2 |
| 1 | B | 1015 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 | 5 | 1 |
| 1 | B | 1016 | VAL | CA-CB-CG1 | 5.22 | 118.74 | 110.90 | 5 | 1 |
| 2 | C | 111 | VAL | CG1-CB-CG2 | -5.22 | 102.55 | 110.90 | 3 | 1 |
| 1 | B | 1047 | ASP | CB-CG-OD2 | 5.22 | 122.99 | 118.30 | 3 | 1 |
| 1 | B | 1232 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 | 7 | 1 |
| 2 | C | 139 | TRP | NE1-CE2-CD2 | 5.20 | 112.50 | 107.30 | 5 | 1 |
| 1 | B | 1368 | TRP | CG-CD2-CE3 | 5.18 | 138.56 | 133.90 | 5 | 1 |
| 1 | A | 1098 | ASN | N-CA-C | 5.17 | 124.96 | 111.00 | 9 | 1 |
| 1 | A | 1304 | GLU | OE1-CD-OE2 | -5.16 | 117.11 | 123.30 | 4 | 1 |
| 1 | A | 1195 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 | 5 | 1 |
| 2 | C | 45 | GLN | CA-CB-CG | 5.15 | 124.73 | 113.40 | 3 | 1 |
| 1 | B | 1234 | PHE | CB-CG-CD2 | 5.14 | 124.40 | 120.80 | 9 | 1 |
| 1 | A | 1343 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 | 4 | 1 |
| 1 | B | 1294 | TYR | CB-CG-CD1 | -5.10 | 117.94 | 121.00 | 7 | 1 |
| 1 | A | 1107 | GLU | OE1-CD-OE2 | -5.10 | 117.18 | 123.30 | 4 | 1 |
| 1 | B | 1007 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 | 4 | 1 |
| 1 | B | 1254 | THR | CA-C-N | -5.09 | 106.00 | 117.20 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | C | 50 | VAL | CG1-CB-CG2 | 5.09 | 119.05 | 110.90 | 4 | 1 |
| 1 | B | 1175 | VAL | CA-CB-CG2 | 5.09 | 118.53 | 110.90 | 6 | 1 |
| 2 | C | 60 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 | 7 | 1 |
| 1 | B | 1100 | GLU | OE1-CD-OE2 | -5.08 | 117.20 | 123.30 | 7 | 1 |
| 1 | A | 1343 | ASP | N-CA-CB | 5.07 | 119.72 | 110.60 | 4 | 1 |
| 1 | A | 1319 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 | 8 | 1 |
| 1 | A | 1079 | GLU | OE1-CD-OE2 | -5.05 | 117.25 | 123.30 | 8 | 1 |
| 1 | A | 1094 | TRP | NE1-CE2-CD2 | 5.04 | 112.34 | 107.30 | 9 | 1 |
| 1 | B | 1239 | MET | CA-CB-CG | 5.04 | 121.87 | 113.30 | 9 | 1 |
| 2 | C | 52 | GLU | OE1-CD-OE2 | -5.04 | 117.25 | 123.30 | 1 | 1 |
| 1 | B | 1108 | ARG | NH1-CZ-NH2 | -5.03 | 113.86 | 119.40 | 4 | 1 |
| 1 | B | 1045 | PHE | N-CA-C | -5.03 | 97.41 | 111.00 | 8 | 1 |
| 1 | B | 1046 | ASP | CB-CG-OD1 | 5.03 | 122.82 | 118.30 | 10 | 1 |
| 1 | A | 1002 | ARG | N-CA-C | -5.02 | 97.44 | 111.00 | 5 | 1 |
| 2 | C | 183 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 | 9 | 1 |
| 1 | A | 1213 | GLU | OE1-CD-OE2 | -5.01 | 117.29 | 123.30 | 8 | 1 |
| 1 | B | 1128 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 | 5 | 1 |
| 1 | B | 1351 | ASP | CB-CG-OD2 | 5.00 | 122.80 | 118.30 | 10 | 1 |
| 1 | A | 1144 | GLU | OE1-CD-OE2 | -5.00 | 117.30 | 123.30 | 6 | 1 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | B | 1139 | TYR | Sidechain | 4 |
| 1 | A | 1294 | TYR | Sidechain | 4 |
| 1 | B | 1318 | ARG | Sidechain | 3 |
| 2 | C | 90 | TYR | Sidechain | 3 |
| 1 | A | 1045 | PHE | Peptide | 3 |
| 1 | B | 1312 | TYR | Sidechain | 3 |
| 1 | A | 1140 | ARG | Sidechain | 3 |
| 2 | C | 48 | TYR | Sidechain | 2 |
| 1 | A | 1318 | ARG | Sidechain | 2 |
| 1 | A | 1362 | ARG | Sidechain | 2 |
| 1 | A | 1108 | ARG | Sidechain | 1 |
| 2 | C | 39 | TYR | Sidechain | 1 |
| 1 | A | 1327 | TYR | Sidechain | 1 |
| 2 | C | 60 | ARG | Sidechain | 1 |
| 1 | B | 1327 | TYR | Sidechain | 1 |
| 2 | C | 155 | TYR | Sidechain | 1 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 1123 | ARG | Sidechain | 1 |
| 1 | A | 1139 | TYR | Sidechain | 1 |
| 2 | C | 58 | ARG | Sidechain | 1 |
| 1 | A | 1007 | ARG | Sidechain | 1 |
| 1 | A | 1192 | ARG | Sidechain | 1 |
| 1 | A | 1255 | THR | Peptide | 1 |
| 1 | A | 1269 | ARG | Sidechain | 1 |
| 1 | B | 998 | HIS | Peptide | 1 |

## 6.2 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 each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 2735 | 579 | 2770 | 35±5 |
| 1 | B | 2729 | 582 | 2778 | 40±5 |
| 2 | C | 1272 | 264 | 1273 | 22±5 |
| 3 | B | 44 | 8 | 26 | 0±0 |
| 4 | C | 48 | 7 | 25 | 1±1 |
| All | All | 68280 | 14400 | 68720 | 892 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1186:SER:HB3 | 1:B:1187:LEU:HA | 0.88 | 1.44 | 8 | 2 |
| 2:C:120:PRO:HG2 | 2:C:160:ASN:HB2 | 0.81 | 1.52 | 4 | 1 |
| 2:C:162:LEU:HA | 2:C:168:THR:HG22 | 0.77 | 1.56 | 9 | 2 |
| 1:B:1016:VAL:HB | 1:B:1043:ALA:HB2 | 0.77 | 1.57 | 8 | 1 |
| 1:A:1187:LEU:HA | 1:B:1186:SER:HB3 | 0.77 | 1.56 | 7 | 2 |
| 1:B:1152:PHE:HB2 | 1:B:1163:VAL:HG11 | 0.76 | 1.57 | 4 | 6 |
| 1:A:1134:ALA:HB1 | 1:A:1176:ALA:HB2 | 0.75 | 1.56 | 8 | 5 |
| 2:C:40:GLY:HA3 | 2:C:113:GLY:HA3 | 0.74 | 1.57 | 2 | 2 |
| 1:A:1152:PHE:HB2 | 1:A:1163:VAL:HG11 | 0.74 | 1.59 | 10 | 4 |
| 1:A:1151:ARG:HA | 1:B:1322:GLN:HB2 | 0.73 | 1.61 | 10 | 8 |
| 2:C:130:ILE:HG12 | 2:C:156:ALA:HB2 | 0.73 | 1.59 | 8 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1015:ARG:HD2 | 1:A:1072:VAL:HG11 | 0.72 | 1.60 | 8 | 3 |
| 1:B:1070:LEU:HD13 | 1:B:1331:LEU:HD13 | 0.71 | 1.62 | 3 | 3 |
| 2:C:148:LYS:HD3 | 2:C:170:MET:SD | 0.71 | 2.25 | 2 | 2 |
| 2:C:41:MET:SD | 2:C:83:LEU:HD11 | 0.70 | 2.27 | 5 | 2 |
| 1:B:1287:GLN:HB3 | 1:B:1313:THR:HG23 | 0.68 | 1.65 | 10 | 3 |
| 2:C:146:VAL:HG21 | 2:C:162:LEU:HB3 | 0.68 | 1.63 | 7 | 2 |
| 1:A:1136:ILE:HD13 | 1:A:1323:SER:HA | 0.68 | 1.66 | 7 | 5 |
| 1:B:1134:ALA:HB1 | 1:B:1176:ALA:HB2 | 0.68 | 1.66 | 4 | 5 |
| 1:A:1135:ASN:HB2 | 1:A:1175:VAL:HG12 | 0.67 | 1.64 | 3 | 3 |
| 1:A:1023:VAL:HG22 | 1:A:1033:VAL:HG11 | 0.67 | 1.64 | 8 | 2 |
| 2:C:121:ALA:HA | 2:C:125:ASP:HB3 | 0.67 | 1.67 | 9 | 1 |
| 1:B:1215:ASP:HB3 | 1:B:1237:ALA:HB1 | 0.67 | 1.67 | 4 | 1 |
| 1:B:1203:GLN:HG2 | 2:C:74:ARG:HG3 | 0.66 | 1.67 | 1 | 3 |
| 1:A:1133:MET:HA | 1:A:1136:ILE:HD12 | 0.66 | 1.66 | 8 | 2 |
| 1:A:1005:ILE:HG23 | 1:A:1017:ALA:HB3 | 0.66 | 1.67 | 3 | 7 |
| 1:A:1141:ALA:HB2 | 1:A:1284:LEU:HD21 | 0.66 | 1.68 | 9 | 5 |
| 1:B:1145:ALA:HB1 | 1:B:1251:ILE:HD12 | 0.65 | 1.68 | 4 | 7 |
| 1:A:1009:ARG:NH1 | 1:A:1079:GLU:HG2 | 0.65 | 2.06 | 1 | 1 |
| 1:A:1070:LEU:HD13 | 1:A:1331:LEU:HD13 | 0.65 | 1.67 | 5 | 3 |
| 1:B:1195:ASP:HB3 | 1:B:1200:VAL:HG21 | 0.65 | 1.67 | 6 | 2 |
| 2:C:162:LEU:HA | 2:C:168:THR:HB | 0.65 | 1.68 | 1 | 1 |
| 1:A:1145:ALA:HB1 | 1:A:1251:ILE:HD12 | 0.65 | 1.67 | 4 | 5 |
| 2:C:107:ASP:HA | 2:C:142:GLN:HB2 | 0.65 | 1.69 | 6 | 2 |
| 1:A:1305:ASN:HA | 1:B:1046:ASP:HB2 | 0.65 | 1.69 | 3 | 2 |
| 2:C:133:MET:SD | 2:C:134:PRO:HD2 | 0.65 | 2.32 | 4 | 7 |
| 1:A:1061:ASN:HA | 1:A:1064:TRP:HD1 | 0.64 | 1.51 | 8 | 1 |
| 2:C:72:ALA:HB3 | 2:C:79:MET:SD | 0.64 | 2.33 | 2 | 1 |
| 2:C:66:PHE:HB2 | 2:C:93:VAL:HA | 0.64 | 1.68 | 7 | 4 |
| 1:B:1083:LEU:HD21 | 1:B:1089:LEU:HD13 | 0.64 | 1.69 | 8 | 1 |
| 1:A:1003:ILE:HG12 | 1:A:1068:ILE:HB | 0.64 | 1.69 | 6 | 1 |
| 1:B:1212:LEU:HB3 | 1:B:1241:LEU:HD21 | 0.64 | 1.67 | 8 | 1 |
| 1:A:1157:ILE:HG21 | 2:C:70:PRO:HB2 | 0.64 | 1.68 | 2 | 1 |
| 1:A:1148:GLU:HB3 | 1:A:1308:LYS:HD2 | 0.63 | 1.68 | 4 | 3 |
| 1:B:1123:ARG:HG3 | 1:B:1354:VAL:HG21 | 0.63 | 1.70 | 2 | 3 |
| 1:B:1199:GLU:HB2 | 2:C:155:TYR:HE1 | 0.63 | 1.53 | 9 | 1 |
| 1:A:1254:THR:HB | 1:A:1283:ASP:HA | 0.63 | 1.68 | 10 | 3 |
| 1:A:1148:GLU:HB2 | 1:A:1310:ILE:HD11 | 0.63 | 1.69 | 2 | 5 |
| 2:C:30:SER:HA | 2:C:107:ASP:HB3 | 0.63 | 1.69 | 4 | 3 |
| 1:A:1018:ALA:HB1 | 1:A:1022:THR:HB | 0.62 | 1.70 | 4 | 1 |
| 1:B:1157:ILE:HG23 | 1:B:1162:LYS:HG2 | 0.62 | 1.71 | 8 | 1 |
| 1:A:1113:MET:SD | 1:A:1338:LEU:HD21 | 0.62 | 2.33 | 7 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1339:CYS:SG | 1:A:1342:LYS:HA | 0.62 | 2.34 | 2 | 1 |
| 2:C:37:PRO:HD2 | 2:C:68:ILE:HG12 | 0.62 | 1.69 | 10 | 4 |
| 2:C:174:ASP:HB3 | 2:C:177:ALA:HB3 | 0.62 | 1.72 | 4 | 5 |
| 2:C:47:GLN:HG2 | 2:C:82:LEU:HB3 | 0.62 | 1.71 | 4 | 2 |
| 2:C:143:ASN:HA | 2:C:167:ASN:HB2 | 0.62 | 1.71 | 1 | 1 |
| 1:B:1080:ILE:HA | 1:B:1083:LEU:HD12 | 0.61 | 1.71 | 5 | 2 |
| 1:B:1267:ILE:HG21 | 1:B:1281:ILE:HD13 | 0.61 | 1.71 | 9 | 2 |
| 1:B:1070:LEU:HD22 | 1:B:1331:LEU:HD22 | 0.61 | 1.72 | 7 | 5 |
| 2:C:41:MET:HA | 2:C:46:ALA:HB3 | 0.61 | 1.72 | 8 | 2 |
| 1:B:1181:ILE:HG22 | 1:B:1207:MET:SD | 0.61 | 2.36 | 8 | 5 |
| 1:A:1151:ARG:NH2 | 1:A:1164:PRO:HB2 | 0.61 | 2.10 | 2 | 1 |
| 2:C:24:ALA:HB1 | 2:C:186:LEU:HA | 0.61 | 1.71 | 7 | 1 |
| 1:B:1169:MET:HB2 | 1:B:1249:VAL:HG11 | 0.61 | 1.71 | 4 | 6 |
| 2:C:151:MET:SD | 2:C:170:MET:SD | 0.61 | 2.98 | 6 | 1 |
| 1:A:1322:GLN:HB2 | 1:B:1151:ARG:HA | 0.61 | 1.73 | 7 | 5 |
| 2:C:145:ILE:HG12 | 2:C:171:LEU:HB2 | 0.61 | 1.73 | 9 | 1 |
| 2:C:99:ILE:HG13 | 2:C:102:ASP:HB2 | 0.61 | 1.71 | 1 | 1 |
| 2:C:25:GLU:HA | 2:C:28:LYS:HE2 | 0.60 | 1.73 | 9 | 2 |
| 1:B:1295:THR:HG23 | 1:B:1311:GLY:HA3 | 0.60 | 1.73 | 10 | 5 |
| 1:A:1014:THR:HB | 1:A:1320:PRO:HB3 | 0.60 | 1.72 | 8 | 1 |
| 1:A:1296:VAL:HB | 1:A:1299:GLU:HB2 | 0.60 | 1.74 | 9 | 1 |
| 1:A:1328:GLY:HA2 | 1:A:1331:LEU:HD12 | 0.59 | 1.74 | 3 | 3 |
| 1:B:1120:ARG:HB2 | 1:B:1375:VAL:HG13 | 0.59 | 1.74 | 3 | 1 |
| 1:B:1181:ILE:HG12 | 1:B:1191:VAL:HG11 | 0.59 | 1.74 | 5 | 2 |
| 1:B:1070:LEU:HB3 | 1:B:1331:LEU:HD13 | 0.59 | 1.72 | 2 | 4 |
| 1:B:1199:GLU:HB2 | 2:C:74:ARG:NH2 | 0.59 | 2.13 | 10 | 1 |
| 1:A:1124:ALA:HB2 | 1:A:1354:VAL:HG11 | 0.59 | 1.75 | 3 | 1 |
| 1:B:1328:GLY:HA2 | 1:B:1331:LEU:HD12 | 0.58 | 1.73 | 4 | 5 |
| 1:A:1246:ALA:HB1 | 1:A:1275:MET:HG2 | 0.58 | 1.75 | 2 | 2 |
| 1:B:1125:GLN:HA | 1:B:1128:ASP:HB3 | 0.58 | 1.74 | 10 | 1 |
| 1:B:1167:LYS:HB2 | 1:B:1249:VAL:HA | 0.58 | 1.74 | 5 | 5 |
| 2:C:111:VAL:HB | 2:C:146:VAL:HA | 0.58 | 1.75 | 8 | 4 |
| 1:A:1118:VAL:HG22 | 1:A:1358:VAL:HG22 | 0.58 | 1.74 | 2 | 2 |
| 1:B:1148:GLU:HB3 | 1:B:1308:LYS:HD2 | 0.58 | 1.74 | 3 | 2 |
| 1:B:1230:MET:N | 1:B:1231:SER:HG | 0.58 | 1.96 | 8 | 3 |
| 1:B:1193:ALA:HB3 | 1:B:1204:VAL:HG11 | 0.58 | 1.74 | 8 | 1 |
| 1:B:1173:ALA:HA | 1:B:1177:GLY:HA3 | 0.58 | 1.75 | 9 | 3 |
| 2:C:39:TYR:HB2 | 2:C:114:ALA:HB2 | 0.58 | 1.76 | 4 | 1 |
| 2:C:70:PRO:HD3 | 2:C:96:MET:HB2 | 0.58 | 1.74 | 4 | 1 |
| 2:C:20:ALA:HA | 2:C:171:LEU:HD21 | 0.58 | 1.76 | 3 | 1 |
| 1:B:1207:MET:SD | 2:C:75:LEU:HG | 0.58 | 2.37 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1127:LEU:HG | 1:B:1334:LEU:HA | 0.58 | 1.76 | 8 | 2 |
| 2:C:90:TYR:HA | 2:C:93:VAL:HB | 0.58 | 1.74 | 7 | 2 |
| 1:B:1214:LEU:HG | 1:B:1241:LEU:HD22 | 0.57 | 1.73 | 5 | 1 |
| 1:B:1335:LEU:HD23 | 1:B:1338:LEU:HD12 | 0.57 | 1.75 | 2 | 2 |
| 1:B:1005:ILE:HG23 | 1:B:1017:ALA:HB3 | 0.57 | 1.75 | 1 | 3 |
| 1:B:1016:VAL:HG21 | 1:B:1039:ALA:HB1 | 0.57 | 1.75 | 3 | 4 |
| 1:B:1113:MET:SD | 1:B:1334:LEU:HD21 | 0.57 | 2.39 | 10 | 2 |
| 1:A:1254:THR:HG21 | 1:A:1291:ASN:HB2 | 0.57 | 1.76 | 2 | 2 |
| 1:B:1118:VAL:HG22 | 1:B:1358:VAL:HG23 | 0.57 | 1.76 | 3 | 1 |
| 1:B:1312:TYR:HB2 | 1:B:1315:LEU:HG | 0.57 | 1.74 | 2 | 3 |
| 1:A:1300:ILE:HG12 | 1:A:1310:ILE:HG12 | 0.57 | 1.75 | 6 | 2 |
| 1:B:1120:ARG:HB2 | 1:B:1375:VAL:HG11 | 0.57 | 1.77 | 10 | 1 |
| 1:A:1280:VAL:HG22 | 1:A:1308:LYS:HB2 | 0.56 | 1.75 | 10 | 2 |
| 2:C:34:ILE:HB | 2:C:109:VAL:HG13 | 0.56 | 1.75 | 1 | 1 |
| 1:A:1157:ILE:HD13 | 2:C:95:GLU:HB3 | 0.56 | 1.77 | 2 | 3 |
| 2:C:116:ASP:HA | 2:C:119:ASN:HB2 | 0.56 | 1.75 | 3 | 3 |
| 1:B:1083:LEU:HD11 | 1:B:1089:LEU:HD22 | 0.56 | 1.78 | 9 | 2 |
| 2:C:68:ILE:HB | 2:C:95:GLU:HA | 0.56 | 1.77 | 5 | 1 |
| 1:B:1083:LEU:HD22 | 1:B:1110:VAL:HG11 | 0.56 | 1.76 | 5 | 1 |
| 1:B:1145:ALA:HA | 1:B:1280:VAL:HG11 | 0.56 | 1.76 | 10 | 5 |
| 1:A:1157:ILE:HG12 | 2:C:70:PRO:HG2 | 0.56 | 1.78 | 10 | 1 |
| 1:A:1267:ILE:HG23 | 1:A:1271:MET:SD | 0.56 | 2.41 | 4 | 1 |
| 1:B:1332:VAL:HG12 | 1:B:1336:LYS:HE3 | 0.55 | 1.76 | 2 | 2 |
| 1:A:1157:ILE:HG13 | 2:C:70:PRO:HB3 | 0.55 | 1.78 | 5 | 2 |
| 1:B:1041:GLN:NE2 | 1:B:1046:ASP:HA | 0.55 | 2.16 | 7 | 1 |
| 1:B:1141:ALA:HA | 1:B:1282:VAL:HG11 | 0.55 | 1.78 | 2 | 3 |
| 2:C:122:ALA:HB1 | 2:C:133:MET:HB3 | 0.55 | 1.77 | 7 | 2 |
| 1:A:1075:PRO:HG2 | 1:A:1089:LEU:HD21 | 0.55 | 1.78 | 5 | 4 |
| 1:B:1120:ARG:HB2 | 1:B:1375:VAL:HG21 | 0.55 | 1.78 | 8 | 1 |
| 2:C:109:VAL:HG11 | 2:C:138:VAL:HG21 | 0.55 | 1.78 | 10 | 1 |
| 2:C:32:SER:HB2 | 2:C:106:THR:HA | 0.55 | 1.78 | 1 | 2 |
| 2:C:148:LYS:HE3 | 2:C:151:MET:HA | 0.55 | 1.79 | 5 | 1 |
| 1:A:1004:GLY:O | 1:A:1006:PRO:HD3 | 0.54 | 2.01 | 7 | 2 |
| 1:B:1043:ALA:HA | 1:B:1320:PRO:HB2 | 0.54 | 1.79 | 10 | 2 |
| 1:B:1118:VAL:HG12 | 1:B:1124:ALA:HB1 | 0.54 | 1.77 | 8 | 3 |
| 1:A:1354:VAL:O | 1:A:1358:VAL:HG23 | 0.54 | 2.02 | 10 | 6 |
| 1:B:1267:ILE:HB | 1:B:1292:CYS:HA | 0.54 | 1.79 | 4 | 2 |
| 1:A:1137:ALA:HB2 | 1:A:1316:PRO:HG3 | 0.54 | 1.80 | 8 | 2 |
| 1:A:1115:MET:SD | 1:A:1334:LEU:HD22 | 0.54 | 2.43 | 8 | 3 |
| 1:A:1090:VAL:HG13 | 1:A:1113:MET:HB2 | 0.54 | 1.78 | 4 | 1 |
| 1:B:1349:ASP:HB3 | 1:B:1355:ILE:HG21 | 0.54 | 1.79 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1136:ILE:HG23 | 1:A:1319:LEU:HD23 | 0.54 | 1.80 | 9 | 1 |
| 1:A:1136:ILE:HD11 | 1:A:1326:LEU:HB2 | 0.54 | 1.80 | 7 | 1 |
| 1:B:1085:PRO:HB3 | 1:B:1109:ASN:HB2 | 0.53 | 1.80 | 3 | 2 |
| 2:C:96:MET:SD | 2:C:134:PRO:HB2 | 0.53 | 2.43 | 6 | 1 |
| 1:A:1070:LEU:HD21 | 1:A:1335:LEU:HD11 | 0.53 | 1.81 | 4 | 1 |
| 1:B:1300:ILE:HG12 | 1:B:1310:ILE:HG12 | 0.53 | 1.79 | 7 | 1 |
| 1:A:1169:MET:HA | 1:A:1192:ARG:O | 0.53 | 2.03 | 4 | 1 |
| 1:B:1022:THR:HG21 | 1:B:1328:GLY:HA3 | 0.53 | 1.80 | 1 | 1 |
| 1:B:1085:PRO:HA | 1:B:1108:ARG:O | 0.53 | 2.04 | 7 | 1 |
| 1:A:1113:MET:SD | 1:A:1334:LEU:HD21 | 0.53 | 2.43 | 9 | 1 |
| 1:B:1286:ALA:HA | 1:B:1290:GLY:HA2 | 0.53 | 1.80 | 9 | 1 |
| 1:A:1132:SER:HB3 | 1:A:1326:LEU:HB3 | 0.53 | 1.80 | 2 | 1 |
| 1:B:1181:ILE:HG22 | 1:B:1207:MET:HG2 | 0.53 | 1.79 | 4 | 1 |
| 1:B:1355:ILE:HA | 1:B:1358:VAL:HG12 | 0.53 | 1.81 | 9 | 4 |
| 1:B:1339:CYS:SG | 1:B:1344:GLY:N | 0.53 | 2.82 | 10 | 1 |
| 1:A:1252:ILE:HB | 1:A:1281:ILE:HG12 | 0.53 | 1.80 | 1 | 1 |
| 2:C:35:ILE:O | 2:C:37:PRO:HD3 | 0.53 | 2.03 | 6 | 1 |
| 1:A:1109:ASN:HA | 1:A:1364:GLY:HA2 | 0.53 | 1.79 | 1 | 1 |
| 1:A:1339:CYS:SG | 1:A:1344:GLY:HA2 | 0.53 | 2.44 | 6 | 3 |
| 2:C:157:GLY:O | 2:C:160:ASN:HB2 | 0.53 | 2.04 | 7 | 1 |
| 2:C:121:ALA:HA | 2:C:124:ASP:HB3 | 0.53 | 1.80 | 10 | 1 |
| 1:A:1145:ALA:HA | 1:A:1280:VAL:HG11 | 0.52 | 1.81 | 1 | 4 |
| 1:B:1029:LEU:HD21 | 1:B:1336:LYS:HG2 | 0.52 | 1.80 | 6 | 2 |
| 1:B:1141:ALA:HB2 | 1:B:1284:LEU:HD21 | 0.52 | 1.82 | 7 | 2 |
| 2:C:148:LYS:O | 2:C:172:PHE:HA | 0.52 | 2.04 | 6 | 4 |
| 1:A:1113:MET:HB3 | 1:A:1358:VAL:HG12 | 0.52 | 1.82 | 10 | 2 |
| 1:A:1031:PHE:HZ | 1:A:1339:CYS:HG | 0.52 | 1.44 | 7 | 1 |
| 1:B:1192:ARG:HG2 | 1:B:1210:GLU:HB2 | 0.52 | 1.80 | 3 | 2 |
| 1:A:1255:THR:HG22 | 1:A:1284:LEU:HD13 | 0.52 | 1.81 | 8 | 2 |
| 2:C:53:ILE:HD13 | 2:C:183:LEU:HA | 0.52 | 1.81 | 7 | 2 |
| 1:A:1031:PHE:HZ | 1:A:1339:CYS:SG | 0.52 | 2.28 | 7 | 1 |
| 2:C:52:GLU:HB3 | 2:C:183:LEU:HB2 | 0.52 | 1.81 | 8 | 2 |
| 1:B:1181:ILE:HG23 | 1:B:1191:VAL:HG11 | 0.52 | 1.81 | 1 | 2 |
| 2:C:145:ILE:HG23 | 2:C:171:LEU:HB2 | 0.52 | 1.82 | 5 | 1 |
| 1:A:1267:ILE:HA | 1:A:1271:MET:SD | 0.51 | 2.45 | 10 | 1 |
| 1:A:1178:LEU:HD13 | 1:A:1203:GLN:HG2 | 0.51 | 1.81 | 1 | 1 |
| 2:C:148:LYS:HE3 | 2:C:151:MET:SD | 0.51 | 2.46 | 4 | 1 |
| 1:B:1124:ALA:HB2 | 1:B:1354:VAL:HG22 | 0.51 | 1.82 | 5 | 1 |
| 1:B:1123:ARG:HD2 | 1:B:1337:LEU:HD21 | 0.51 | 1.81 | 1 | 1 |
| 1:B:1254:THR:HG23 | 1:B:1283:ASP:HA | 0.51 | 1.82 | 8 | 1 |
| 1:A:1067:GLU:HB3 | 1:A:1068:ILE:HD12 | 0.51 | 1.82 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1110:VAL:HG23 | 1:A:1112:VAL:HG23 | 0.51 | 1.82 | 6 | 1 |
| 1:A:1024:GLU:O | 1:A:1028:LYS:HG2 | 0.51 | 2.06 | 8 | 1 |
| 1:A:1161:GLY:HA3 | 1:B:1326:LEU:HA | 0.51 | 1.83 | 8 | 1 |
| 1:B:1125:GLN:NE2 | 1:B:1131:SER:HB3 | 0.51 | 2.19 | 8 | 1 |
| 2:C:41:MET:SD | 2:C:79:MET:HB2 | 0.51 | 2.46 | 8 | 1 |
| 1:A:1236:LYS:O | 1:A:1240:GLU:HG3 | 0.51 | 2.06 | 9 | 2 |
| 1:B:1003:ILE:HG12 | 1:B:1068:ILE:HD12 | 0.51 | 1.81 | 7 | 1 |
| 2:C:73:GLY:C | 2:C:74:ARG:HD2 | 0.50 | 2.26 | 1 | 1 |
| 1:A:1149:PHE:CZ | 1:A:1250:ASP:HB3 | 0.50 | 2.41 | 10 | 2 |
| 1:B:1258:ILE:HB | 1:B:1261:LYS:HB2 | 0.50 | 1.84 | 3 | 1 |
| 1:A:1026:LEU:HD21 | 1:A:1332:VAL:HG22 | 0.50 | 1.83 | 4 | 1 |
| 1:B:1015:ARG:HG3 | 1:B:1317:GLY:HA2 | 0.50 | 1.82 | 2 | 4 |
| 1:A:1320:PRO:HD2 | 1:B:1150:GLY:HA2 | 0.50 | 1.84 | 5 | 3 |
| 1:B:1007:ARG:HB2 | 1:B:1039:ALA:HA | 0.50 | 1.84 | 10 | 1 |
| 1:B:1118:VAL:HG21 | 1:B:1128:ASP:HA | 0.50 | 1.83 | 2 | 1 |
| 2:C:165:LYS:HB2 | 2:C:168:THR:HB | 0.50 | 1.80 | 10 | 2 |
| 1:B:1083:LEU:HB3 | 1:B:1110:VAL:HG11 | 0.50 | 1.84 | 9 | 4 |
| 2:C:156:ALA:HB1 | 2:C:158:VAL:HG22 | 0.50 | 1.84 | 9 | 1 |
| 1:B:1122:SER:HB2 | 2:C:133:MET:HA | 0.50 | 1.82 | 4 | 3 |
| 1:B:1148:GLU:HB2 | 1:B:1310:ILE:HD11 | 0.50 | 1.83 | 10 | 2 |
| 1:A:1181:ILE:HA | 1:A:1191:VAL:HG11 | 0.50 | 1.84 | 1 | 1 |
| 1:B:1088:THR:HA | 1:B:1111:THR:HB | 0.50 | 1.83 | 1 | 2 |
| 2:C:123:GLN:HB2 | 2:C:135:VAL:HG22 | 0.50 | 1.82 | 2 | 1 |
| 1:A:1292:CYS:HB3 | 1:A:1295:THR:OG1 | 0.50 | 2.06 | 10 | 3 |
| 1:B:1292:CYS:HB3 | 1:B:1295:THR:OG1 | 0.50 | 2.07 | 8 | 4 |
| 3:B:1:NAD:H3D | 3:B:1:NAD:O1N | 0.50 | 2.07 | 3 | 1 |
| 1:B:1338:LEU:HD13 | 1:B:1346:ILE:HG23 | 0.50 | 1.84 | 10 | 1 |
| 1:A:1140:ARG:HG3 | 1:A:1315:LEU:HD22 | 0.49 | 1.82 | 4 | 2 |
| 1:B:1127:LEU:HD23 | 1:B:1334:LEU:HD12 | 0.49 | 1.83 | 5 | 2 |
| 1:A:1019:THR:HG21 | 1:A:1325:GLN:HA | 0.49 | 1.84 | 10 | 1 |
| 1:A:1140:ARG:HD3 | 1:A:1319:LEU:HD13 | 0.49 | 1.82 | 3 | 1 |
| 1:A:1194:PHE:HB2 | 1:A:1212:LEU:HD12 | 0.49 | 1.84 | 6 | 1 |
| 1:B:1275:MET:SD | 1:B:1281:ILE:HD11 | 0.49 | 2.48 | 6 | 1 |
| 1:B:998:HIS:HB2 | 1:B:1000:HIS:HB2 | 0.49 | 1.82 | 10 | 1 |
| 1:B:1025:GLN:HE22 | 1:B:1329:THR:HG23 | 0.49 | 1.68 | 3 | 1 |
| 1:B:1203:GLN:OE1 | 2:C:74:ARG:HA | 0.49 | 2.07 | 8 | 3 |
| 1:A:1089:LEU:HD23 | 1:A:1112:VAL:HG22 | 0.49 | 1.83 | 7 | 1 |
| 1:B:1250:ASP:O | 1:B:1279:SER:HB3 | 0.49 | 2.08 | 6 | 2 |
| 1:B:1121:ILE:HG22 | 2:C:131:ALA:HB1 | 0.49 | 1.82 | 8 | 1 |
| 1:A:1174:GLY:HA2 | 1:A:1197:ARG:NH2 | 0.49 | 2.23 | 10 | 1 |
| 2:C:35:ILE:HG22 | 2:C:37:PRO:HD3 | 0.49 | 1.84 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1252:ILE:HD12 | 1:A:1281:ILE:HG12 | 0.49 | 1.84 | 10 | 2 |
| 1:A:1157:ILE:HB | 2:C:95:GLU:HG2 | 0.49 | 1.85 | 9 | 1 |
| 1:B:1333:ASN:HA | 1:B:1336:LYS:HD2 | 0.49 | 1.85 | 1 | 4 |
| 1:A:1015:ARG:HB3 | 1:A:1072:VAL:HG11 | 0.49 | 1.84 | 7 | 1 |
| 1:B:1058:VAL:HB | 1:B:1062:SER:HB2 | 0.49 | 1.84 | 8 | 1 |
| 1:A:1277:ALA:HB1 | 1:B:1045:PHE:HA | 0.49 | 1.83 | 7 | 2 |
| 1:B:1155:GLY:HA3 | 1:B:1165:PRO:HG3 | 0.49 | 1.84 | 8 | 1 |
| 1:A:1036:GLU:HB3 | 1:A:1039:ALA:HB2 | 0.48 | 1.85 | 1 | 1 |
| 2:C:107:ASP:HA | 2:C:142:GLN:HB3 | 0.48 | 1.83 | 1 | 1 |
| 1:A:1070:LEU:HB3 | 1:A:1331:LEU:HD13 | 0.48 | 1.84 | 7 | 2 |
| 1:A:1096:ALA:HB3 | 1:A:1097:GLN:NE2 | 0.48 | 2.23 | 6 | 1 |
| 2:C:153:THR:HG23 | 2:C:157:GLY:HA3 | 0.48 | 1.85 | 7 | 2 |
| 2:C:160:ASN:HB3 | 2:C:162:LEU:HD12 | 0.48 | 1.84 | 9 | 1 |
| 1:A:1080:ILE:HD11 | 1:A:1101:LEU:HG | 0.48 | 1.84 | 5 | 1 |
| 2:C:115:ASN:ND2 | 2:C:116:ASP:H | 0.48 | 2.06 | 10 | 1 |
| 2:C:75:LEU:HB2 | 2:C:78:HIS:HB2 | 0.48 | 1.85 | 8 | 1 |
| 1:B:1235:ILE:O | 1:B:1239:MET:HG2 | 0.48 | 2.09 | 5 | 2 |
| 1:B:1298:GLY:HA2 | 1:B:1312:TYR:HA | 0.48 | 1.84 | 4 | 1 |
| 1:B:1268:THR:HA | 1:B:1293:GLU:HG3 | 0.48 | 1.85 | 5 | 2 |
| 1:B:1015:ARG:NH1 | 1:B:1133:MET:SD | 0.48 | 2.87 | 9 | 1 |
| 1:B:1067:GLU:HB2 | 1:B:1068:ILE:HD12 | 0.48 | 1.86 | 9 | 1 |
| 1:A:1152:PHE:CD1 | 1:B:1322:GLN:HG2 | 0.48 | 2.43 | 9 | 4 |
| 1:B:1094:TRP:HB2 | 1:B:1098:ASN:ND2 | 0.48 | 2.24 | 1 | 2 |
| 2:C:109:VAL:HG11 | 2:C:138:VAL:HG23 | 0.48 | 1.86 | 6 | 1 |
| 2:C:79:MET:HA | 2:C:82:LEU:HD12 | 0.48 | 1.85 | 10 | 1 |
| 2:C:148:LYS:HE3 | 4:C:1001:NAP:O2B | 0.48 | 2.09 | 10 | 1 |
| 1:B:1123:ARG:HA | 2:C:134:PRO:HD3 | 0.48 | 1.84 | 3 | 2 |
| 1:B:1300:ILE:HG23 | 1:B:1310:ILE:HG12 | 0.48 | 1.85 | 4 | 1 |
| 1:B:1002:ARG:HG3 | 1:B:1032:THR:HB | 0.48 | 1.85 | 6 | 1 |
| 2:C:37:PRO:HG2 | 2:C:68:ILE:HG13 | 0.48 | 1.83 | 1 | 1 |
| 2:C:144:VAL:HB | 2:C:168:THR:HG23 | 0.48 | 1.85 | 5 | 2 |
| 1:A:1127:LEU:HD21 | 1:A:1337:LEU:HD22 | 0.48 | 1.85 | 6 | 1 |
| 2:C:145:ILE:HG13 | 2:C:171:LEU:HB2 | 0.48 | 1.86 | 7 | 2 |
| 1:A:1016:VAL:HG21 | 1:A:1039:ALA:HB1 | 0.48 | 1.84 | 10 | 1 |
| 1:B:1251:ILE:HA | 1:B:1280:VAL:O | 0.47 | 2.09 | 1 | 1 |
| 1:A:1022:THR:HB | 1:A:1332:VAL:HG21 | 0.47 | 1.85 | 2 | 1 |
| 1:A:1140:ARG:HD3 | 1:A:1319:LEU:HB2 | 0.47 | 1.85 | 8 | 1 |
| 2:C:71:VAL:HG22 | 2:C:76:PRO:HB3 | 0.47 | 1.85 | 8 | 1 |
| 2:C:115:ASN:ND2 | 2:C:154:GLY:HA3 | 0.47 | 2.24 | 10 | 1 |
| 1:A:1214:LEU:HG | 1:A:1216:PHE:HB2 | 0.47 | 1.84 | 1 | 1 |
| 1:A:1167:LYS:HB2 | 1:A:1249:VAL:HA | 0.47 | 1.85 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1003:ILE:HG12 | 1:B:1068:ILE:HB | 0.47 | 1.85 | 5 | 2 |
| 1:A:1025:GLN:OE1 | 1:A:1336:LYS:HE2 | 0.47 | 2.10 | 10 | 1 |
| 2:C:118:VAL:HG12 | 2:C:136:LEU:HB2 | 0.47 | 1.86 | 1 | 1 |
| 1:B:1105:LEU:HD13 | 1:B:1112:VAL:HG21 | 0.47 | 1.85 | 7 | 4 |
| 1:B:1264:PRO:O | 1:B:1291:ASN:HA | 0.47 | 2.09 | 5 | 1 |
| 1:A:1250:ASP:O | 1:A:1279:SER:HB3 | 0.47 | 2.08 | 8 | 2 |
| 1:A:1312:TYR:HB2 | 1:A:1315:LEU:HG | 0.47 | 1.84 | 6 | 1 |
| 1:A:1029:LEU:HA | 1:A:1342:LYS:HE3 | 0.47 | 1.84 | 10 | 1 |
| 2:C:34:ILE:HG12 | 2:C:106:THR:HG21 | 0.47 | 1.87 | 1 | 1 |
| 1:B:1284:LEU:HD23 | 1:B:1315:LEU:HD13 | 0.47 | 1.85 | 2 | 1 |
| 2:C:144:VAL:HB | 2:C:168:THR:HA | 0.47 | 1.86 | 2 | 2 |
| 1:A:1061:ASN:HA | 1:A:1064:TRP:CD1 | 0.47 | 2.40 | 8 | 1 |
| 1:A:1178:LEU:HB3 | 1:A:1207:MET:SD | 0.47 | 2.49 | 6 | 1 |
| 1:A:1185:ASN:ND2 | 1:A:1208:GLY:HA3 | 0.47 | 2.25 | 7 | 1 |
| 2:C:160:ASN:HD22 | 2:C:162:LEU:HD12 | 0.47 | 1.70 | 1 | 1 |
| 2:C:30:SER:CA | 2:C:107:ASP:HB3 | 0.47 | 2.40 | 4 | 1 |
| 1:B:1253:VAL:HG12 | 1:B:1255:THR:HG23 | 0.47 | 1.86 | 8 | 2 |
| 1:B:1104:LYS:O | 1:B:1108:ARG:HG2 | 0.47 | 2.08 | 6 | 1 |
| 2:C:49:PRO:O | 2:C:183:LEU:HD11 | 0.47 | 2.09 | 6 | 1 |
| 1:B:1064:TRP:CZ3 | 1:B:1083:LEU:HG | 0.47 | 2.45 | 2 | 1 |
| 1:A:1172:GLY:O | 1:A:1255:THR:HB | 0.47 | 2.09 | 4 | 1 |
| 1:A:1019:THR:HG21 | 1:A:1321:THR:HG23 | 0.47 | 1.87 | 5 | 1 |
| 1:A:1029:LEU:HA | 1:A:1342:LYS:HE2 | 0.47 | 1.86 | 5 | 1 |
| 1:B:1111:THR:HG23 | 1:B:1362:ARG:HA | 0.47 | 1.86 | 7 | 2 |
| 1:A:1148:GLU:HB3 | 1:A:1308:LYS:HG3 | 0.47 | 1.86 | 2 | 1 |
| 2:C:179:VAL:HA | 2:C:182:ILE:HG12 | 0.47 | 1.86 | 2 | 2 |
| 2:C:48:TYR:HB2 | 2:C:49:PRO:HD3 | 0.47 | 1.87 | 3 | 2 |
| 1:B:1248:GLU:O | 1:B:1276:LYS:NZ | 0.47 | 2.47 | 4 | 1 |
| 1:B:1357:GLY:CA | 1:B:1370:ALA:HB2 | 0.47 | 2.39 | 1 | 1 |
| 1:B:1272:VAL:HG11 | 1:B:1303:THR:HG21 | 0.47 | 1.86 | 4 | 1 |
| 1:A:1152:PHE:HE1 | 1:B:1136:ILE:HD13 | 0.47 | 1.68 | 10 | 1 |
| 1:A:1071:LYS:HE3 | 1:A:1073:ASN:O | 0.47 | 2.10 | 1 | 1 |
| 2:C:109:VAL:HB | 2:C:144:VAL:HA | 0.47 | 1.86 | 4 | 1 |
| 2:C:35:ILE:HG12 | 2:C:110:LEU:HB2 | 0.47 | 1.85 | 8 | 1 |
| 1:A:1178:LEU:HD23 | 1:A:1181:ILE:HD12 | 0.47 | 1.86 | 9 | 1 |
| 1:A:1069:ILE:HG12 | 1:A:1087:THR:HG21 | 0.46 | 1.87 | 1 | 1 |
| 1:B:1169:MET:O | 1:B:1252:ILE:HA | 0.46 | 2.09 | 2 | 1 |
| 1:A:1080:ILE:HA | 1:A:1083:LEU:HD23 | 0.46 | 1.86 | 4 | 2 |
| 1:B:1199:GLU:O | 1:B:1203:GLN:HG2 | 0.46 | 2.09 | 3 | 1 |
| 1:A:1322:GLN:HG2 | 1:B:1152:PHE:CD1 | 0.46 | 2.46 | 7 | 1 |
| 1:B:1302:THR:HG23 | 1:B:1308:LYS:HG2 | 0.46 | 1.86 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1275:MET:HB2 | 1:B:1307:VAL:HG21 | 0.46 | 1.87 | 4 | 2 |
| 1:B:1265:LYS:NZ | 1:B:1289:GLY:O | 0.46 | 2.49 | 6 | 3 |
| 1:A:1157:ILE:HD13 | 2:C:95:GLU:HB2 | 0.46 | 1.86 | 9 | 1 |
| 1:B:1169:MET:HA | 1:B:1192:ARG:O | 0.46 | 2.10 | 2 | 2 |
| 1:B:1350:PHE:HE1 | 1:B:1359:THR:HB | 0.46 | 1.70 | 3 | 1 |
| 1:A:1339:CYS:HB3 | 1:A:1344:GLY:HA2 | 0.46 | 1.87 | 7 | 1 |
| 1:B:1200:VAL:HB | 1:B:1203:GLN:NE2 | 0.46 | 2.25 | 7 | 1 |
| 1:A:1120:ARG:HD3 | 1:A:1130:LEU:HD13 | 0.46 | 1.88 | 8 | 1 |
| 1:B:1146:ALA:HB2 | 1:B:1153:PHE:HE1 | 0.46 | 1.70 | 3 | 2 |
| 1:B:1252:ILE:HB | 1:B:1281:ILE:HG12 | 0.46 | 1.87 | 1 | 1 |
| 1:B:1016:VAL:HG12 | 1:B:1043:ALA:HB2 | 0.46 | 1.87 | 5 | 1 |
| 1:B:1267:ILE:HG22 | 1:B:1272:VAL:HG22 | 0.46 | 1.87 | 8 | 1 |
| 1:A:1150:GLY:HA2 | 1:B:1320:PRO:HG2 | 0.46 | 1.87 | 5 | 3 |
| 1:A:1301:PHE:HB3 | 1:A:1309:VAL:HB | 0.46 | 1.87 | 2 | 1 |
| 1:B:1051:VAL:HG23 | 1:B:1057:ILE:HG12 | 0.46 | 1.88 | 5 | 1 |
| 2:C:44:ALA:HB2 | 4:C:1001:NAP:N6A | 0.46 | 2.25 | 10 | 1 |
| 1:A:1070:LEU:HD22 | 1:A:1331:LEU:HD22 | 0.46 | 1.87 | 8 | 3 |
| 1:B:1109:ASN:HA | 1:B:1364:GLY:HA3 | 0.46 | 1.88 | 2 | 1 |
| 1:B:1178:LEU:HA | 1:B:1181:ILE:HD12 | 0.46 | 1.86 | 3 | 1 |
| 1:A:1132:SER:HB2 | 1:A:1330:ASN:OD1 | 0.46 | 2.11 | 4 | 1 |
| 1:A:1080:ILE:HG21 | 1:A:1104:LYS:HB3 | 0.46 | 1.87 | 5 | 1 |
| 1:B:1193:ALA:HB3 | 1:B:1204:VAL:HG21 | 0.46 | 1.88 | 5 | 2 |
| 2:C:34:ILE:HG13 | 2:C:103:PHE:HA | 0.46 | 1.88 | 5 | 1 |
| 1:A:1268:THR:O | 1:A:1272:VAL:HG23 | 0.46 | 2.10 | 7 | 3 |
| 1:B:1008:GLU:HG3 | 1:B:1072:VAL:HB | 0.46 | 1.87 | 7 | 2 |
| 2:C:109:VAL:HG21 | 2:C:138:VAL:HG23 | 0.46 | 1.86 | 7 | 1 |
| 1:A:1338:LEU:HD23 | 1:A:1346:ILE:HG23 | 0.46 | 1.88 | 5 | 1 |
| 1:A:1368:TRP:CD1 | 1:A:1369:PRO:HA | 0.46 | 2.46 | 5 | 1 |
| 1:B:1133:MET:HB3 | 1:B:1316:PRO:HB3 | 0.45 | 1.88 | 5 | 4 |
| 1:A:1161:GLY:HA3 | 1:B:1329:THR:HG21 | 0.45 | 1.88 | 4 | 2 |
| 1:B:1010:LEU:HB3 | 1:B:1013:GLU:HB2 | 0.45 | 1.89 | 6 | 2 |
| 1:B:1035:VAL:HB | 1:B:1057:ILE:HD13 | 0.45 | 1.88 | 7 | 1 |
| 1:A:1329:THR:HB | 1:B:1160:ALA:HB1 | 0.45 | 1.86 | 9 | 1 |
| 1:B:1007:ARG:NH1 | 1:B:1038:GLY:HA3 | 0.45 | 2.26 | 9 | 1 |
| 1:B:1113:MET:SD | 1:B:1338:LEU:HD11 | 0.45 | 2.51 | 5 | 1 |
| 1:B:1080:ILE:HG22 | 1:B:1108:ARG:HG3 | 0.45 | 1.86 | 9 | 1 |
| 1:B:1112:VAL:HB | 1:B:1361:ILE:HB | 0.45 | 1.86 | 2 | 1 |
| 1:B:1070:LEU:HD22 | 1:B:1331:LEU:HB3 | 0.45 | 1.88 | 4 | 1 |
| 2:C:113:GLY:HA2 | 2:C:147:PHE:O | 0.45 | 2.11 | 5 | 1 |
| 1:A:1204:VAL:HG13 | 1:A:1209:ALA:HB3 | 0.45 | 1.87 | 6 | 2 |
| 1:A:1167:LYS:N | 1:A:1167:LYS:HD2 | 0.45 | 2.27 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1115:MET:HB3 | 1:B:1129:ALA:CB | 0.45 | 2.41 | 7 | 1 |
| 1:A:1263:ALA:HB1 | 1:A:1291:ASN:ND2 | 0.45 | 2.26 | 8 | 1 |
| 1:B:1139:TYR:HD2 | 1:B:1319:LEU:HD21 | 0.45 | 1.71 | 8 | 1 |
| 1:A:1083:LEU:HD12 | 1:A:1110:VAL:HG11 | 0.45 | 1.88 | 9 | 1 |
| 1:A:1335:LEU:HA | 1:A:1338:LEU:HB2 | 0.45 | 1.86 | 1 | 1 |
| 1:A:1025:GLN:HB3 | 1:A:1332:VAL:HG11 | 0.45 | 1.87 | 6 | 2 |
| 1:B:1132:SER:HB3 | 1:B:1326:LEU:HB3 | 0.45 | 1.89 | 6 | 2 |
| 1:A:1337:LEU:HD13 | 1:A:1355:ILE:HD11 | 0.45 | 1.88 | 8 | 1 |
| 1:A:1058:VAL:HB | 1:A:1062:SER:HB2 | 0.45 | 1.88 | 5 | 1 |
| 1:A:1112:VAL:HB | 1:A:1361:ILE:HB | 0.45 | 1.88 | 6 | 2 |
| 1:A:1158:THR:O | 2:C:70:PRO:HB3 | 0.45 | 2.12 | 3 | 1 |
| 1:A:1034:ALA:HA | 1:A:1056:GLU:HB3 | 0.45 | 1.88 | 4 | 1 |
| 2:C:146:VAL:HB | 2:C:170:MET:HA | 0.45 | 1.86 | 8 | 2 |
| 1:B:1167:LYS:HA | 1:B:1190:ILE:O | 0.45 | 2.12 | 7 | 1 |
| 1:B:1132:SER:O | 1:B:1136:ILE:HG12 | 0.45 | 2.11 | 8 | 1 |
| 1:B:1199:GLU:HB2 | 2:C:155:TYR:CE1 | 0.45 | 2.41 | 9 | 1 |
| 1:A:1173:ALA:HA | 1:A:1177:GLY:HA3 | 0.45 | 1.86 | 10 | 1 |
| 2:C:174:ASP:HA | 4:C:1001:NAP:N1A | 0.45 | 2.27 | 1 | 1 |
| 1:A:1275:MET:SD | 1:A:1281:ILE:HD11 | 0.45 | 2.52 | 4 | 1 |
| 1:A:1186:SER:O | 1:B:1186:SER:HB3 | 0.45 | 2.12 | 6 | 1 |
| 2:C:116:ASP:HB2 | 4:C:1001:NAP:H51N | 0.45 | 1.88 | 6 | 1 |
| 2:C:151:MET:HG2 | 2:C:170:MET:SD | 0.45 | 2.51 | 9 | 1 |
| 1:B:1115:MET:SD | 1:B:1334:LEU:HD13 | 0.45 | 2.51 | 2 | 1 |
| 2:C:130:ILE:HB | 2:C:133:MET:HB2 | 0.45 | 1.88 | 2 | 1 |
| 1:B:1089:LEU:O | 1:B:1112:VAL:HA | 0.45 | 2.12 | 5 | 1 |
| 1:A:1111:THR:HG21 | 1:A:1348:VAL:HG21 | 0.45 | 1.88 | 8 | 1 |
| 1:A:1176:ALA:HB3 | 1:A:1255:THR:HG21 | 0.45 | 1.88 | 10 | 1 |
| 2:C:149:ARG:NH2 | 4:C:1001:NAP:N6A | 0.45 | 2.65 | 10 | 1 |
| 1:A:1071:LYS:HB2 | 1:A:1091:SER:OG | 0.45 | 2.12 | 3 | 1 |
| 1:A:1135:ASN:ND2 | 1:A:1179:ALA:HB2 | 0.45 | 2.27 | 4 | 1 |
| 1:A:1010:LEU:HD12 | 1:A:1076:LEU:HD11 | 0.45 | 1.89 | 5 | 1 |
| 1:B:1328:GLY:O | 1:B:1332:VAL:HG23 | 0.45 | 2.12 | 10 | 2 |
| 1:A:1047:ASP:HA | 1:A:1050:PHE:HD2 | 0.45 | 1.71 | 4 | 1 |
| 1:B:1016:VAL:CG2 | 1:B:1039:ALA:HB1 | 0.45 | 2.42 | 5 | 1 |
| 1:B:1050:PHE:HB2 | 1:B:1057:ILE:HD11 | 0.45 | 1.86 | 5 | 2 |
| 1:B:1279:SER:O | 1:B:1307:VAL:HA | 0.45 | 2.12 | 5 | 1 |
| 1:A:1015:ARG:HG3 | 1:A:1317:GLY:HA2 | 0.45 | 1.88 | 6 | 2 |
| 1:A:1113:MET:SD | 1:A:1348:VAL:HG13 | 0.45 | 2.51 | 8 | 1 |
| 1:B:1207:MET:SD | 2:C:75:LEU:HD22 | 0.44 | 2.52 | 1 | 1 |
| 2:C:144:VAL:HB | 2:C:168:THR:HG22 | 0.44 | 1.87 | 1 | 1 |
| 1:A:1312:TYR:CB | 1:A:1315:LEU:HG | 0.44 | 2.42 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1255:THR:HA | 1:B:1284:LEU:HD22 | 0.44 | 1.89 | 8 | 1 |
| 2:C:115:ASN:HD21 | 2:C:154:GLY:HA3 | 0.44 | 1.72 | 10 | 1 |
| 1:B:1339:CYS:SG | 1:B:1342:LYS:HA | 0.44 | 2.52 | 4 | 2 |
| 1:B:1178:LEU:HD22 | 2:C:75:LEU:HG | 0.44 | 1.89 | 5 | 1 |
| 1:B:1338:LEU:O | 1:B:1347:THR:HB | 0.44 | 2.11 | 8 | 1 |
| 1:A:1328:GLY:O | 1:A:1332:VAL:HG23 | 0.44 | 2.13 | 1 | 1 |
| 1:B:1018:ALA:HB1 | 1:B:1022:THR:HB | 0.44 | 1.89 | 1 | 2 |
| 2:C:68:ILE:HD11 | 2:C:93:VAL:HG13 | 0.44 | 1.88 | 7 | 1 |
| 1:B:1125:GLN:HG3 | 1:B:1131:SER:HB3 | 0.44 | 1.88 | 10 | 1 |
| 1:B:1080:ILE:HD11 | 1:B:1101:LEU:HD12 | 0.44 | 1.89 | 1 | 1 |
| 1:A:1275:MET:HB2 | 1:A:1307:VAL:HG21 | 0.44 | 1.88 | 2 | 1 |
| 1:A:1140:ARG:NH1 | 1:A:1318:ARG:O | 0.44 | 2.50 | 6 | 2 |
| 2:C:128:SER:OG | 2:C:158:VAL:HG21 | 0.44 | 2.11 | 5 | 1 |
| 2:C:33:VAL:O | 2:C:64:VAL:HA | 0.44 | 2.12 | 7 | 3 |
| 1:B:1068:ILE:HA | 1:B:1088:THR:HB | 0.44 | 1.88 | 7 | 1 |
| 1:B:1091:SER:O | 1:B:1114:ALA:HA | 0.44 | 2.12 | 7 | 1 |
| 1:A:1021:LYS:HB2 | 1:A:1325:GLN:NE2 | 0.44 | 2.27 | 10 | 1 |
| 2:C:66:PHE:HB2 | 2:C:93:VAL:HG22 | 0.44 | 1.89 | 10 | 1 |
| 2:C:137:GLU:HB3 | 2:C:139:TRP:NE1 | 0.44 | 2.28 | 2 | 1 |
| 1:B:1090:VAL:HG13 | 1:B:1113:MET:HB2 | 0.44 | 1.90 | 3 | 1 |
| 2:C:34:ILE:HG12 | 2:C:106:THR:OG1 | 0.44 | 2.12 | 5 | 1 |
| 1:A:1255:THR:HA | 1:A:1284:LEU:HB2 | 0.44 | 1.89 | 7 | 1 |
| 1:B:1021:LYS:O | 1:B:1025:GLN:HG3 | 0.44 | 2.12 | 3 | 1 |
| 1:B:1079:GLU:HA | 1:B:1082:LEU:HD12 | 0.44 | 1.88 | 9 | 2 |
| 2:C:122:ALA:HA | 2:C:128:SER:CB | 0.44 | 2.43 | 5 | 1 |
| 1:B:1113:MET:HA | 1:B:1358:VAL:O | 0.44 | 2.12 | 9 | 1 |
| 1:B:1036:GLU:HB3 | 1:B:1039:ALA:HB2 | 0.44 | 1.89 | 10 | 2 |
| 2:C:30:SER:HB3 | 2:C:32:SER:O | 0.43 | 2.12 | 5 | 1 |
| 1:A:1312:TYR:O | 1:A:1315:LEU:HG | 0.43 | 2.13 | 3 | 1 |
| 1:B:1002:ARG:NH2 | 1:B:1065:GLN:O | 0.43 | 2.50 | 10 | 2 |
| 1:B:1156:GLN:H | 1:B:1163:VAL:HB | 0.43 | 1.74 | 8 | 1 |
| 1:A:1016:VAL:HG23 | 1:A:1039:ALA:HB1 | 0.43 | 1.90 | 3 | 1 |
| 1:A:1045:PHE:HD1 | 1:B:1277:ALA:HB3 | 0.43 | 1.73 | 5 | 1 |
| 2:C:27:LEU:HD21 | 2:C:110:LEU:HD21 | 0.43 | 1.90 | 5 | 1 |
| 1:B:1080:ILE:HG21 | 1:B:1104:LYS:HB3 | 0.43 | 1.89 | 6 | 1 |
| 1:A:1269:ARG:HG3 | 1:A:1293:GLU:HB3 | 0.43 | 1.90 | 7 | 1 |
| 1:A:1214:LEU:HD11 | 1:A:1238:GLU:HA | 0.43 | 1.89 | 6 | 1 |
| 1:A:1275:MET:HB3 | 1:A:1307:VAL:HG21 | 0.43 | 1.89 | 9 | 2 |
| 1:A:1169:MET:O | 1:A:1252:ILE:HA | 0.43 | 2.14 | 10 | 1 |
| 1:A:1342:LYS:N | 1:A:1343:ASP:HB3 | 0.43 | 2.29 | 1 | 1 |
| 1:B:1111:THR:HA | 1:B:1363:ALA:H | 0.43 | 1.74 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1127:LEU:HD11 | 1:B:1337:LEU:HD13 | 0.43 | 1.89 | 1 | 1 |
| 1:B:1332:VAL:O | 1:B:1336:LYS:HG3 | 0.43 | 2.12 | 2 | 1 |
| 1:A:1003:ILE:HA | 1:A:1068:ILE:O | 0.43 | 2.12 | 7 | 1 |
| 1:A:1097:GLN:NE2 | 1:A:1260:GLY:HA2 | 0.43 | 2.29 | 7 | 1 |
| 1:A:1131:SER:HA | 1:A:1175:VAL:HG21 | 0.43 | 1.89 | 9 | 1 |
| 1:A:1044:SER:HB3 | 1:B:1278:GLY:HA2 | 0.43 | 1.91 | 10 | 1 |
| 1:A:1169:MET:HG3 | 1:A:1212:LEU:HD11 | 0.43 | 1.90 | 10 | 1 |
| 1:B:1102:MET:HA | 1:B:1105:LEU:HD12 | 0.43 | 1.90 | 10 | 1 |
| 1:A:1167:LYS:HB3 | 1:A:1249:VAL:HG12 | 0.43 | 1.89 | 2 | 1 |
| 2:C:148:LYS:NZ | 2:C:152:ASN:OD1 | 0.43 | 2.51 | 2 | 2 |
| 2:C:34:ILE:HD11 | 2:C:102:ASP:HB3 | 0.43 | 1.90 | 3 | 1 |
| 1:A:1323:SER:O | 1:A:1327:TYR:HB3 | 0.43 | 2.14 | 5 | 1 |
| 1:A:1140:ARG:NH2 | 1:B:1147:HIS:O | 0.43 | 2.51 | 8 | 1 |
| 2:C:133:MET:HG2 | 4:C:1001:NAP:O3D | 0.43 | 2.14 | 8 | 1 |
| 1:B:1280:VAL:HG22 | 1:B:1308:LYS:HB2 | 0.43 | 1.90 | 2 | 2 |
| 1:A:1331:LEU:O | 1:A:1335:LEU:HG | 0.43 | 2.14 | 5 | 1 |
| 1:B:1356:ARG:HG3 | 1:B:1371:PRO:HD3 | 0.43 | 1.90 | 7 | 1 |
| 1:B:1121:ILE:HD12 | 1:B:1123:ARG:HB3 | 0.43 | 1.91 | 9 | 1 |
| 1:A:1045:PHE:HA | 1:B:1277:ALA:HB1 | 0.43 | 1.91 | 10 | 1 |
| 1:B:1230:MET:SD | 1:B:1234:PHE:CD2 | 0.43 | 3.12 | 2 | 1 |
| 1:A:1132:SER:O | 1:A:1135:ASN:HB3 | 0.43 | 2.14 | 3 | 1 |
| 2:C:31:HIS:O | 2:C:62:ILE:HG23 | 0.43 | 2.13 | 4 | 1 |
| 1:A:1146:ALA:HA | 1:A:1149:PHE:HB2 | 0.43 | 1.91 | 4 | 2 |
| 1:B:1024:GLU:O | 1:B:1028:LYS:HG3 | 0.43 | 2.13 | 6 | 1 |
| 1:B:1008:GLU:OE2 | 1:B:1071:LYS:HG2 | 0.43 | 2.14 | 7 | 1 |
| 1:B:1256:ALA:HB3 | 1:B:1291:ASN:OD1 | 0.43 | 2.14 | 7 | 1 |
| 1:A:1111:THR:HG23 | 1:A:1362:ARG:HG3 | 0.43 | 1.91 | 10 | 1 |
| 2:C:42:ALA:HB2 | 2:C:79:MET:HB3 | 0.43 | 1.89 | 2 | 1 |
| 1:B:1305:ASN:OD1 | 1:B:1307:VAL:HG23 | 0.43 | 2.14 | 7 | 1 |
| 2:C:39:TYR:CD1 | 2:C:74:ARG:HD3 | 0.43 | 2.49 | 9 | 1 |
| 1:B:1092:PHE:CD1 | 1:B:1116:ASP:HB3 | 0.42 | 2.48 | 1 | 1 |
| 1:B:1069:ILE:HG22 | 1:B:1071:LYS:HB2 | 0.42 | 1.89 | 2 | 1 |
| 1:A:1330:ASN:ND2 | 1:B:1160:ALA:HB2 | 0.42 | 2.29 | 4 | 1 |
| 1:A:1342:LYS:HA | 1:A:1344:GLY:H | 0.42 | 1.73 | 5 | 1 |
| 1:A:1070:LEU:HD23 | 1:A:1090:VAL:HB | 0.42 | 1.91 | 8 | 1 |
| 1:B:1136:ILE:HG21 | 1:B:1316:PRO:HA | 0.42 | 1.89 | 6 | 1 |
| 2:C:148:LYS:NZ | 4:C:1001:NAP:O3B | 0.42 | 2.52 | 8 | 1 |
| 2:C:116:ASP:HB3 | 2:C:130:ILE:HD13 | 0.42 | 1.91 | 9 | 1 |
| 2:C:118:VAL:HG23 | 2:C:162:LEU:HD13 | 0.42 | 1.90 | 1 | 1 |
| 1:A:1339:CYS:HB3 | 1:A:1342:LYS:HG2 | 0.42 | 1.91 | 4 | 1 |
| 1:A:1060:GLY:O | 1:A:1063:VAL:HG12 | 0.42 | 2.14 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 2:C:24:ALA:HB2 | 2:C:182:ILE:HG22 | 0.42 | 1.90 | 10 | 1 |
| 1:A:1287:GLN:HA | 1:A:1313:THR:HG23 | 0.42 | 1.92 | 1 | 1 |
| 1:B:1023:VAL:HG22 | 1:B:1033:VAL:HG11 | 0.42 | 1.91 | 3 | 1 |
| 1:A:1173:ALA:HB3 | 1:A:1200:VAL:HG21 | 0.42 | 1.91 | 10 | 2 |
| 2:C:115:ASN:HB3 | 4:C:1001:NAP:O1N | 0.42 | 2.13 | 9 | 1 |
| 1:B:1000:HIS:HA | 1:B:1067:GLU:HB2 | 0.42 | 1.92 | 1 | 1 |
| 2:C:118:VAL:O | 2:C:162:LEU:HD11 | 0.42 | 2.14 | 1 | 1 |
| 1:B:1119:PRO:HG2 | 1:B:1357:GLY:HA3 | 0.42 | 1.90 | 4 | 1 |
| 1:A:1196:THR:HG23 | 1:A:1234:PHE:CE2 | 0.42 | 2.49 | 5 | 1 |
| 1:A:1163:VAL:HG22 | 1:B:1326:LEU:HD21 | 0.42 | 1.91 | 6 | 1 |
| 1:A:1174:GLY:HA2 | 1:A:1200:VAL:HG11 | 0.42 | 1.92 | 7 | 1 |
| 1:A:1253:VAL:HA | 1:A:1282:VAL:HG23 | 0.42 | 1.91 | 2 | 1 |
| 2:C:146:VAL:HG21 | 2:C:162:LEU:HG | 0.42 | 1.90 | 2 | 1 |
| 1:A:1040:GLY:HA2 | 1:A:1043:ALA:HB3 | 0.42 | 1.91 | 5 | 1 |
| 1:A:1083:LEU:HD11 | 1:A:1089:LEU:HD13 | 0.42 | 1.92 | 10 | 1 |
| 1:A:1127:LEU:HD23 | 1:A:1334:LEU:HD12 | 0.42 | 1.91 | 7 | 1 |
| 1:B:1254:THR:HG23 | 1:B:1291:ASN:HB2 | 0.42 | 1.92 | 7 | 1 |
| 1:A:1045:PHE:CZ | 1:A:1321:THR:HG23 | 0.42 | 2.50 | 10 | 1 |
| 2:C:48:TYR:CZ | 2:C:86:ALA:HA | 0.42 | 2.50 | 10 | 1 |
| 1:A:1149:PHE:CE1 | 1:A:1151:ARG:HD2 | 0.42 | 2.50 | 4 | 1 |
| 1:B:1120:ARG:HB3 | 3:B:1:NAD:H1D | 0.42 | 1.92 | 10 | 1 |
| 2:C:44:ALA:HB2 | 4:C:1001:NAP:H62A | 0.42 | 1.74 | 10 | 1 |
| 2:C:111:VAL:HG13 | 2:C:114:ALA:HB3 | 0.42 | 1.91 | 10 | 1 |
| 2:C:72:ALA:HA | 4:C:1001:NAP:H52N | 0.42 | 1.91 | 2 | 1 |
| 2:C:38:GLY:HA3 | 2:C:114:ALA:HB2 | 0.42 | 1.91 | 7 | 1 |
| 1:A:1041:GLN:HE22 | 1:A:1047:ASP:HB2 | 0.42 | 1.75 | 9 | 1 |
| 1:B:1119:PRO:HB2 | 1:B:1121:ILE:HG12 | 0.42 | 1.91 | 2 | 1 |
| 1:A:1036:GLU:HG2 | 1:A:1063:VAL:HG11 | 0.42 | 1.91 | 4 | 1 |
| 2:C:64:VAL:HG13 | 2:C:92:ILE:HD12 | 0.42 | 1.92 | 4 | 1 |
| 1:A:1022:THR:O | 1:A:1026:LEU:HG | 0.42 | 2.15 | 5 | 1 |
| 1:A:1272:VAL:HG21 | 1:A:1292:CYS:SG | 0.42 | 2.55 | 6 | 1 |
| 1:A:1140:ARG:HH11 | 1:A:1319:LEU:HD13 | 0.42 | 1.75 | 9 | 1 |
| 1:B:1068:ILE:HD11 | 1:B:1346:ILE:HD11 | 0.42 | 1.91 | 10 | 1 |
| 1:A:1065:GLN:NE2 | 1:A:1084:ASN:HD21 | 0.41 | 2.13 | 2 | 1 |
| 1:B:1146:ALA:HA | 1:B:1149:PHE:HB2 | 0.41 | 1.92 | 2 | 1 |
| 1:A:1193:ALA:O | 1:A:1211:PHE:HA | 0.41 | 2.15 | 6 | 1 |
| 1:A:1071:LYS:HE2 | 1:A:1075:PRO:HA | 0.41 | 1.91 | 7 | 1 |
| 1:B:1126:SER:OG | 1:B:1127:LEU:HD12 | 0.41 | 2.14 | 7 | 1 |
| 1:A:1239:MET:SD | 1:A:1266:LEU:O | 0.41 | 2.78 | 9 | 1 |
| 1:B:1140:ARG:HH11 | 1:B:1319:LEU:HD13 | 0.41 | 1.75 | 9 | 1 |
| 1:B:1164:PRO:HA | 1:B:1165:PRO:HD3 | 0.41 | 1.74 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:1263:ALA:CB | 1:B:1285:ALA:HB1 | 0.41 | 2.45 | 4 | 1 |
| 1:A:1135:ASN:HA | 1:A:1176:ALA:HA | 0.41 | 1.92 | 5 | 1 |
| 2:C:129:PRO:HD2 | 2:C:156:ALA:HB2 | 0.41 | 1.92 | 1 | 1 |
| 1:A:1068:ILE:HG12 | 1:A:1088:THR:HB | 0.41 | 1.92 | 2 | 1 |
| 1:B:1119:PRO:CG | 1:B:1357:GLY:HA3 | 0.41 | 2.45 | 4 | 1 |
| 2:C:65:ARG:NH2 | 2:C:94:LEU:HD22 | 0.41 | 2.30 | 7 | 1 |
| 1:B:1125:GLN:HE21 | 1:B:1131:SER:HB3 | 0.41 | 1.75 | 8 | 1 |
| 1:A:1338:LEU:HG | 1:A:1347:THR:O | 0.41 | 2.15 | 10 | 1 |
| 1:A:1069:ILE:HG12 | 1:A:1087:THR:CG2 | 0.41 | 2.45 | 1 | 1 |
| 1:A:1292:CYS:SG | 1:A:1309:VAL:HG11 | 0.41 | 2.55 | 7 | 1 |
| 1:B:1115:MET:HB3 | 1:B:1129:ALA:HB2 | 0.41 | 1.91 | 7 | 1 |
| 1:B:1118:VAL:CG1 | 1:B:1124:ALA:HB1 | 0.41 | 2.45 | 7 | 1 |
| 1:A:1254:THR:HG22 | 1:A:1291:ASN:HB2 | 0.41 | 1.92 | 10 | 1 |
| 2:C:26:LEU:HA | 2:C:29:ASN:HB3 | 0.41 | 1.90 | 5 | 1 |
| 1:A:1216:PHE:HE1 | 1:A:1233:ALA:HB1 | 0.41 | 1.74 | 8 | 1 |
| 1:A:1239:MET:SD | 1:A:1242:PHE:HD2 | 0.41 | 2.39 | 1 | 1 |
| 1:B:1109:ASN:HA | 1:B:1364:GLY:CA | 0.41 | 2.46 | 2 | 1 |
| 1:A:1264:PRO:HG2 | 1:A:1291:ASN:ND2 | 0.41 | 2.31 | 5 | 1 |
| 1:A:1356:ARG:NH1 | 1:A:1367:THR:O | 0.41 | 2.53 | 6 | 1 |
| 1:B:1127:LEU:HD22 | 1:B:1354:VAL:HG11 | 0.41 | 1.92 | 7 | 1 |
| 1:A:1215:ASP:H | 1:A:1241:LEU:HD21 | 0.41 | 1.75 | 8 | 1 |
| 1:A:1333:ASN:HA | 1:A:1336:LYS:HD2 | 0.41 | 1.92 | 9 | 1 |
| 1:B:1015:ARG:HG2 | 1:B:1323:SER:HB3 | 0.41 | 1.93 | 2 | 1 |
| 2:C:148:LYS:HE3 | 2:C:150:SER:O | 0.41 | 2.16 | 3 | 1 |
| 1:A:1098:ASN:HB3 | 1:A:1101:LEU:HB3 | 0.41 | 1.93 | 5 | 1 |
| 2:C:58:ARG:NH1 | 2:C:63:ASN:HA | 0.41 | 2.30 | 5 | 1 |
| 1:B:1346:ILE:HG22 | 1:B:1348:VAL:HG23 | 0.41 | 1.91 | 10 | 1 |
| 1:A:1043:ALA:HA | 1:A:1320:PRO:HB2 | 0.41 | 1.92 | 1 | 1 |
| 1:A:1020:PRO:HD2 | 1:A:1045:PHE:CD2 | 0.41 | 2.50 | 4 | 1 |
| 1:A:1164:PRO:HA | 1:A:1165:PRO:HD2 | 0.41 | 1.79 | 7 | 1 |
| 1:A:1169:MET:SD | 1:A:1245:GLN:HB3 | 0.41 | 2.55 | 8 | 1 |
| 1:B:1121:ILE:HB | 2:C:131:ALA:O | 0.41 | 2.16 | 10 | 1 |
| 1:B:1148:GLU:HG3 | 1:B:1300:ILE:HD13 | 0.41 | 1.92 | 1 | 1 |
| 1:B:1295:THR:O | 1:B:1297:PRO:HD3 | 0.41 | 2.16 | 1 | 1 |
| 2:C:47:GLN:O | 2:C:50:VAL:HG12 | 0.41 | 2.15 | 3 | 1 |
| 1:A:1003:ILE:HD13 | 1:A:1335:LEU:HD13 | 0.41 | 1.93 | 4 | 1 |
| 1:A:1264:PRO:HG2 | 1:A:1291:ASN:HD21 | 0.41 | 1.76 | 5 | 1 |
| 1:B:1258:ILE:HG23 | 3:B:1:NAD:H8A | 0.41 | 1.93 | 7 | 1 |
| 2:C:48:TYR:CD1 | 2:C:49:PRO:HD3 | 0.41 | 2.50 | 7 | 1 |
| 1:B:1149:PHE:CZ | 1:B:1250:ASP:HB3 | 0.41 | 2.51 | 8 | 1 |
| 2:C:26:LEU:HB3 | 2:C:108:THR:OG1 | 0.41 | 2.15 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:1125:GLN:HA | 1:A:1128:ASP:HB3 | 0.41 | 1.92 | 10 | 1 |
| 1:A:1009:ARG:HH11 | 1:A:1079:GLU:HG2 | 0.41 | 1.75 | 2 | 1 |
| 1:B:1092:PHE:HZ | 1:B:1133:MET:HG3 | 0.41 | 1.75 | 6 | 1 |
| 1:A:1114:ALA:HB3 | 1:A:1117:SER:HB2 | 0.41 | 1.92 | 7 | 1 |
| 2:C:37:PRO:HG3 | 2:C:41:MET:SD | 0.41 | 2.57 | 7 | 1 |
| 1:B:1015:ARG:HD3 | 1:B:1133:MET:SD | 0.41 | 2.55 | 9 | 1 |
| 1:B:1176:ALA:HB3 | 1:B:1255:THR:HG21 | 0.41 | 1.91 | 9 | 1 |
| 2:C:128:SER:HB3 | 2:C:158:VAL:HG21 | 0.41 | 1.93 | 9 | 1 |
| 1:B:1177:GLY:O | 1:B:1181:ILE:HG13 | 0.40 | 2.17 | 1 | 1 |
| 1:B:1350:PHE:HB2 | 1:B:1362:ARG:NH1 | 0.40 | 2.31 | 3 | 1 |
| 1:A:1332:VAL:O | 1:A:1336:LYS:HG3 | 0.40 | 2.17 | 2 | 1 |
| 1:A:1148:GLU:HG3 | 1:A:1300:ILE:HD13 | 0.40 | 1.92 | 3 | 1 |
| 1:B:1092:PHE:HD1 | 1:B:1116:ASP:HB3 | 0.40 | 1.75 | 3 | 1 |
| 1:B:1152:PHE:HE2 | 1:B:1156:GLN:NE2 | 0.40 | 2.13 | 3 | 1 |
| 2:C:35:ILE:HG12 | 2:C:110:LEU:HD12 | 0.40 | 1.93 | 3 | 1 |
| 2:C:70:PRO:HG3 | 2:C:96:MET:SD | 0.40 | 2.56 | 4 | 1 |
| 1:B:1003:ILE:HA | 1:B:1068:ILE:O | 0.40 | 2.16 | 5 | 1 |
| 1:A:1348:VAL:HB | 1:A:1362:ARG:NH2 | 0.40 | 2.30 | 6 | 1 |
| 1:A:1151:ARG:NH2 | 1:A:1279:SER:OG | 0.40 | 2.54 | 7 | 1 |
| 1:B:1064:TRP:HA | 1:B:1069:ILE:HD11 | 0.40 | 1.92 | 7 | 1 |
| 1:A:1016:VAL:HG12 | 1:A:1043:ALA:HB2 | 0.40 | 1.93 | 9 | 1 |
| 1:A:1340:LYS:HD2 | 1:A:1347:THR:HG21 | 0.40 | 1.92 | 9 | 1 |
| 1:B:1024:GLU:HA | 1:B:1027:LEU:HD12 | 0.40 | 1.93 | 10 | 1 |
| 2:C:108:THR:HA | 2:C:143:ASN:O | 0.40 | 2.16 | 10 | 1 |
| 2:C:50:VAL:HA | 2:C:53:ILE:HG22 | 0.40 | 1.93 | 5 | 1 |
| 1:A:1235:ILE:O | 1:A:1239:MET:HG2 | 0.40 | 2.16 | 6 | 1 |
| 2:C:32:SER:HB2 | 2:C:106:THR:OG1 | 0.40 | 2.17 | 9 | 1 |
| 2:C:180:ASP:O | 2:C:183:LEU:HG | 0.40 | 2.16 | 10 | 1 |
| 1:A:1140:ARG:CZ | 1:A:1318:ARG:HB3 | 0.40 | 2.46 | 3 | 1 |
| 2:C:45:GLN:HG3 | 2:C:176:LYS:HG3 | 0.40 | 1.92 | 7 | 1 |
| 1:A:1152:PHE:HB2 | 1:A:1163:VAL:CG1 | 0.40 | 2.47 | 9 | 1 |
| 2:C:52:GLU:O | 2:C:56:LYS:HE2 | 0.40 | 2.16 | 9 | 1 |
| 1:A:1113:MET:HA | 1:A:1358:VAL:O | 0.40 | 2.17 | 1 | 1 |
| 1:A:1231:SER:O | 1:A:1234:PHE:HB3 | 0.40 | 2.16 | 1 | 1 |
| 2:C:116:ASP:HA | 2:C:119:ASN:CB | 0.40 | 2.46 | 4 | 1 |
| 1:B:1036:GLU:HB2 | 1:B:1063:VAL:HG11 | 0.40 | 1.94 | 5 | 1 |
| 1:B:1200:VAL:HA | 1:B:1203:GLN:HG2 | 0.40 | 1.92 | 6 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 363/401 (91%) | 323±5 (89±1%) | 36±5 (10±1%) | 4±1 (1±0%) | 18 66 |
| 1 | B | 361/401 (90%) | 322±3 (89±1%) | 34±3 (9±1%) | 6±2 (2±1%) | 13 57 |
| 2 | C | 165/186 (89%) | 132±3 (80±2%) | 25±3 (15±2%) | 8±1 (5±1%) | 4 26 |
| All | All | 8890/9880 (90%) | 7769 (87%) | 941 (11%) | 180 (2%) | 11 52 |

All 90 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 2 | C | 75 | LEU | 8 |
| 1 | A | 1343 | ASP | 7 |
| 1 | B | 1320 | PRO | 6 |
| 2 | C | 159 | GLN | 6 |
| 1 | A | 1286 | ALA | 6 |
| 2 | C | 31 | HIS | 5 |
| 2 | C | 137 | GLU | 5 |
| 1 | B | 1318 | ARG | 4 |
| 2 | C | 78 | HIS | 4 |
| 1 | B | 1372 | PRO | 4 |
| 1 | B | 1259 | PRO | 4 |
| 2 | C | 115 | ASN | 4 |
| 1 | B | 1231 | SER | 4 |
| 1 | B | 1175 | VAL | 3 |
| 1 | B | 1256 | ALA | 3 |
| 2 | C | 114 | ALA | 3 |
| 1 | B | 1233 | ALA | 3 |
| 2 | C | 158 | VAL | 3 |
| 1 | A | 1001 | GLY | 3 |
| 1 | A | 1363 | ALA | 3 |
| 2 | C | 45 | GLN | 3 |
| 1 | A | 1372 | PRO | 3 |
| 1 | A | 1154 | THR | 2 |
| 1 | A | 1208 | GLY | 2 |
| 1 | B | 1122 | SER | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 1232 | ASP | 2 |
| 2 | C | 71 | VAL | 2 |
| 2 | C | 99 | ILE | 2 |
| 2 | C | 140 | LYS | 2 |
| 1 | B | 1346 | ILE | 2 |
| 2 | C | 138 | VAL | 2 |
| 1 | B | 1235 | ILE | 2 |
| 2 | C | 37 | PRO | 2 |
| 2 | C | 70 | PRO | 2 |
| 2 | C | 127 | LYS | 2 |
| 2 | C | 96 | MET | 2 |
| 2 | C | 63 | ASN | 2 |
| 1 | A | 1256 | ALA | 2 |
| 1 | B | 1363 | ALA | 2 |
| 2 | C | 132 | GLY | 2 |
| 1 | A | 1037 | SER | 1 |
| 1 | A | 1092 | PHE | 1 |
| 1 | B | 1054 | GLY | 1 |
| 1 | B | 1295 | THR | 1 |
| 2 | C | 130 | ILE | 1 |
| 2 | C | 141 | ALA | 1 |
| 2 | C | 156 | ALA | 1 |
| 1 | B | 1160 | ALA | 1 |
| 1 | B | 1286 | ALA | 1 |
| 1 | B | 1369 | PRO | 1 |
| 1 | A | 1010 | LEU | 1 |
| 1 | A | 1015 | ARG | 1 |
| 2 | C | 68 | ILE | 1 |
| 2 | C | 100 | ASN | 1 |
| 2 | C | 154 | GLY | 1 |
| 1 | B | 1099 | PRO | 1 |
| 1 | B | 1159 | ALA | 1 |
| 2 | C | 105 | ASP | 1 |
| 1 | A | 1020 | PRO | 1 |
| 1 | B | 1043 | ALA | 1 |
| 2 | C | 185 | ALA | 1 |
| 1 | A | 1060 | GLY | 1 |
| 1 | A | 1074 | ALA | 1 |
| 1 | A | 1085 | PRO | 1 |
| 1 | B | 1011 | THR | 1 |
| 1 | B | 1198 | PRO | 1 |
| 1 | B | 1314 | ASP | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 2 | C | 76 | PRO | 1 |
| 2 | C | 107 | ASP | 1 |
| 2 | C | 117 | THR | 1 |
| 1 | A | 1297 | PRO | 1 |
| 1 | B | 1012 | ASN | 1 |
| 1 | B | 1030 | GLY | 1 |
| 1 | B | 1085 | PRO | 1 |
| 1 | B | 1290 | GLY | 1 |
| 1 | B | 1297 | PRO | 1 |
| 2 | C | 157 | GLY | 1 |
| 2 | C | 160 | ASN | 1 |
| 1 | A | 1054 | GLY | 1 |
| 1 | A | 1072 | VAL | 1 |
| 1 | A | 1120 | ARG | 1 |
| 1 | A | 1359 | THR | 1 |
| 2 | C | 69 | HIS | 1 |
| 2 | C | 87 | LYS | 1 |
| 2 | C | 121 | ALA | 1 |
| 2 | C | 162 | LEU | 1 |
| 2 | C | 183 | LEU | 1 |
| 1 | B | 1289 | GLY | 1 |
| 2 | C | 86 | ALA | 1 |
| 2 | C | 89 | PRO | 1 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 288/317 (91%) | 272±3 (95±1%) | 16±3 (5±1%) | 25 | 74 |
| 1 | B | 290/317 (91%) | 274±2 (94±1%) | 16±2 (6±1%) | 24 | 73 |
| 2 | C | 135/153 (88%) | 122±2 (90±1%) | 13±2 (10±1%) | 12 | 58 |
| All | All | 7130/7870 (91%) | 6677 (94%) | 453 (6%) | 21 | 70 |

All 198 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 2 | C | 47 | GLN | 10 |
| 2 | C | 79 | MET | 10 |
| 1 | B | 1287 | GLN | 9 |
| 2 | C | 159 | GLN | 9 |
| 2 | C | 176 | LYS | 9 |
| 1 | B | 1045 | PHE | 8 |
| 1 | A | 1020 | PRO | 7 |
| 1 | A | 1282 | VAL | 7 |
| 1 | B | 1014 | THR | 7 |
| 1 | A | 1083 | LEU | 6 |
| 1 | A | 1254 | THR | 6 |
| 1 | B | 1020 | PRO | 6 |
| 1 | A | 1045 | PHE | 6 |
| 1 | A | 1149 | PHE | 6 |
| 1 | B | 1048 | LYS | 6 |
| 1 | B | 1199 | GLU | 6 |
| 1 | B | 1019 | THR | 5 |
| 1 | B | 1063 | VAL | 5 |
| 1 | B | 1135 | ASN | 5 |
| 2 | C | 21 | GLU | 5 |
| 2 | C | 45 | GLN | 5 |
| 1 | A | 1343 | ASP | 5 |
| 1 | B | 1149 | PHE | 5 |
| 1 | B | 1350 | PHE | 5 |
| 1 | A | 1032 | THR | 4 |
| 1 | A | 1067 | GLU | 4 |
| 2 | C | 140 | LYS | 4 |
| 1 | B | 1077 | ASP | 4 |
| 1 | A | 1100 | GLU | 4 |
| 2 | C | 25 | GLU | 4 |
| 1 | A | 1014 | THR | 4 |
| 1 | A | 1046 | ASP | 3 |
| 1 | B | 1022 | THR | 3 |
| 1 | B | 1084 | ASN | 3 |
| 2 | C | 50 | VAL | 3 |
| 2 | C | 115 | ASN | 3 |
| 2 | C | 151 | MET | 3 |
| 1 | A | 1072 | VAL | 3 |
| 1 | A | 1152 | PHE | 3 |
| 1 | A | 1196 | THR | 3 |
| 1 | B | 1196 | THR | 3 |
| 1 | B | 1373 | ILE | 3 |
| 2 | C | 52 | GLU | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 2 | C | 90 | TYR | 3 |
| 2 | C | 102 | ASP | 3 |
| 2 | C | 155 | TYR | 3 |
| 1 | A | 1077 | ASP | 3 |
| 1 | A | 1084 | ASN | 3 |
| 1 | A | 1130 | LEU | 3 |
| 1 | B | 1214 | LEU | 3 |
| 2 | C | 22 | GLU | 3 |
| 2 | C | 123 | GLN | 3 |
| 2 | C | 152 | ASN | 3 |
| 1 | A | 1022 | THR | 3 |
| 1 | A | 1313 | THR | 3 |
| 2 | C | 74 | ARG | 3 |
| 2 | C | 166 | GLU | 3 |
| 1 | A | 1019 | THR | 3 |
| 1 | B | 1113 | MET | 3 |
| 1 | B | 1367 | THR | 3 |
| 1 | A | 1108 | ARG | 2 |
| 1 | A | 1119 | PRO | 2 |
| 1 | A | 1301 | PHE | 2 |
| 1 | B | 1288 | ASN | 2 |
| 1 | B | 1294 | TYR | 2 |
| 1 | B | 1313 | THR | 2 |
| 1 | B | 1352 | ASP | 2 |
| 2 | C | 58 | ARG | 2 |
| 2 | C | 142 | GLN | 2 |
| 1 | A | 1158 | THR | 2 |
| 1 | A | 1268 | THR | 2 |
| 1 | A | 1312 | TYR | 2 |
| 1 | A | 1321 | THR | 2 |
| 1 | A | 1369 | PRO | 2 |
| 1 | A | 1371 | PRO | 2 |
| 1 | B | 1064 | TRP | 2 |
| 1 | B | 1120 | ARG | 2 |
| 1 | B | 1365 | GLU | 2 |
| 2 | C | 75 | LEU | 2 |
| 2 | C | 161 | PRO | 2 |
| 2 | C | 186 | LEU | 2 |
| 1 | A | 1122 | SER | 2 |
| 1 | A | 1123 | ARG | 2 |
| 1 | A | 1247 | LYS | 2 |
| 1 | A | 1294 | TYR | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 1213 | GLU | 2 |
| 2 | C | 117 | THR | 2 |
| 1 | A | 1048 | LYS | 2 |
| 1 | A | 1065 | GLN | 2 |
| 1 | B | 1041 | GLN | 2 |
| 1 | B | 1268 | THR | 2 |
| 1 | B | 1230 | MET | 2 |
| 1 | B | 1273 | ASP | 2 |
| 1 | B | 1321 | THR | 2 |
| 2 | C | 103 | PHE | 2 |
| 1 | B | 1067 | GLU | 2 |
| 1 | B | 1085 | PRO | 2 |
| 1 | B | 1100 | GLU | 2 |
| 1 | A | 1255 | THR | 2 |
| 2 | C | 26 | LEU | 2 |
| 1 | A | 1047 | ASP | 2 |
| 1 | A | 1273 | ASP | 2 |
| 1 | A | 1092 | PHE | 1 |
| 1 | A | 1110 | VAL | 1 |
| 1 | A | 1203 | GLN | 1 |
| 1 | A | 1216 | PHE | 1 |
| 1 | A | 1224 | ASP | 1 |
| 1 | A | 1367 | THR | 1 |
| 1 | B | 1008 | GLU | 1 |
| 1 | B | 1047 | ASP | 1 |
| 1 | B | 1062 | SER | 1 |
| 1 | B | 1068 | ILE | 1 |
| 1 | B | 1312 | TYR | 1 |
| 2 | C | 23 | THR | 1 |
| 2 | C | 83 | LEU | 1 |
| 2 | C | 101 | ASP | 1 |
| 1 | A | 1085 | PRO | 1 |
| 1 | A | 1116 | ASP | 1 |
| 1 | A | 1126 | SER | 1 |
| 1 | A | 1151 | ARG | 1 |
| 1 | A | 1226 | TYR | 1 |
| 1 | A | 1270 | GLU | 1 |
| 1 | A | 1365 | GLU | 1 |
| 1 | B | 1099 | PRO | 1 |
| 1 | B | 1103 | GLN | 1 |
| 1 | B | 1152 | PHE | 1 |
| 1 | B | 1231 | SER | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 1372 | PRO | 1 |
| 2 | C | 37 | PRO | 1 |
| 1 | A | 1202 | GLU | 1 |
| 1 | B | 1032 | THR | 1 |
| 1 | B | 1059 | GLU | 1 |
| 1 | B | 1088 | THR | 1 |
| 1 | B | 1125 | GLN | 1 |
| 1 | B | 1232 | ASP | 1 |
| 2 | C | 78 | HIS | 1 |
| 2 | C | 85 | GLU | 1 |
| 1 | A | 1036 | GLU | 1 |
| 1 | A | 1207 | MET | 1 |
| 1 | A | 1338 | LEU | 1 |
| 1 | A | 1354 | VAL | 1 |
| 1 | B | 1051 | VAL | 1 |
| 1 | B | 1065 | GLN | 1 |
| 1 | B | 1078 | ASP | 1 |
| 1 | B | 1234 | PHE | 1 |
| 1 | B | 1248 | GLU | 1 |
| 1 | B | 1270 | GLU | 1 |
| 1 | B | 1282 | VAL | 1 |
| 2 | C | 49 | PRO | 1 |
| 2 | C | 80 | ASN | 1 |
| 2 | C | 92 | ILE | 1 |
| 1 | B | 1021 | LYS | 1 |
| 1 | B | 1058 | VAL | 1 |
| 1 | B | 1061 | ASN | 1 |
| 1 | B | 1297 | PRO | 1 |
| 2 | C | 125 | ASP | 1 |
| 1 | A | 1058 | VAL | 1 |
| 1 | A | 1350 | PHE | 1 |
| 1 | B | 1036 | GLU | 1 |
| 1 | B | 1158 | THR | 1 |
| 1 | B | 1200 | VAL | 1 |
| 1 | B | 1271 | MET | 1 |
| 1 | B | 1308 | LYS | 1 |
| 2 | C | 108 | THR | 1 |
| 2 | C | 116 | ASP | 1 |
| 2 | C | 120 | PRO | 1 |
| 2 | C | 135 | VAL | 1 |
| 1 | A | 1093 | ILE | 1 |
| 1 | A | 1232 | ASP | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 1097 | GLN | 1 |
| 1 | B | 1258 | ILE | 1 |
| 1 | B | 1342 | LYS | 1 |
| 2 | C | 147 | PHE | 1 |
| 1 | A | 1154 | THR | 1 |
| 1 | A | 1156 | GLN | 1 |
| 1 | B | 998 | HIS | 1 |
| 1 | B | 1000 | HIS | 1 |
| 1 | B | 1012 | ASN | 1 |
| 1 | B | 1109 | ASN | 1 |
| 1 | A | 1015 | ARG | 1 |
| 1 | A | 1175 | VAL | 1 |
| 1 | A | 1199 | GLU | 1 |
| 1 | A | 1248 | GLU | 1 |
| 1 | A | 1275 | MET | 1 |
| 1 | A | 1334 | LEU | 1 |
| 1 | B | 1275 | MET | 1 |
| 2 | C | 56 | LYS | 1 |
| 2 | C | 107 | ASP | 1 |
| 2 | C | 150 | SER | 1 |
| 1 | A | 1041 | GLN | 1 |
| 1 | A | 1063 | VAL | 1 |
| 1 | A | 1316 | PRO | 1 |
| 1 | B | 1339 | CYS | 1 |
| 1 | B | 1340 | LYS | 1 |
| 2 | C | 96 | MET | 1 |
| 2 | C | 119 | ASN | 1 |
| 2 | C | 139 | TRP | 1 |
| 2 | C | 169 | HIS | 1 |

### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | NAD | B | 1 | - | 42,48,48 | 1.40±0.11 | 5±1 (11±3%) |
| 4 | NAP | C | 1001 | - | 46,52,52 | 1.50±0.11 | 6±1 (13±2%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | NAD | B | 1 | - | 50,73,73 | 2.06±0.26 | 8±1 (16±2%) |
| 4 | NAP | C | 1001 | - | 61,80,80 | 1.88±0.19 | 8±2 (13±3%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAD | B | 1 | - | - | 0±0,26,62,62 | 0±0,5,5,5 |
| 4 | NAP | C | 1001 | - | - | 0±0,31,67,67 | 0±0,5,5,5 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 3 | B | 1 | NAD | C2N-N1N | 7.29 | 1.43 | 1.35 | 1 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 4 | C | 1001 | NAP | C2N-N1N | 7.04 | 1.42 | 1.35 | 1 | 10 |
| 4 | C | 1001 | NAP | PA-O3 | 4.76 | 1.64 | 1.59 | 1 | 6 |
| 3 | B | 1 | NAD | O4D-C1D | 4.63 | 1.47 | 1.40 | 4 | 8 |
| 4 | C | 1001 | NAP | O4D-C1D | 3.85 | 1.45 | 1.40 | 9 | 10 |
| 4 | C | 1001 | NAP | O4B-C1B | 3.75 | 1.45 | 1.40 | 8 | 7 |
| 4 | C | 1001 | NAP | PN-O3 | 3.67 | 1.63 | 1.59 | 3 | 2 |
| 4 | C | 1001 | NAP | C3N-C7N | 3.44 | 1.55 | 1.50 | 3 | 4 |
| 3 | B | 1 | NAD | O4B-C1B | 3.34 | 1.45 | 1.40 | 9 | 7 |
| 3 | B | 1 | NAD | PA-O3 | 3.24 | 1.63 | 1.59 | 5 | 3 |
| 3 | B | 1 | NAD | C6N-N1N | 3.19 | 1.42 | 1.35 | 6 | 9 |
| 4 | C | 1001 | NAP | C6N-N1N | 3.10 | 1.42 | 1.35 | 5 | 9 |
| 3 | B | 1 | NAD | C3N-C7N | 2.68 | 1.54 | 1.50 | 9 | 3 |
| 4 | C | 1001 | NAP | P2B-O2X | 2.50 | 1.45 | 1.54 | 8 | 4 |
| 3 | B | 1 | NAD | C5A-N7A | 2.50 | 1.30 | 1.39 | 4 | 7 |
| 4 | C | 1001 | NAP | C5A-N7A | 2.37 | 1.31 | 1.39 | 2 | 6 |
| 4 | C | 1001 | NAP | C2A-N3A | 2.23 | 1.35 | 1.32 | 3 | 2 |
| 3 | B | 1 | NAD | C5N-C4N | 2.12 | 1.42 | 1.38 | 8 | 1 |
| 4 | C | 1001 | NAP | P2B-O2B | 2.09 | 1.63 | 1.59 | 8 | 1 |
| 3 | B | 1 | NAD | C2N-C3N | 2.01 | 1.42 | 1.39 | 5 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 3 | B | 1 | NAD | C4B-O4B-C1B | 11.56 | 99.34 | 109.92 | 3 | 9 |
| 4 | C | 1001 | NAP | C4D-O4D-C1D | 10.37 | 100.43 | 109.92 | 10 | 9 |
| 4 | C | 1001 | NAP | O4B-C1B-N9A | 9.12 | 120.84 | 108.75 | 4 | 8 |
| 4 | C | 1001 | NAP | C4B-O4B-C1B | 8.81 | 101.85 | 109.92 | 3 | 10 |
| 3 | B | 1 | NAD | C4D-O4D-C1D | 8.60 | 102.05 | 109.92 | 8 | 9 |
| 3 | B | 1 | NAD | O4B-C1B-N9A | 7.56 | 118.77 | 108.75 | 7 | 10 |
| 3 | B | 1 | NAD | N3A-C2A-N1A | 5.89 | 120.68 | 128.67 | 9 | 10 |
| 4 | C | 1001 | NAP | N3A-C2A-N1A | 5.58 | 121.10 | 128.67 | 5 | 10 |
| 3 | B | 1 | NAD | C4A-C5A-N7A | 5.04 | 114.66 | 109.34 | 4 | 10 |
| 4 | C | 1001 | NAP | C4A-C5A-N7A | 4.53 | 114.12 | 109.34 | 2 | 10 |
| 3 | B | 1 | NAD | C6A-C5A-C4A | 3.83 | 125.36 | 117.90 | 2 | 10 |
| 4 | C | 1001 | NAP | C6N-N1N-C2N | 3.75 | 118.68 | 121.88 | 1 | 8 |
| 4 | C | 1001 | NAP | O2B-P2B-O1X | 3.25 | 97.75 | 109.33 | 4 | 7 |
| 3 | B | 1 | NAD | C5N-C4N-C3N | 3.24 | 123.55 | 120.36 | 5 | 3 |
| 3 | B | 1 | NAD | C6N-N1N-C2N | 2.98 | 119.35 | 121.88 | 4 | 7 |
| 3 | B | 1 | NAD | C5A-C6A-N1A | 2.80 | 113.55 | 120.23 | 2 | 1 |
| 4 | C | 1001 | NAP | N6A-C6A-N1A | 2.77 | 124.25 | 118.33 | 1 | 6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 4 | C | 1001 | NAP | C6A-C5A-C4A | 2.64 | 123.03 | 117.90 | 4 | 4 |
| 3 | B | 1 | NAD | O5D-C5D-C4D | 2.63 | 117.96 | 108.99 | 8 | 1 |
| 3 | B | 1 | NAD | N6A-C6A-N1A | 2.63 | 123.95 | 118.33 | 2 | 4 |
| 4 | C | 1001 | NAP | C5N-C4N-C3N | 2.60 | 122.92 | 120.36 | 4 | 1 |
| 4 | C | 1001 | NAP | O4B-C4B-C5B | 2.57 | 117.58 | 109.33 | 10 | 1 |
| 4 | C | 1001 | NAP | C2D-C3D-C4D | 2.55 | 97.69 | 102.61 | 2 | 1 |
| 4 | C | 1001 | NAP | C2N-C3N-C4N | 2.47 | 121.13 | 118.26 | 9 | 1 |
| 3 | B | 1 | NAD | C5A-C6A-N6A | 2.42 | 123.99 | 120.31 | 9 | 1 |
| 4 | C | 1001 | NAP | O7N-C7N-C3N | 2.36 | 122.49 | 119.60 | 4 | 2 |
| 3 | B | 1 | NAD | O4B-C4B-C5B | 2.32 | 116.78 | 109.33 | 7 | 6 |
| 4 | C | 1001 | NAP | C5A-C6A-N1A | 2.32 | 114.71 | 120.23 | 7 | 2 |
| 4 | C | 1001 | NAP | C3N-C7N-N7N | 2.26 | 114.95 | 117.74 | 4 | 2 |
| 3 | B | 1 | NAD | C1B-N9A-C4A | 2.17 | 122.82 | 126.64 | 4 | 2 |
| 4 | C | 1001 | NAP | C3B-C2B-C1B | 2.06 | 106.75 | 102.81 | 9 | 1 |
| 4 | C | 1001 | NAP | O2X-P2B-O1X | 2.06 | 118.85 | 110.83 | 4 | 1 |

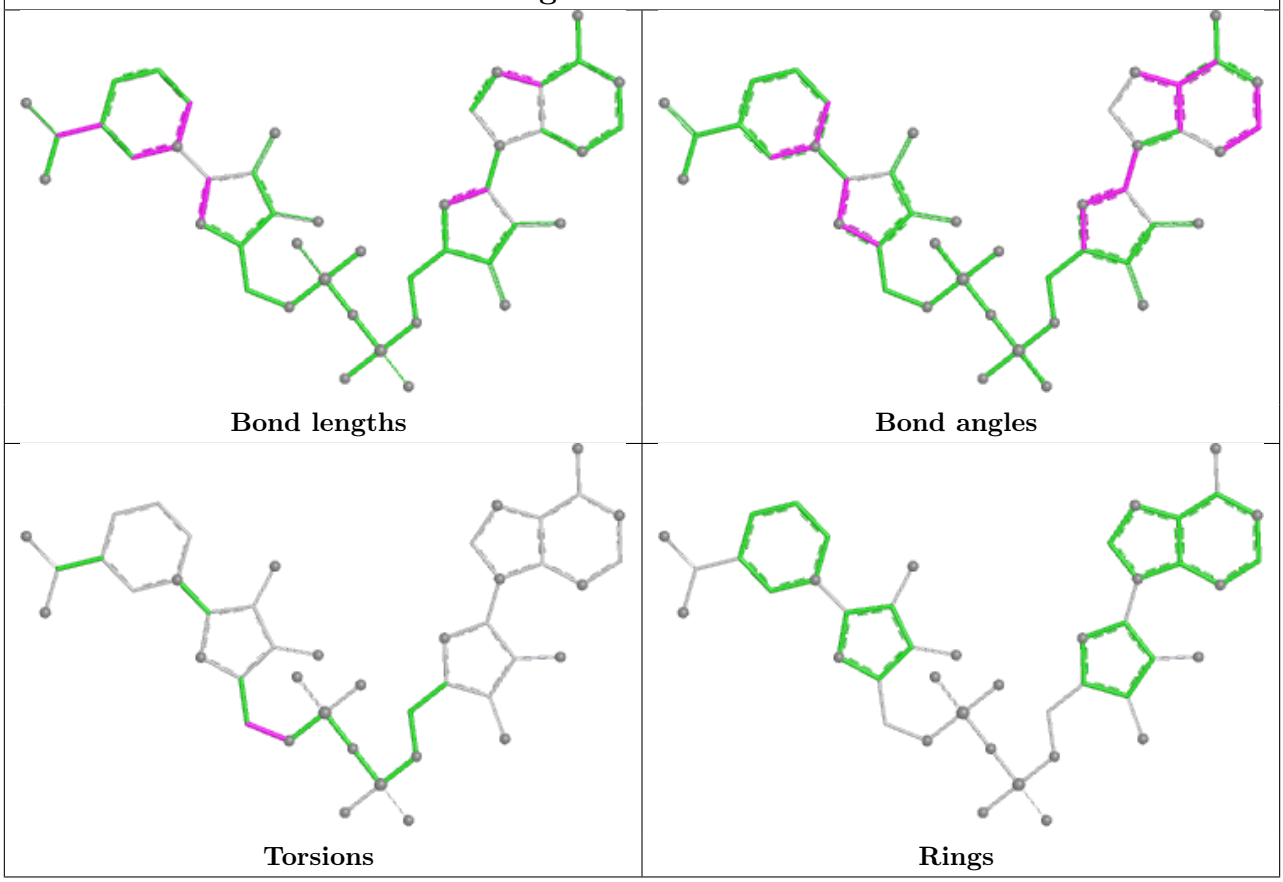
There are no chirality outliers.

There are no torsion outliers.

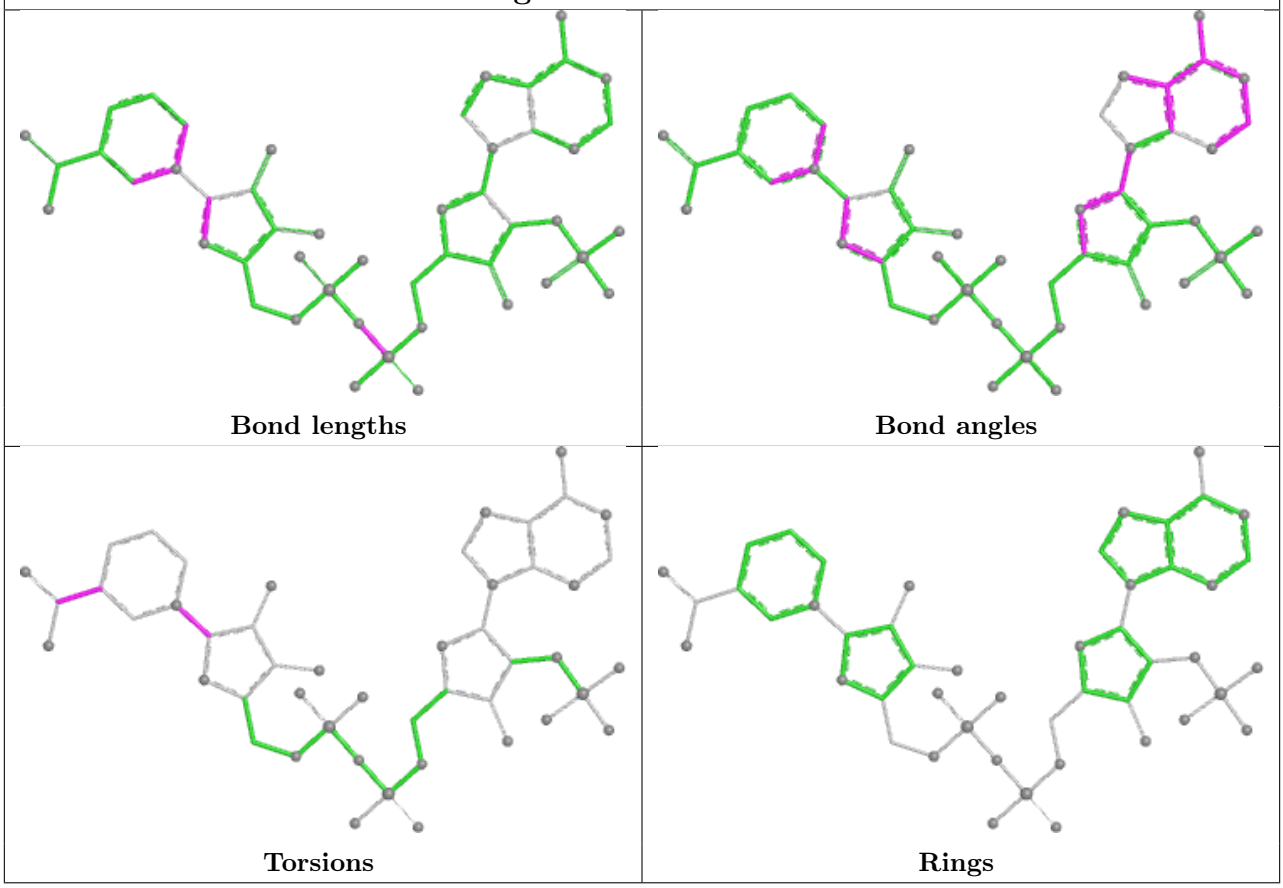
There are no ring outliers.

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

**Ligand NAD B 1**



**Ligand NAP C 1001**




## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided