



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:20 PM BST

PDB ID : 1PJZ  
Title : Solution structure of thiopurine methyltransferase from *Pseudomonas syringae*  
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Deposited on : 2003-06-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

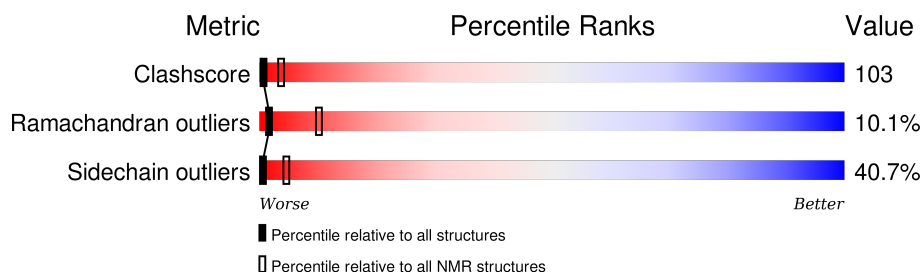
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 203    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:3-A:201 (199)       | 0.42              | 2            |

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 2 single-model clusters were found.

| Cluster number        | Models  |
|-----------------------|---|
| 1                     | 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 19 |
| 2                     | 1, 6  |
| Single-model clusters | 17; 20  |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3097 atoms, of which 1520 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thiopurine S-methyltransferase.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|-------|
| 1   | A     | 201      | Total | C   | H    | N   | O   | S  | 0     |
|     |       |          | 3097  | 998 | 1520 | 275 | 294 | 10 |       |

There are 2 discrepancies between the modelled and reference sequences:

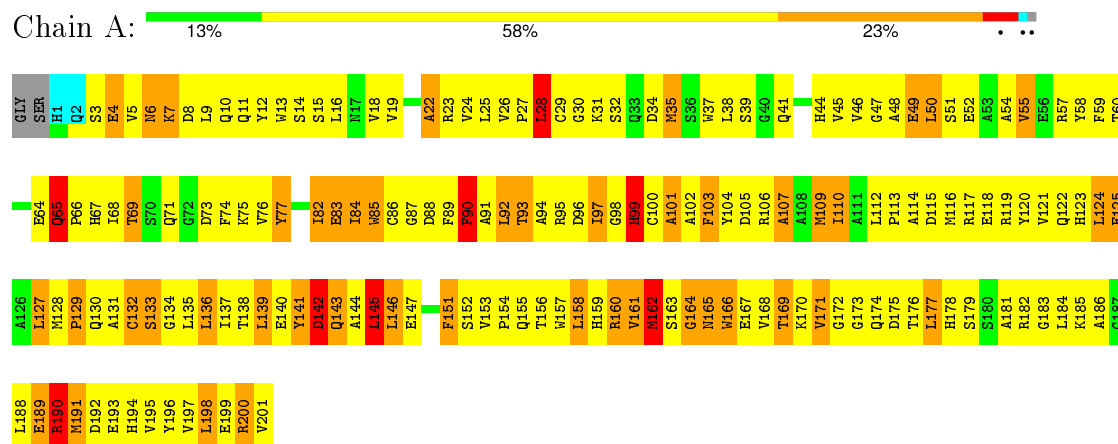
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | -1      | GLY      | -      | CLONING ARTIFACT | UNP O86262 |
| A     | 0       | SER      | -      | CLONING ARTIFACT | UNP O86262 |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Thiopurine S-methyltransferase

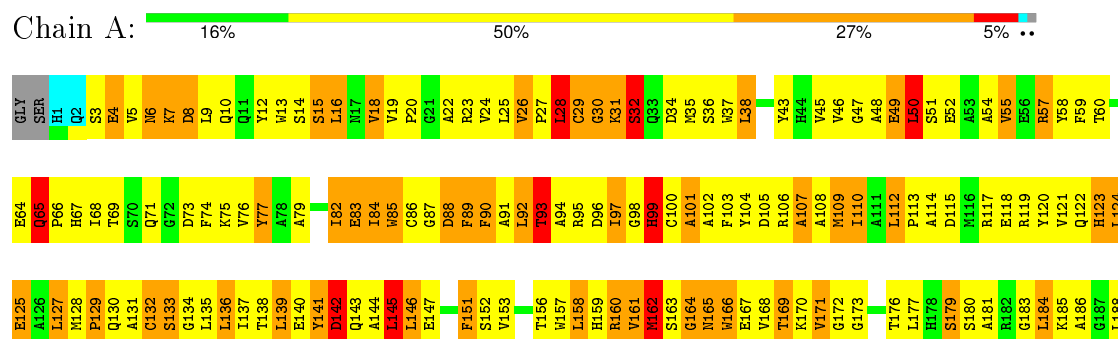


### 4.2 Scores per residue for each member of the ensemble

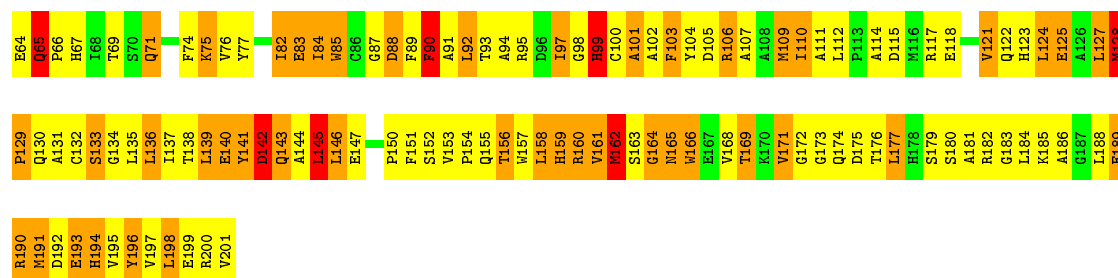
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Thiopurine S-methyltransferase

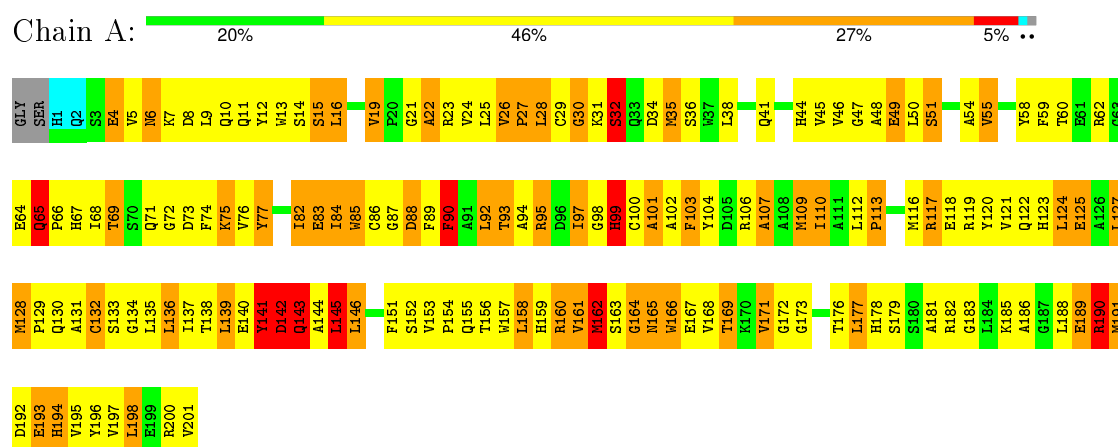






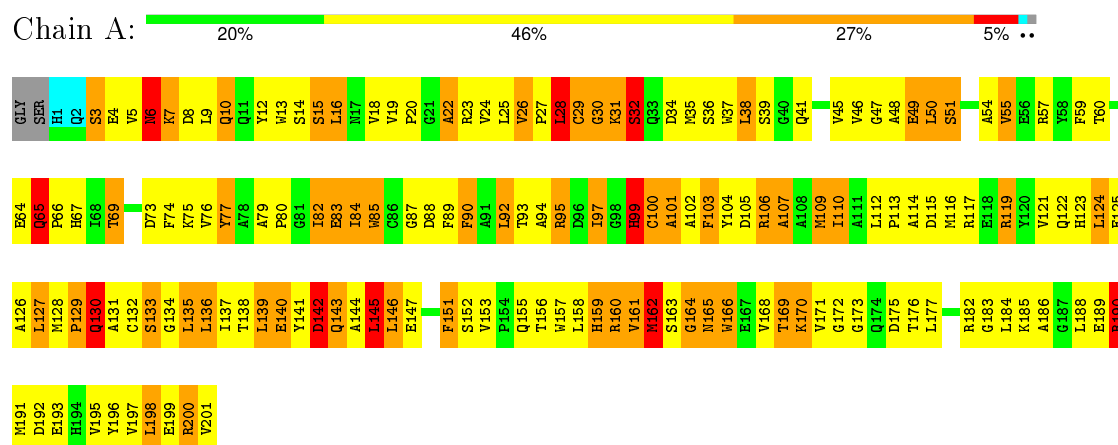
#### 4.2.5 Score per residue for model 5

- Molecule 1: Thiopurine S-methyltransferase



#### 4.2.6 Score per residue for model 6

- Molecule 1: Thiopurine S-methyltransferase

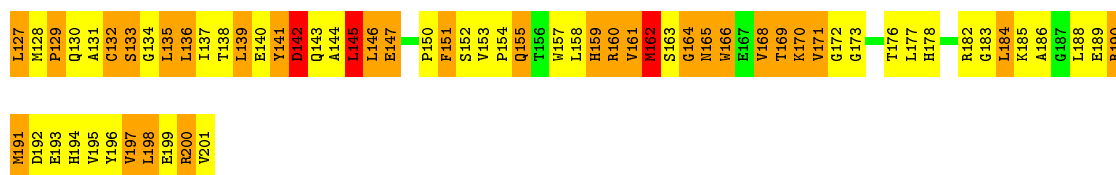


- Molecule 1: Thiopurine S-methyltransferase

- Molecule 1: Thiopurine S-methyltransferase

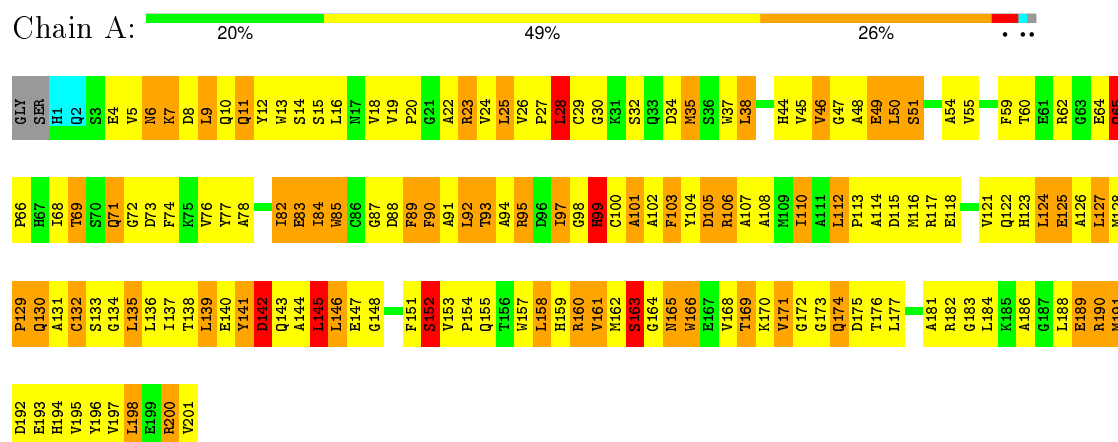
- Molecule 1: Thiopurine S-methyltransferase





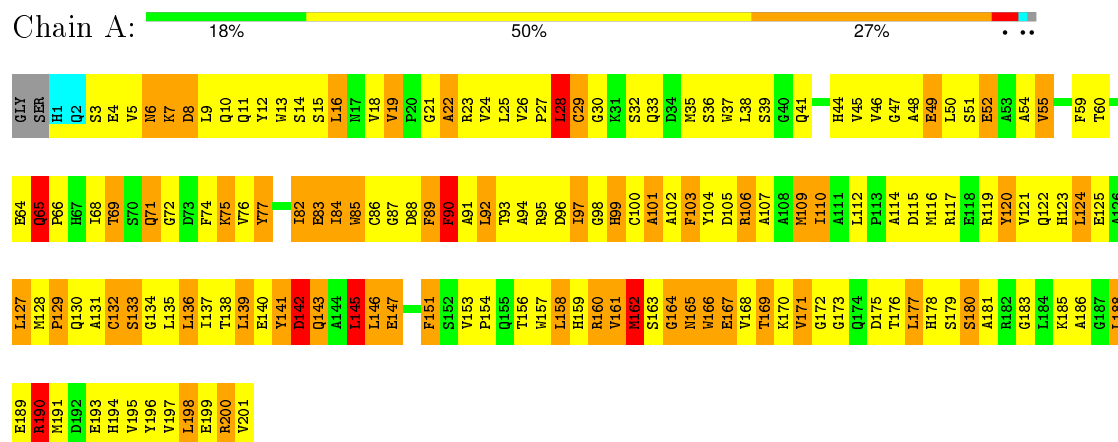
#### 4.2.10 Score per residue for model 10

- Molecule 1: Thiopurine S-methyltransferase



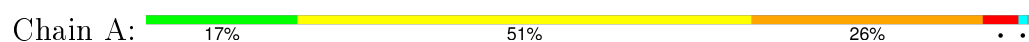
#### 4.2.11 Score per residue for model 11

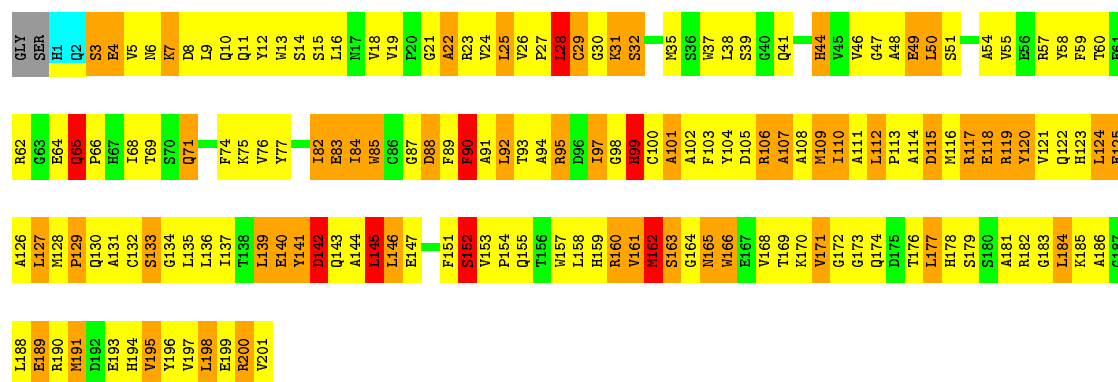
- Molecule 1: Thiopurine S-methyltransferase



#### 4.2.12 Score per residue for model 12

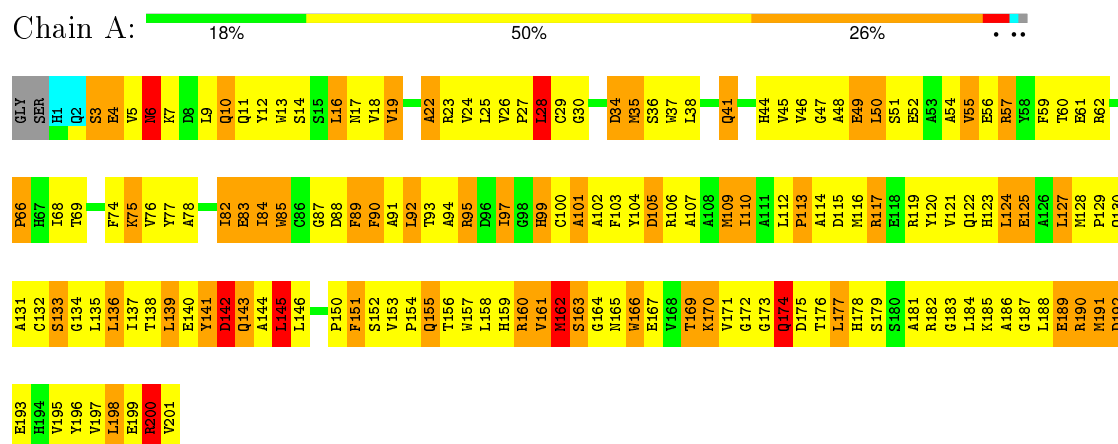
- Molecule 1: Thiopurine S-methyltransferase





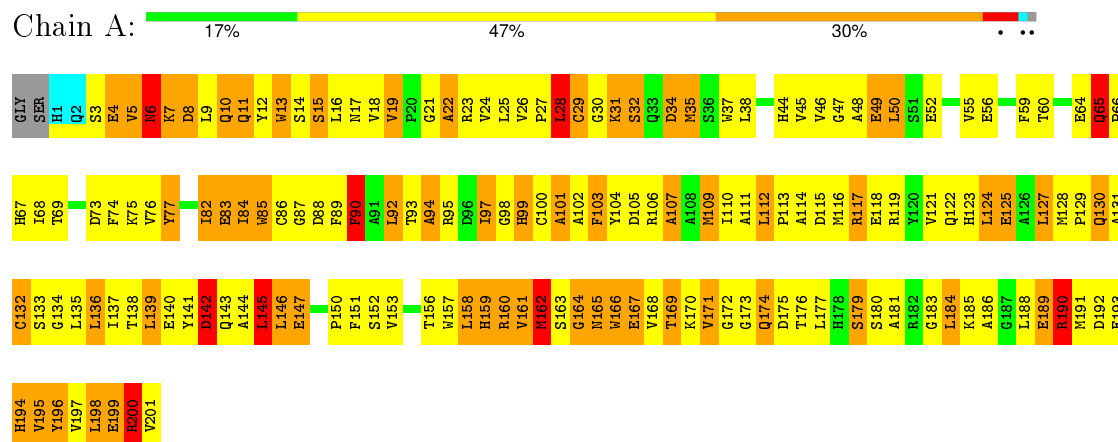
#### 4.2.13 Score per residue for model 13

- Molecule 1: Thiopurine S-methyltransferase



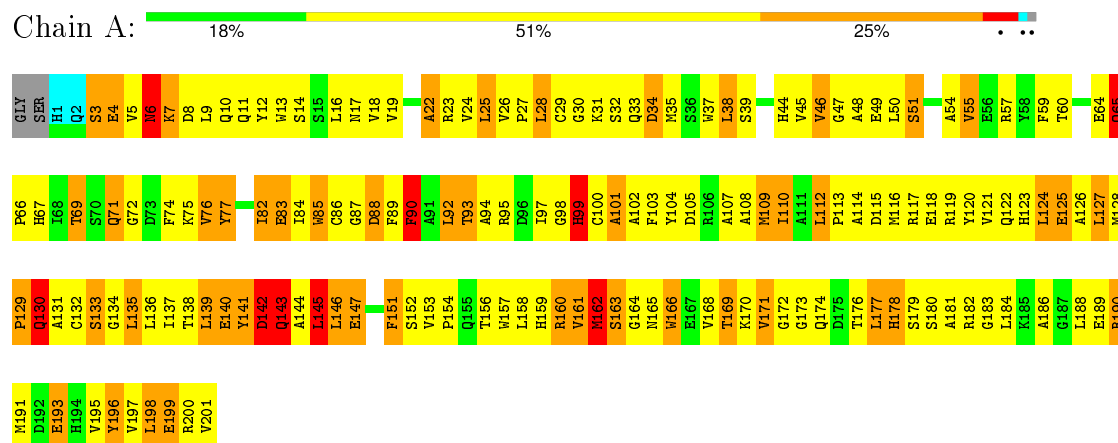
#### 4.2.14 Score per residue for model 14

- Molecule 1: Thiopurine S-methyltransferase



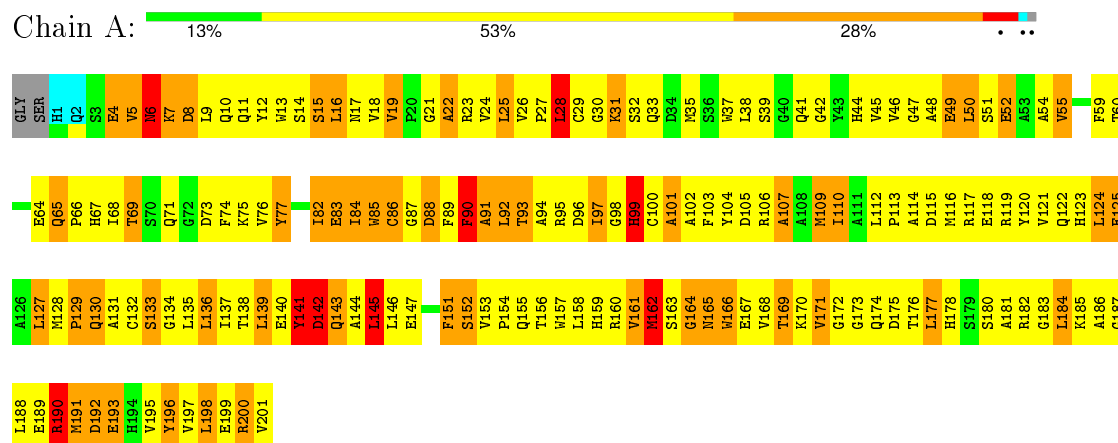
### 4.2.15 Score per residue for model 15

- Molecule 1: Thiopurine S-methyltransferase



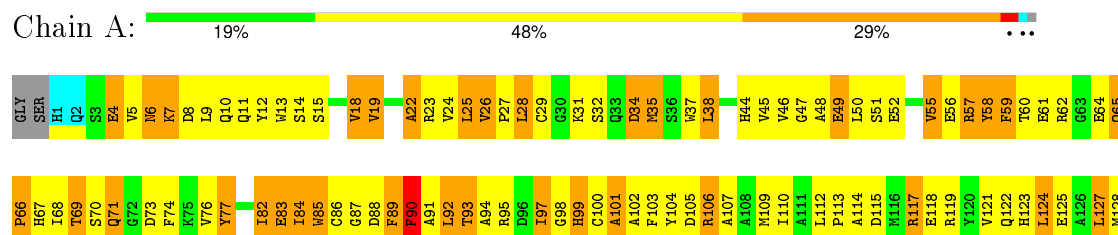
### 4.2.16 Score per residue for model 16

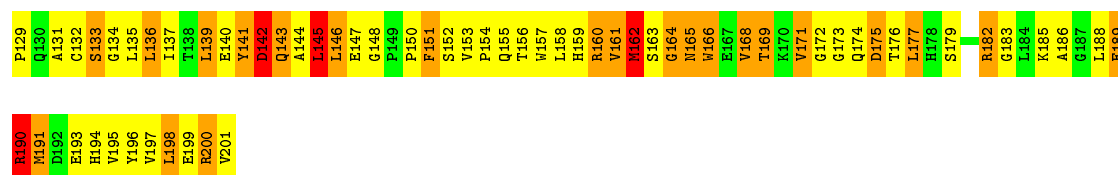
- Molecule 1: Thiopurine S-methyltransferase



### 4.2.17 Score per residue for model 17

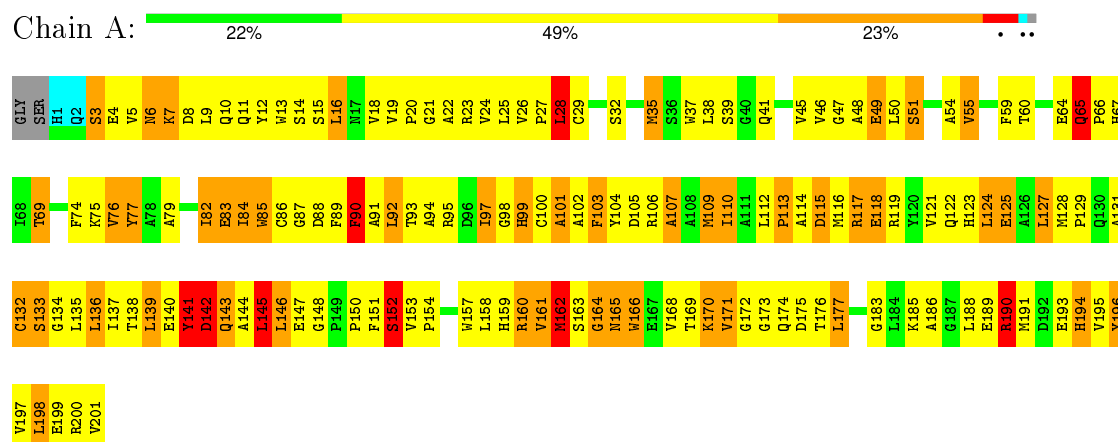
- Molecule 1: Thiopurine S-methyltransferase





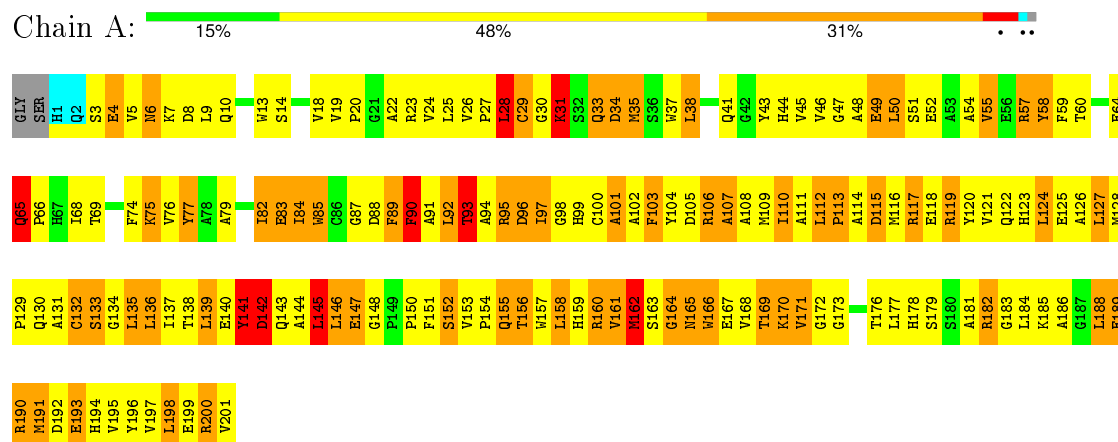
#### 4.2.18 Score per residue for model 18

- Molecule 1: Thiopurine S-methyltransferase



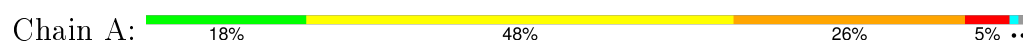
#### 4.2.19 Score per residue for model 19

- Molecule 1: Thiopurine S-methyltransferase



#### 4.2.20 Score per residue for model 20

- Molecule 1: Thiopurine S-methyltransferase



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-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------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| D192 | E193 | H194 | V195 | Y196 | P197 | L198 | E199 | R200 | V201 | P129 | Q130 | A131 | C132 | S133 | G134 | L135 | L136 | T137 | T138 | L139 | E140 | Y141 | D142 | Q143 | L144 | L145 | L146 | E147 | F151 | S152 | V153 | P154 | Q155 | T156 | M157 | L158 | H159 | R160 | V161 | M162 | S163 | G164 | L165 | H166 | E167 | V168 | T169 | K170 | V171 | G172 | G173 | Q174 | T175 | T176 | L177 | H178 | S179 | R182 | G183 | L184 | K185 | A186 | G187 | L188 | E189 | R190 | M191 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P66  | H67  | I68  | T69  | S70  | Q71  | G72  | D73  | K74  | K75  | V76  | Y77  | T82  | E83  | I84  | W85  | C86  | G87  | D88  | F89  | F90  | A91  | L92  | T93  | A94  | R95  | D96  | I97  | G98  | H99  | C100 | A101 | A102 | F103 | I104 | D105 | R106 | A107 | A108 | M109 | I110 | A111 | L112 | P113 | A114 | D115 | M116 | R117 | E118 | R119 | Y120 | V121 | Q122 | R123 | L124 | A125 | A126 | L127 | M128 | V129 | E130 | H131 | S132 | P133 | C134 | L135 | T136 | R137 | E138 | S139 | P140 | C141 | L142 | A143 | D144 | H145 | S146 | P147 | C148 | L149 | T150 | E151 | S152 | P153 | C154 | L155 | T156 | E157 | S158 | P159 | C160 | L161 | T162 | E163 | S164 | P165 | C166 | L167 | T168 | E169 | S170 | P171 | C172 | L173 | T174 | E175 | S176 | P177 | C178 | L179 | T180 | E181 | S182 | P183 | C184 | L185 | T186 | E187 | S188 | P189 | C190 | L191 | T192 | E193 | S194 | P195 | C196 | L197 | T198 | E199 | S200 | P201 | C202 | L203 | T204 | E205 | S206 | P207 | C208 | L209 | T210 | E211 | S212 | P213 | C214 | L215 | T216 | E217 | S218 | P219 | C220 | L221 | T222 | E223 | S224 | P225 | C226 | L227 | T228 | E229 | S230 | P231 | C232 | L233 | T234 | E235 | S236 | P237 | C238 | L239 | T240 | E241 | S242 | P243 | C244 | L245 | T246 | E247 | S248 | P249 | C250 | L251 | T252 | E253 | S254 | P255 | C256 | L257 | T258 | E259 | S260 | P261 | C262 | L263 | T264 | E265 | S266 | P267 | C268 | L269 | T270 | E271 | S272 | P273 | C274 | L275 | T276 | E277 | S278 | P279 | C280 | L281 | T282 | E283 | S284 | P285 | C286 | L287 | T288 | E289 | S290 | P291 | C292 | L293 | T294 | E295 | S296 | P297 | C298 | L299 | T300 | E301 | S302 | P303 | C304 | L305 | T306 | E307 | S308 | P309 | C310 | L311 | T312 | E313 | S314 | P315 | C316 | L317 | T318 | E319 | S320 | P321 | C322 | L323 | T324 | E325 | S326 | P327 | C328 | L329 | T330 | E331 | S332 | P333 | C334 | L335 | T336 | E337 | S338 | P339 | C340 | L341 | T342 | E343 | S344 | P345 | C346 | L347 | T348 | E349 | S350 | P351 | C352 | L353 | T354 | E355 | S356 | P357 | C358 | L359 | T360 | E361 | S362 | P363 | C364 | L365 | T366 | E367 | S368 | P369 | C370 | L371 | T372 | E373 | S374 | P375 | C376 | L377 | T378 | E379 | S380 | P381 | C382 | L383 | T384 | E385 | S386 | P387 | C388 | L389 | T390 | E391 | S392 | P393 | C394 | L395 | T396 | E397 | S398 | P399 | C400 | L401 | T402 | E403 | S404 | P405 | C406 | L407 | T408 | E409 | S410 | P411 | C412 | L413 | T414 | E415 | S416 | P417 | C418 | L419 | T420 | E421 | S422 | P423 | C424 | L425 | T426 | E427 | S428 | P429 | C430 | L431 | T432 | E433 | S434 | P435 | C436 | L437 | T438 | E439 | S440 | P441 | C442 | L443 | T444 | E445 | S446 | P447 | C448 | L449 | T450 | E451 | S452 | P453 | C454 | L455 | T456 | E457 | S458 | P459 | C460 | L461 | T462 | E463 | S464 | P465 | C466 | L467 | T468 | E469 | S470 | P471 | C472 | L473 | T474 | E475 | S476 | P477 | C478 | L479 | T480 | E481 | S482 | P483 | C484 | L485 | T486 | E487 | S488 | P489 | C490 | L491 | T492 | E493 | S494 | P495 | C496 | L497 | T498 | E499 | S500 | P501 | C502 | L503 | T504 | E505 | S506 | P507 | C508 | L509 | T510 | E511 | S512 | P513 | C514 | L515 | T516 | E517 | S518 | P519 | C520 | L521 | T522 | E523 | S524 | P525 | C526 | L527 | T528 | E529 | S530 | P531 | C532 | L533 | T534 | E535 | S536 | P537 | C538 | L539 | T540 | E541 | S542 | P543 | C544 | L545 | T546 | E547 | S548 | P549 | C550 | L551 | T552 | E553 | S554 | P555 | C556 | L557 | T558 | E559 | S560 | P561 | C562 | L563 | T564 | E565 | S566 | P567 | C568 | L569 | T570 | E571 | S572 | P573 | C574 | L575 | T576 | E577 | S578 | P579 | C580 | L581 | T582 | E583 | S584 | P585 | C586 | L587 | T588 | E589 | S590 | P591 | C592 | L593 | T594 | E595 | S596 | P597 | C598 | L599 | T600 | E601 | S602 | P603 | C604 | L605 | T606 | E607 | S608 | P609 | C610 | L611 | T612 | E613 | S614 | P615 | C616 | L617 | T618 | E619 | S620 | P621 | C622 | L623 | T624 | E625 | S626 | P627 | C628 | L629 | T630 | E631 | S632 | P633 | C634 | L635 | T636 | E637 | S638 | P639 | C640 | L641 | T642 | E643 | S644 | P645 | C646 | L647 | T648 | E649 | S650 | P651 | C652 | L653 | T654 | E655 | S656 | P657 | C658 | L659 | T660 | E661 | S662 | P663 | C664 | L665 | T666 | E667 | S668 | P669 | C670 | L671 | T672 | E673 | S674 | P675 | C676 | L677 | T678 | E679 | S680 | P681 | C682 | L683 | T684 | E685 | S686 | P687 | C688 | L689 | T690 | E691 | S692 | P693 | C694 | L695 | T696 | E697 | S698 | P699 | C700 | L701 | T702 | E703 | S704 | P705 | C706 | L707 | T708 | E709 | S710 | P711 | C712 | L713 | T714 | E715 | S716 | P717 | C718 | L719 | T720 | E721 | S722 | P723 | C724 | L725 | T726 | E727 | S728 | P729 | C730 | L731 | T732 | E733 | S734 | P735 | C736 | L737 | T738 | E739 | S740 | P741 | C742 | L743 | T744 | E745 | S746 | P747 | C748 | L749 | T750 | E751 | S752 | P753 | C754 | L755 | T756 | E757 | S758 | P759 | C760 | L761 | T762 | E763 | S764 | P765 | C766 | L767 | T768 | E769 | S770 | P771 | C772 | L773 | T774 | E775 | S776 | P777 | C778 | L779 | T780 | E781 | S782 | P783 | C784 | L785 | T786 | E787 | S788 | P789 | C790 | L791 | T792 | E793 | S794 | P795 | C796 | L797 | T798 | E799 | S800 | P801 | C802 | L803 | T804 | E805 | S806 | P807 | C808 | L809 | T810 | E811 | S812 | P813 | C814 | L815 | T816 | E817 | S818 | P819 | C820 | L821 | T822 | E823 | S824 | P825 | C826 | L827 | T828 | E829 | S830 | P831 | C832 | L833 | T834 | E835 | S836 | P837 | C838 | L839 | T840 | E841 | S842 | P843 | C844 | L845 | T846 | E847 | S848 | P849 | C850 | L851 | T852 | E853 | S854 | P855 | C856 | L857 | T858 | E859 | S860 | P861 | C862 | L863 | T864 | E865 | S866 | P867 | C868 | L869 | T870 | E871 | S872 | P873 | C874 | L875 | T876 | E877 | S878 | P879 | C880 | L881 | T882 | E883 | S884 | P885 | C886 | L887 | T888 | E889 | S890 | P891 | C892 | L893 | T894 | E895 | S896 | P897 | C898 | L899 | T900 | E901 | S902 | P903 | C904 | L905 | T906 | E907 | S908 | P909 | C910 | L911 | T912 | E913 | S914 | P915 | C916 | L917 | T918 | E919 | S920 | P921 | C922 | L923 | T924 | E925 | S926 | P927 | C928 | L929 | T930 | E931 | S932 | P933 | C934 | L935 | T936 | E937 | S938 | P939 | C940 | L941 | T942 | E943 | S944 | P945 | C946 | L947 | T948 | E949 | S950 | P951 | C952 | L953 | T954 | E955 | S956 | P957 | C958 | L959 | T960 | E961 | S962 | P963 | C964 | L965 | T966 | E967 | S968 | P969 | C970 | L971 | T972 | E973 | S974 | P975 | C976 | L977 | T978 | E979 | S980 | P981 | C982 | L983 | T984 | E985 | S986 | P987 | C988 | L989 | T990 | E991 | S992 | P993 | C994 | L995 | T996 | E997 | S998 | P999 | C1000 | L1001 | T1002 | E1003 | S1004 | P1005 | C1006 | L1007 | T1008 | E1009 | S1010 | P1011 | C1012 | L1013 | T1014 | E1015 | S1016 | P1017 | C1018 | L1019 | T1020 | E1021 | S1022 | P1023 | C1024 | L1025 | T1026 | E1027 | S1028 | P1029 | C1030 | L1031 | T1032 | E1033 | S1034 | P1035 | C1036 | L1037 | T1038 | E1039 | S1040 | P1041 | C1042 | L1043 | T1044 | E1045 | S1046 | P1047 | C1048 | L1049 | T1050 | E1051 | S1052 | P1053 | C1054 | L1055 | T1056 | E1057 | S1058 | P1059 | C1060 | L1061 | T1062 | E1063 | S1064 | P1065 | C1066 | L1067 | T1068 | E1069 | S1070 | P1071 | C1072 | L1073 | T1074 | E1075 | S1076 | P1077 | C1078 | L1079 | T1080 | E1081 | S1082 | P1083 | C1084 | L1085 | T1086 | E1087 | S1088 | P1089 | C1090 | L1091 | T1092 | E1093 | S1094 | P1095 | C1096 | L1097 | T1098 | E1099 | S1100 | P1101 | C1102 | L1103 | T1104 | E1105 | S1106 | P1107 | C1108 | L1109 | T1110 | E1111 | S1112 | P1113 | C1114 | L1115 | T1116 | E1117 | S1118 | P1119 | C1120 | L1121 | T1122 | E1123 | S1124 | P1125 | C1126 | L1127 | T1128 | E1129 | S1130 | P1131 | C1132 | L1133 | T1134 | E1135 | S1136 | P1137 | C1138 | L1139 | T1140 | E1141 | S1142 | P1143 | C1144 | L1145 | T1146 | E1147 | S1148 | P1149 | C1150 | L1151 | T1152 | E1153 | S1154 | P1155 | C1156 | L1157 | T1158 | E1159 | S1160 | P1161 | C1162 | L1163 | T1164 | E1165 | S1166 | P1167 | C1168 | L1169 | T1170 | E1171 | S1172 | P1173 | C1174 | L1175 | T1176 | E1177 | S1178 | P1179 | C1180 | L1181 | T1182 | E1183 | S1184 | P1185 | C1186 | L1187 | T1188 | E1189 | S1190 | P1191 | C1192 | L1193 | T1194 | E1195 | S1196 | P1197 | C1198 | L1199 | T1200 | E1201 | S1202 | P1203 | C1204 | L1205 | T1206 | E1207 | S1208 | P1209 | C1210 | L1211 | T1212 | E1213 | S1214 | P1215 | C1216 | L1217 | T1218 | E1219 | S1220 | P1221 | C1222 | L1223 | T1224 | E1225 | S1226 | P1227 | C1228 | L1229 | T1230 | E1231 | S1232 | P1233 | C1234 | L1235 | T1236 | E1237 | S1238 | P1239 | C1240 | L1241 | T1242 | E1243 | S1244 | P1245 | C1246 | L1247 | T1248 | E1249 | S1250 | P1251 | C1252 | L1253 | T1254 | E1255 | S1256 | P1257 | C1258 | L1259 | T1260 | E1261 | S1262 | P1263 | C1264 | L1265 | T1266 | E1267 | S1268 | P1269 | C1270 | L1271 | T1272 | E1273 | S1274 | P1275 | C1276 | L1277 | T1278 | E1279 | S1280 | P1281 | C1282 | L1283 | T1284 | E1285 | S1286 | P1287 | C1288 | L1289 | T1290 | E1291 | S1292 | P1293 | C1294 | L1295 | T1296 | E1297 | S1298 | P1299 | C1300 | L1301 | T1302 | E1303 | S1304 | P1305 | C1306 | L1307 | T1308 | E1309 | S1310 | P1311 | C1312 | L1313 | T1314 | E1315 | S1316 | P1317 | C1318 | L1319 | T1320 | E1321 | S1322 | P1323 | C1324 | L1325 | T1326 | E1327 | S1328 | P1329 | C1330 | L1331 | T1332 | E1333 | S1334 | P1335 | C1336 | L1337 | T1338 | E1339 | S1340 | P1341 | C1342 | L1343 | T1344 | E1345 | S1346 | P1347 | C1348 | L1349 | T1350 | E1351 | S1352 | P1353 | C1354 | L1355 | T1356 | E1357 | S1358 | P1359 | C1360 | L1361 | T1362 | E1363 | S1364 | P1365 | C1366 | L1367 | T1368 | E1369 | S1370 | P1371 | C1372 | L1373 | T1374 | E1375 | S1376 | P1377 | C1378 | L1379 | T1380 | E1381 | S1382 | P1383 | C1384 | L1385 | T1386 | E1387 | S1388 | P1389 | C1390 | L1391 | T1392 | E1393 | S1394 | P1395 | C1396 | L1397 | T1398 | E1399 | S1400 | P1401 | C1402 | L1403 | T1404 | E1405 | S1406 | P1407 | C1408 | L1409 | T1410 | E1411 | S1412 | P1413 | C1414 | L1415 | T1416 | E1417 | S1418 | P1419 | C1420 | L1421 | T1422 | E1423 | S1424 | P1425 | C1426 | L1427 | T1428 | E1429 | S1430 | P1431 | C1432 | L1433 | T1434 | E1435 | S1436 | P1437 | C1438 | L1439 | T1440 | E1441 | S1442 | P1443 | C1444 | L1445 | T1446 | E1447 | S1448 | P1449 | C1450 | L1451 | T1452 | E1453 | S1454 | P1455 | C1456 | L1457 | T1458 | E1459 | S1460 | P1461 | C1462 | L1463 | T1464 | E1465 | S1466 | P1467 | C1468 | L1469 | T1470 | E1471 | S1472 | P1473 | C1474 | L1475 | T1476 | E1477 | S1478 | P1479 | C1480 | L1481 | T1482 | E1483 | S1484 | P1485 | C1486 | L1487 | T1488 | E1489 |

## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| Cyana         | structure solution | 1.05    |
| Cyana         | refinement         | 1.05    |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

|  |                 |
|--|-----------------|
| Chemical shift file(s)                       | BMRB entry 5820 |
| Number of chemical shift lists               | 1               |
| Total number of shifts                       | 2157            |
| Number of shifts mapped to atoms             | 2157            |
| Number of unparsed shifts                    | 0               |
| Number of shifts with mapping errors         | 0               |
| Number of shifts with mapping warnings       | 0               |
| Assignment completeness (well-defined parts) | 79%             |

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1558  | 1505     | 1505     | 316±17  |
| All | All   | 31160 | 30100    | 30100    | 6326    |

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 103.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:196:TYR:CE1  | 1:A:198:LEU:HD22 | 1.10     | 1.82        | 18     | 1     |
| 1:A:19:VAL:HG23  | 1:A:22:ALA:HB2   | 1.09     | 1.23        | 5      | 12    |
| 1:A:135:LEU:HD13 | 1:A:137:ILE:HD11 | 1.05     | 1.28        | 15     | 2     |
| 1:A:19:VAL:HG13  | 1:A:22:ALA:HB2   | 1.04     | 1.21        | 20     | 8     |
| 1:A:19:VAL:CG1   | 1:A:22:ALA:HB2   | 1.03     | 1.84        | 1      | 7     |
| 1:A:48:ALA:HB2   | 1:A:85:TRP:CE2   | 1.03     | 1.89        | 16     | 20    |
| 1:A:92:LEU:HD13  | 1:A:92:LEU:C     | 1.03     | 1.74        | 4      | 9     |
| 1:A:13:TRP:CH2   | 1:A:102:ALA:HB3  | 1.01     | 1.90        | 18     | 19    |
| 1:A:94:ALA:HB3   | 1:A:127:LEU:HD13 | 1.01     | 1.26        | 15     | 16    |
| 1:A:104:TYR:CE2  | 1:A:135:LEU:HD12 | 1.00     | 1.90        | 10     | 1     |
| 1:A:24:VAL:HG11  | 1:A:38:LEU:HD13  | 1.00     | 1.27        | 12     | 7     |
| 1:A:22:ALA:HB1   | 1:A:101:ALA:CB   | 0.98     | 1.88        | 18     | 20    |
| 1:A:97:ILE:HD13  | 1:A:98:GLY:N     | 0.97     | 1.75        | 5      | 2     |
| 1:A:92:LEU:C     | 1:A:92:LEU:HD13  | 0.97     | 1.80        | 12     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:45:VAL:HG12  | 1:A:82:ILE:HD11  | 0.96     | 1.37        | 13     | 19    |
| 1:A:117:ARG:O    | 1:A:121:VAL:HG13 | 0.96     | 1.59        | 9      | 18    |
| 1:A:168:VAL:HG13 | 1:A:198:LEU:HD22 | 0.96     | 1.38        | 14     | 2     |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:HD13 | 0.95     | 1.38        | 4      | 12    |
| 1:A:104:TYR:CZ   | 1:A:137:ILE:HD13 | 0.95     | 1.95        | 16     | 4     |
| 1:A:92:LEU:HD22  | 1:A:92:LEU:O     | 0.95     | 1.59        | 10     | 3     |
| 1:A:27:PRO:O     | 1:A:28:LEU:HD22  | 0.95     | 1.61        | 1      | 13    |
| 1:A:177:LEU:HD22 | 1:A:177:LEU:O    | 0.95     | 1.60        | 17     | 5     |
| 1:A:177:LEU:O    | 1:A:177:LEU:HD22 | 0.95     | 1.62        | 18     | 2     |
| 1:A:135:LEU:CD1  | 1:A:137:ILE:HD11 | 0.95     | 1.92        | 15     | 1     |
| 1:A:92:LEU:O     | 1:A:92:LEU:HD22  | 0.95     | 1.60        | 1      | 5     |
| 1:A:136:LEU:O    | 1:A:137:ILE:HD13 | 0.94     | 1.62        | 15     | 6     |
| 1:A:136:LEU:HD22 | 1:A:137:ILE:N    | 0.94     | 1.77        | 20     | 1     |
| 1:A:138:THR:O    | 1:A:139:LEU:HD13 | 0.93     | 1.61        | 9      | 5     |
| 1:A:28:LEU:HD13  | 1:A:28:LEU:N     | 0.92     | 1.79        | 16     | 7     |
| 1:A:46:VAL:HG21  | 1:A:97:ILE:CD1   | 0.92     | 1.95        | 8      | 4     |
| 1:A:137:ILE:HG23 | 1:A:195:VAL:HG22 | 0.91     | 1.41        | 20     | 2     |
| 1:A:139:LEU:HD21 | 1:A:150:PRO:CG   | 0.90     | 1.96        | 3      | 1     |
| 1:A:171:VAL:HG11 | 1:A:197:VAL:HG23 | 0.90     | 1.39        | 15     | 7     |
| 1:A:109:MET:SD   | 1:A:136:LEU:HD21 | 0.90     | 2.06        | 13     | 4     |
| 1:A:168:VAL:HG22 | 1:A:198:LEU:HB3  | 0.90     | 1.44        | 19     | 3     |
| 1:A:23:ARG:O     | 1:A:101:ALA:HB3  | 0.90     | 1.67        | 8      | 20    |
| 1:A:102:ALA:HB1  | 1:A:133:SER:O    | 0.90     | 1.67        | 1      | 19    |
| 1:A:139:LEU:HD23 | 1:A:142:ASP:CG   | 0.90     | 1.87        | 3      | 1     |
| 1:A:146:LEU:HD12 | 1:A:147:GLU:N    | 0.89     | 1.82        | 2      | 8     |
| 1:A:26:VAL:HG22  | 1:A:29:CYS:SG    | 0.89     | 2.07        | 1      | 2     |
| 1:A:28:LEU:N     | 1:A:28:LEU:HD13  | 0.89     | 1.82        | 3      | 7     |
| 1:A:24:VAL:HG11  | 1:A:38:LEU:CD1   | 0.89     | 1.98        | 9      | 8     |
| 1:A:128:MET:SD   | 1:A:200:ARG:CZ   | 0.89     | 2.60        | 15     | 1     |
| 1:A:198:LEU:HD23 | 1:A:198:LEU:N    | 0.89     | 1.82        | 14     | 5     |
| 1:A:46:VAL:HG22  | 1:A:97:ILE:HD12  | 0.89     | 1.44        | 2      | 5     |
| 1:A:92:LEU:HD13  | 1:A:93:THR:N     | 0.89     | 1.83        | 3      | 11    |
| 1:A:198:LEU:N    | 1:A:198:LEU:HD23 | 0.89     | 1.83        | 13     | 5     |
| 1:A:25:LEU:HD23  | 1:A:97:ILE:HD11  | 0.89     | 1.43        | 2      | 5     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:CD1  | 0.88     | 1.98        | 6      | 12    |
| 1:A:139:LEU:HD23 | 1:A:191:MET:CE   | 0.88     | 1.99        | 12     | 7     |
| 1:A:107:ALA:CB   | 1:A:139:LEU:HD11 | 0.88     | 1.98        | 16     | 3     |
| 1:A:138:THR:C    | 1:A:139:LEU:HD13 | 0.88     | 1.89        | 4      | 4     |
| 1:A:105:ASP:HB2  | 1:A:136:LEU:HD12 | 0.87     | 1.42        | 2      | 3     |
| 1:A:178:HIS:CD2  | 1:A:184:LEU:HD21 | 0.87     | 2.05        | 15     | 1     |
| 1:A:34:ASP:O     | 1:A:38:LEU:HD22  | 0.87     | 1.69        | 6      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:92:LEU:HD13  | 1:A:92:LEU:O     | 0.87     | 1.70        | 9      | 4     |
| 1:A:105:ASP:HB3  | 1:A:136:LEU:HD12 | 0.87     | 1.45        | 12     | 6     |
| 1:A:145:LEU:C    | 1:A:145:LEU:HD22 | 0.87     | 1.89        | 5      | 7     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:HG23 | 0.87     | 1.43        | 16     | 3     |
| 1:A:171:VAL:HG13 | 1:A:195:VAL:HG23 | 0.87     | 1.47        | 12     | 2     |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:HG   | 0.86     | 1.46        | 18     | 4     |
| 1:A:97:ILE:O     | 1:A:97:ILE:HD13  | 0.86     | 1.70        | 19     | 1     |
| 1:A:51:SER:O     | 1:A:55:VAL:HG13  | 0.86     | 1.70        | 16     | 7     |
| 1:A:46:VAL:CG2   | 1:A:97:ILE:HD12  | 0.86     | 1.99        | 2      | 5     |
| 1:A:186:ALA:HB3  | 1:A:188:LEU:HD11 | 0.86     | 1.47        | 11     | 7     |
| 1:A:92:LEU:CD2   | 1:A:97:ILE:HG21  | 0.85     | 2.00        | 4      | 17    |
| 1:A:171:VAL:HG13 | 1:A:195:VAL:CG2  | 0.85     | 2.01        | 12     | 2     |
| 1:A:94:ALA:HB3   | 1:A:127:LEU:CD1  | 0.85     | 2.01        | 15     | 9     |
| 1:A:112:LEU:HD23 | 1:A:116:MET:HG2  | 0.85     | 1.48        | 18     | 8     |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:CD1  | 0.85     | 2.02        | 3      | 16    |
| 1:A:112:LEU:HD23 | 1:A:116:MET:CG   | 0.84     | 2.02        | 16     | 8     |
| 1:A:196:TYR:OH   | 1:A:198:LEU:HD13 | 0.84     | 1.73        | 18     | 1     |
| 1:A:93:THR:HG22  | 1:A:95:ARG:HG2   | 0.84     | 1.50        | 1      | 4     |
| 1:A:183:GLY:HA2  | 1:A:188:LEU:HD23 | 0.84     | 1.49        | 13     | 12    |
| 1:A:196:TYR:CZ   | 1:A:198:LEU:HD22 | 0.84     | 2.07        | 18     | 1     |
| 1:A:46:VAL:HG13  | 1:A:83:GLU:HB3   | 0.84     | 1.47        | 9      | 2     |
| 1:A:168:VAL:HB   | 1:A:196:TYR:CE1  | 0.84     | 2.08        | 20     | 1     |
| 1:A:177:LEU:HD13 | 1:A:178:HIS:N    | 0.84     | 1.86        | 15     | 1     |
| 1:A:19:VAL:CG2   | 1:A:22:ALA:HB2   | 0.83     | 2.02        | 15     | 4     |
| 1:A:27:PRO:HB2   | 1:A:28:LEU:HD13  | 0.83     | 1.50        | 5      | 1     |
| 1:A:85:TRP:CZ2   | 1:A:92:LEU:HB3   | 0.83     | 2.08        | 16     | 9     |
| 1:A:165:ASN:O    | 1:A:201:VAL:HG22 | 0.83     | 1.73        | 8      | 17    |
| 1:A:92:LEU:O     | 1:A:92:LEU:HD13  | 0.83     | 1.71        | 5      | 5     |
| 1:A:109:MET:SD   | 1:A:136:LEU:HD11 | 0.83     | 2.13        | 12     | 7     |
| 1:A:139:LEU:HD22 | 1:A:142:ASP:OD2  | 0.83     | 1.73        | 12     | 4     |
| 1:A:26:VAL:HG13  | 1:A:47:GLY:HA3   | 0.83     | 1.50        | 6      | 3     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:CG2  | 0.83     | 2.04        | 10     | 3     |
| 1:A:171:VAL:HG12 | 1:A:196:TYR:HA   | 0.83     | 1.51        | 14     | 2     |
| 1:A:28:LEU:HD12  | 1:A:89:PHE:CD1   | 0.82     | 2.07        | 1      | 1     |
| 1:A:92:LEU:HD23  | 1:A:97:ILE:HG21  | 0.82     | 1.49        | 11     | 12    |
| 1:A:24:VAL:HG11  | 1:A:38:LEU:HG    | 0.82     | 1.49        | 1      | 4     |
| 1:A:82:ILE:HD12  | 1:A:84:ILE:HB    | 0.82     | 1.52        | 9      | 14    |
| 1:A:27:PRO:C     | 1:A:28:LEU:HD22  | 0.82     | 1.95        | 19     | 13    |
| 1:A:77:TYR:CD1   | 1:A:77:TYR:O     | 0.82     | 2.33        | 17     | 10    |
| 1:A:109:MET:CB   | 1:A:117:ARG:CZ   | 0.82     | 2.58        | 16     | 3     |
| 1:A:55:VAL:HG13  | 1:A:59:PHE:CZ    | 0.82     | 2.10        | 12     | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:136:LEU:HD23 | 1:A:138:THR:HG23 | 0.82     | 1.52        | 8      | 4     |
| 1:A:90:PHE:CZ    | 1:A:123:HIS:CE1  | 0.82     | 2.67        | 15     | 1     |
| 1:A:196:TYR:CE1  | 1:A:198:LEU:HG   | 0.81     | 2.10        | 20     | 1     |
| 1:A:145:LEU:N    | 1:A:145:LEU:HD12 | 0.81     | 1.89        | 19     | 2     |
| 1:A:196:TYR:CD1  | 1:A:196:TYR:C    | 0.81     | 2.52        | 20     | 1     |
| 1:A:145:LEU:HD12 | 1:A:145:LEU:N    | 0.81     | 1.90        | 11     | 2     |
| 1:A:138:THR:C    | 1:A:139:LEU:HD22 | 0.81     | 1.96        | 2      | 2     |
| 1:A:25:LEU:HD22  | 1:A:128:MET:HE1  | 0.81     | 1.50        | 17     | 4     |
| 1:A:139:LEU:HD12 | 1:A:142:ASP:CG   | 0.81     | 1.95        | 19     | 1     |
| 1:A:93:THR:HG22  | 1:A:95:ARG:HG3   | 0.81     | 1.49        | 15     | 1     |
| 1:A:93:THR:O     | 1:A:97:ILE:HG23  | 0.81     | 1.76        | 18     | 10    |
| 1:A:92:LEU:HD21  | 1:A:97:ILE:HD13  | 0.81     | 1.50        | 18     | 5     |
| 1:A:197:VAL:C    | 1:A:198:LEU:HD23 | 0.80     | 1.96        | 18     | 4     |
| 1:A:82:ILE:HD13  | 1:A:83:GLU:N     | 0.80     | 1.91        | 6      | 20    |
| 1:A:171:VAL:HG22 | 1:A:172:GLY:H    | 0.80     | 1.35        | 12     | 2     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:CD2  | 0.80     | 2.07        | 5      | 4     |
| 1:A:105:ASP:CB   | 1:A:136:LEU:HD12 | 0.80     | 2.05        | 4      | 9     |
| 1:A:27:PRO:O     | 1:A:28:LEU:HD23  | 0.80     | 1.77        | 9      | 1     |
| 1:A:25:LEU:HB2   | 1:A:97:ILE:HD11  | 0.80     | 1.53        | 10     | 2     |
| 1:A:26:VAL:HG13  | 1:A:29:CYS:HB2   | 0.80     | 1.52        | 15     | 2     |
| 1:A:47:GLY:O     | 1:A:85:TRP:CD1   | 0.80     | 2.33        | 4      | 20    |
| 1:A:135:LEU:HD13 | 1:A:197:VAL:HG22 | 0.80     | 1.54        | 5      | 4     |
| 1:A:76:VAL:HG13  | 1:A:85:TRP:HB2   | 0.80     | 1.50        | 6      | 9     |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:CE1  | 0.80     | 2.12        | 9      | 6     |
| 1:A:138:THR:C    | 1:A:139:LEU:HD23 | 0.80     | 1.97        | 19     | 1     |
| 1:A:89:PHE:CD1   | 1:A:89:PHE:O     | 0.79     | 2.35        | 1      | 4     |
| 1:A:22:ALA:HB1   | 1:A:101:ALA:HB2  | 0.79     | 1.53        | 18     | 20    |
| 1:A:107:ALA:HB1  | 1:A:110:ILE:HD11 | 0.79     | 1.53        | 17     | 1     |
| 1:A:103:PHE:CE1  | 1:A:134:GLY:CA   | 0.79     | 2.65        | 15     | 3     |
| 1:A:50:LEU:HD21  | 1:A:89:PHE:HB3   | 0.79     | 1.54        | 15     | 5     |
| 1:A:48:ALA:HB3   | 1:A:89:PHE:HB2   | 0.79     | 1.55        | 1      | 5     |
| 1:A:145:LEU:O    | 1:A:186:ALA:HB1  | 0.79     | 1.77        | 19     | 3     |
| 1:A:46:VAL:HG13  | 1:A:97:ILE:HD12  | 0.79     | 1.54        | 17     | 1     |
| 1:A:104:TYR:CE2  | 1:A:137:ILE:HD13 | 0.79     | 2.12        | 18     | 2     |
| 1:A:9:LEU:HD13   | 1:A:9:LEU:C      | 0.79     | 1.97        | 10     | 10    |
| 1:A:145:LEU:HD22 | 1:A:145:LEU:C    | 0.79     | 1.98        | 17     | 9     |
| 1:A:46:VAL:HG13  | 1:A:97:ILE:CD1   | 0.79     | 2.08        | 7      | 2     |
| 1:A:169:THR:O    | 1:A:171:VAL:HG12 | 0.79     | 1.78        | 15     | 11    |
| 1:A:46:VAL:HG21  | 1:A:97:ILE:HD13  | 0.79     | 1.55        | 8      | 4     |
| 1:A:12:TYR:CE1   | 1:A:197:VAL:HG21 | 0.79     | 2.13        | 18     | 2     |
| 1:A:139:LEU:HD22 | 1:A:139:LEU:N    | 0.79     | 1.93        | 4      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:CG   | 0.78     | 2.07        | 7      | 5     |
| 1:A:162:MET:SD   | 1:A:198:LEU:HD13 | 0.78     | 2.17        | 5      | 6     |
| 1:A:169:THR:HG22 | 1:A:197:VAL:HG12 | 0.78     | 1.52        | 14     | 9     |
| 1:A:25:LEU:HD13  | 1:A:25:LEU:C     | 0.78     | 1.98        | 8      | 6     |
| 1:A:135:LEU:CD2  | 1:A:197:VAL:HG22 | 0.78     | 2.09        | 15     | 1     |
| 1:A:100:CYS:HA   | 1:A:131:ALA:O    | 0.78     | 1.79        | 15     | 20    |
| 1:A:23:ARG:O     | 1:A:101:ALA:CB   | 0.78     | 2.30        | 7      | 20    |
| 1:A:92:LEU:HD13  | 1:A:93:THR:H     | 0.78     | 1.39        | 13     | 5     |
| 1:A:46:VAL:HG11  | 1:A:97:ILE:HD12  | 0.78     | 1.52        | 3      | 2     |
| 1:A:94:ALA:HB1   | 1:A:128:MET:HE1  | 0.78     | 1.52        | 15     | 1     |
| 1:A:46:VAL:HG23  | 1:A:83:GLU:HB3   | 0.78     | 1.54        | 20     | 9     |
| 1:A:25:LEU:HD13  | 1:A:27:PRO:HD3   | 0.77     | 1.53        | 7      | 4     |
| 1:A:92:LEU:C     | 1:A:92:LEU:CD1   | 0.77     | 2.52        | 2      | 6     |
| 1:A:97:ILE:HD12  | 1:A:97:ILE:C     | 0.77     | 1.99        | 10     | 3     |
| 1:A:139:LEU:HD21 | 1:A:150:PRO:HG3  | 0.77     | 1.56        | 3      | 1     |
| 1:A:26:VAL:O     | 1:A:26:VAL:HG12  | 0.77     | 1.76        | 1      | 2     |
| 1:A:136:LEU:HD23 | 1:A:138:THR:CG2  | 0.77     | 2.08        | 8      | 4     |
| 1:A:162:MET:O    | 1:A:166:TRP:CD1  | 0.77     | 2.37        | 2      | 16    |
| 1:A:125:GLU:OE2  | 1:A:166:TRP:CG   | 0.77     | 2.37        | 19     | 2     |
| 1:A:109:MET:CE   | 1:A:158:LEU:HD21 | 0.77     | 2.08        | 18     | 2     |
| 1:A:169:THR:CG2  | 1:A:197:VAL:HG12 | 0.77     | 2.09        | 14     | 9     |
| 1:A:93:THR:O     | 1:A:97:ILE:HG22  | 0.77     | 1.79        | 14     | 6     |
| 1:A:104:TYR:CZ   | 1:A:135:LEU:HD12 | 0.77     | 2.15        | 10     | 1     |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:CE2  | 0.77     | 2.14        | 10     | 2     |
| 1:A:196:TYR:CZ   | 1:A:198:LEU:HD23 | 0.77     | 2.13        | 20     | 1     |
| 1:A:26:VAL:HG11  | 1:A:30:GLY:O     | 0.77     | 1.79        | 15     | 1     |
| 1:A:12:TYR:CE2   | 1:A:171:VAL:HG21 | 0.77     | 2.14        | 14     | 12    |
| 1:A:110:ILE:HD12 | 1:A:111:ALA:N    | 0.77     | 1.95        | 9      | 2     |
| 1:A:135:LEU:HD13 | 1:A:137:ILE:CD1  | 0.77     | 2.09        | 15     | 1     |
| 1:A:5:VAL:HG21   | 1:A:37:TRP:HB2   | 0.76     | 1.56        | 10     | 10    |
| 1:A:177:LEU:HD21 | 1:A:183:GLY:HA3  | 0.76     | 1.58        | 18     | 4     |
| 1:A:105:ASP:CG   | 1:A:136:LEU:HD12 | 0.76     | 2.01        | 4      | 6     |
| 1:A:168:VAL:HG23 | 1:A:196:TYR:CZ   | 0.76     | 2.16        | 15     | 1     |
| 1:A:23:ARG:N     | 1:A:101:ALA:HB2  | 0.76     | 1.95        | 15     | 20    |
| 1:A:25:LEU:HD13  | 1:A:26:VAL:N     | 0.76     | 1.96        | 4      | 11    |
| 1:A:48:ALA:HB2   | 1:A:85:TRP:CZ2   | 0.76     | 2.16        | 5      | 14    |
| 1:A:176:THR:HG23 | 1:A:176:THR:O    | 0.76     | 1.80        | 19     | 10    |
| 1:A:109:MET:CE   | 1:A:158:LEU:HD11 | 0.76     | 2.11        | 5      | 1     |
| 1:A:103:PHE:CG   | 1:A:200:ARG:NH2  | 0.76     | 2.54        | 15     | 1     |
| 1:A:117:ARG:CG   | 1:A:157:TRP:CH2  | 0.76     | 2.69        | 12     | 1     |
| 1:A:46:VAL:HG13  | 1:A:97:ILE:HD13  | 0.75     | 1.57        | 11     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:25:LEU:C     | 1:A:25:LEU:HD13  | 0.75     | 2.00        | 4      | 6     |
| 1:A:93:THR:HG22  | 1:A:95:ARG:CG    | 0.75     | 2.12        | 15     | 5     |
| 1:A:189:GLU:O    | 1:A:190:ARG:CB   | 0.75     | 2.33        | 20     | 16    |
| 1:A:24:VAL:HG11  | 1:A:38:LEU:CD2   | 0.75     | 2.11        | 17     | 3     |
| 1:A:90:PHE:CG    | 1:A:90:PHE:O     | 0.75     | 2.40        | 18     | 1     |
| 1:A:166:TRP:CD1  | 1:A:166:TRP:N    | 0.75     | 2.54        | 10     | 9     |
| 1:A:51:SER:OG    | 1:A:54:ALA:HB3   | 0.75     | 1.80        | 3      | 2     |
| 1:A:107:ALA:HB2  | 1:A:138:THR:HA   | 0.75     | 1.56        | 15     | 3     |
| 1:A:145:LEU:CD2  | 1:A:188:LEU:HD13 | 0.75     | 2.11        | 4      | 12    |
| 1:A:92:LEU:CD1   | 1:A:92:LEU:C     | 0.75     | 2.50        | 4      | 4     |
| 1:A:55:VAL:O     | 1:A:59:PHE:CD1   | 0.74     | 2.39        | 13     | 11    |
| 1:A:117:ARG:HA   | 1:A:117:ARG:CZ   | 0.74     | 2.11        | 13     | 2     |
| 1:A:103:PHE:O    | 1:A:103:PHE:CG   | 0.74     | 2.39        | 10     | 5     |
| 1:A:28:LEU:HD12  | 1:A:50:LEU:HD23  | 0.74     | 1.57        | 10     | 5     |
| 1:A:127:LEU:HD12 | 1:A:127:LEU:C    | 0.74     | 2.03        | 4      | 12    |
| 1:A:66:PRO:CG    | 1:A:77:TYR:CE2   | 0.74     | 2.69        | 20     | 8     |
| 1:A:176:THR:HG23 | 1:A:193:GLU:HB3  | 0.74     | 1.58        | 15     | 2     |
| 1:A:9:LEU:CD2    | 1:A:104:TYR:CE2  | 0.74     | 2.71        | 10     | 1     |
| 1:A:25:LEU:HD22  | 1:A:128:MET:CE   | 0.74     | 2.12        | 20     | 4     |
| 1:A:168:VAL:CG1  | 1:A:198:LEU:HD22 | 0.74     | 2.11        | 14     | 2     |
| 1:A:168:VAL:HG12 | 1:A:196:TYR:OH   | 0.74     | 1.81        | 20     | 1     |
| 1:A:100:CYS:O    | 1:A:101:ALA:HB2  | 0.74     | 1.82        | 19     | 20    |
| 1:A:76:VAL:HG23  | 1:A:85:TRP:HB2   | 0.74     | 1.59        | 7      | 6     |
| 1:A:109:MET:HE2  | 1:A:158:LEU:HD21 | 0.74     | 1.59        | 18     | 1     |
| 1:A:77:TYR:C     | 1:A:77:TYR:CD1   | 0.74     | 2.61        | 8      | 6     |
| 1:A:177:LEU:HD23 | 1:A:191:MET:HG2  | 0.74     | 1.60        | 11     | 2     |
| 1:A:135:LEU:HD21 | 1:A:197:VAL:HG22 | 0.74     | 1.59        | 15     | 1     |
| 1:A:158:LEU:HD13 | 1:A:196:TYR:CD2  | 0.73     | 2.17        | 2      | 5     |
| 1:A:22:ALA:HB1   | 1:A:101:ALA:CA   | 0.73     | 2.13        | 7      | 20    |
| 1:A:98:GLY:O     | 1:A:100:CYS:N    | 0.73     | 2.22        | 18     | 17    |
| 1:A:155:GLN:CG   | 1:A:196:TYR:CE1  | 0.73     | 2.71        | 4      | 2     |
| 1:A:139:LEU:HD23 | 1:A:191:MET:HE1  | 0.73     | 1.59        | 17     | 5     |
| 1:A:146:LEU:HG   | 1:A:188:LEU:HD21 | 0.73     | 1.60        | 6      | 6     |
| 1:A:139:LEU:HD12 | 1:A:139:LEU:N    | 0.73     | 1.98        | 16     | 5     |
| 1:A:46:VAL:CG1   | 1:A:97:ILE:HD13  | 0.73     | 2.14        | 11     | 4     |
| 1:A:168:VAL:CG2  | 1:A:198:LEU:HB3  | 0.73     | 2.12        | 19     | 2     |
| 1:A:139:LEU:HD12 | 1:A:146:LEU:HD23 | 0.73     | 1.59        | 14     | 2     |
| 1:A:24:VAL:HG23  | 1:A:45:VAL:HA    | 0.73     | 1.58        | 8      | 2     |
| 1:A:89:PHE:CG    | 1:A:90:PHE:N     | 0.73     | 2.57        | 19     | 1     |
| 1:A:49:GLU:OE1   | 1:A:84:ILE:HD12  | 0.73     | 1.83        | 1      | 2     |
| 1:A:13:TRP:CH2   | 1:A:102:ALA:CB   | 0.73     | 2.72        | 19     | 19    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:12:TYR:O     | 1:A:16:LEU:N     | 0.73     | 2.20        | 12     | 8     |
| 1:A:23:ARG:N     | 1:A:101:ALA:CB   | 0.73     | 2.52        | 15     | 20    |
| 1:A:177:LEU:HD21 | 1:A:190:ARG:H    | 0.72     | 1.45        | 11     | 3     |
| 1:A:137:ILE:HG23 | 1:A:195:VAL:CG2  | 0.72     | 2.13        | 20     | 2     |
| 1:A:127:LEU:C    | 1:A:127:LEU:HD12 | 0.72     | 2.05        | 9      | 7     |
| 1:A:168:VAL:HG13 | 1:A:198:LEU:CD2  | 0.72     | 2.14        | 14     | 2     |
| 1:A:124:LEU:HD13 | 1:A:128:MET:CG   | 0.72     | 2.15        | 13     | 15    |
| 1:A:139:LEU:HD12 | 1:A:142:ASP:OD2  | 0.72     | 1.84        | 19     | 1     |
| 1:A:105:ASP:N    | 1:A:105:ASP:OD1  | 0.72     | 2.18        | 2      | 1     |
| 1:A:92:LEU:CD2   | 1:A:97:ILE:HD13  | 0.72     | 2.14        | 20     | 6     |
| 1:A:159:HIS:O    | 1:A:163:SER:CB   | 0.72     | 2.38        | 20     | 20    |
| 1:A:25:LEU:HG    | 1:A:94:ALA:HB1   | 0.72     | 1.61        | 7      | 12    |
| 1:A:162:MET:SD   | 1:A:166:TRP:CE2  | 0.72     | 2.83        | 10     | 9     |
| 1:A:100:CYS:O    | 1:A:101:ALA:CB   | 0.71     | 2.38        | 18     | 20    |
| 1:A:168:VAL:HG23 | 1:A:196:TYR:CE1  | 0.71     | 2.20        | 15     | 2     |
| 1:A:104:TYR:CE2  | 1:A:135:LEU:CD1  | 0.71     | 2.69        | 10     | 1     |
| 1:A:28:LEU:HD21  | 1:A:120:TYR:OH   | 0.71     | 1.85        | 13     | 5     |
| 1:A:19:VAL:HG12  | 1:A:22:ALA:HB2   | 0.71     | 1.61        | 1      | 3     |
| 1:A:77:TYR:O     | 1:A:77:TYR:CD2   | 0.71     | 2.43        | 14     | 1     |
| 1:A:35:MET:HG2   | 1:A:45:VAL:HG11  | 0.71     | 1.61        | 2      | 6     |
| 1:A:46:VAL:HG13  | 1:A:83:GLU:CB    | 0.71     | 2.15        | 9      | 2     |
| 1:A:107:ALA:HB1  | 1:A:110:ILE:CD1  | 0.71     | 2.15        | 1      | 10    |
| 1:A:76:VAL:HG13  | 1:A:85:TRP:CB    | 0.71     | 2.16        | 20     | 9     |
| 1:A:189:GLU:O    | 1:A:190:ARG:CG   | 0.71     | 2.38        | 20     | 6     |
| 1:A:196:TYR:O    | 1:A:198:LEU:HD23 | 0.71     | 1.85        | 3      | 4     |
| 1:A:177:LEU:C    | 1:A:177:LEU:HD13 | 0.71     | 2.06        | 1      | 2     |
| 1:A:89:PHE:CD2   | 1:A:89:PHE:O     | 0.71     | 2.43        | 11     | 3     |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:HD11 | 0.71     | 1.63        | 17     | 2     |
| 1:A:168:VAL:HG13 | 1:A:198:LEU:HG   | 0.71     | 1.62        | 17     | 2     |
| 1:A:196:TYR:OH   | 1:A:198:LEU:HD23 | 0.71     | 1.84        | 20     | 1     |
| 1:A:76:VAL:HG23  | 1:A:85:TRP:CB    | 0.70     | 2.16        | 2      | 6     |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:CD1  | 0.70     | 2.16        | 10     | 4     |
| 1:A:177:LEU:HD12 | 1:A:190:ARG:H    | 0.70     | 1.44        | 15     | 1     |
| 1:A:137:ILE:HG13 | 1:A:195:VAL:HG22 | 0.70     | 1.62        | 16     | 6     |
| 1:A:97:ILE:C     | 1:A:97:ILE:HD12  | 0.70     | 2.07        | 11     | 2     |
| 1:A:85:TRP:CH2   | 1:A:89:PHE:HA    | 0.70     | 2.22        | 16     | 20    |
| 1:A:9:LEU:C      | 1:A:9:LEU:HD13   | 0.70     | 2.05        | 15     | 9     |
| 1:A:137:ILE:HD13 | 1:A:195:VAL:HB   | 0.70     | 1.63        | 12     | 2     |
| 1:A:28:LEU:HD11  | 1:A:120:TYR:OH   | 0.70     | 1.86        | 7      | 3     |
| 1:A:103:PHE:CE1  | 1:A:134:GLY:HA3  | 0.70     | 2.22        | 1      | 4     |
| 1:A:8:ASP:OD2    | 1:A:195:VAL:HG21 | 0.70     | 1.86        | 20     | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:77:TYR:CD1   | 1:A:77:TYR:C     | 0.70     | 2.65        | 16     | 5     |
| 1:A:26:VAL:CG2   | 1:A:26:VAL:O     | 0.70     | 2.40        | 11     | 4     |
| 1:A:35:MET:CG    | 1:A:45:VAL:HG11  | 0.70     | 2.17        | 7      | 7     |
| 1:A:139:LEU:N    | 1:A:139:LEU:HD12 | 0.70     | 2.02        | 10     | 6     |
| 1:A:132:CYS:O    | 1:A:200:ARG:CB   | 0.70     | 2.39        | 15     | 2     |
| 1:A:158:LEU:O    | 1:A:162:MET:CB   | 0.69     | 2.39        | 19     | 19    |
| 1:A:69:THR:HG22  | 1:A:76:VAL:CG1   | 0.69     | 2.16        | 8      | 7     |
| 1:A:142:ASP:OD1  | 1:A:142:ASP:N    | 0.69     | 2.24        | 3      | 9     |
| 1:A:89:PHE:CZ    | 1:A:127:LEU:HD21 | 0.69     | 2.22        | 8      | 3     |
| 1:A:171:VAL:HG21 | 1:A:197:VAL:HG23 | 0.69     | 1.64        | 6      | 2     |
| 1:A:177:LEU:HD23 | 1:A:191:MET:HG3  | 0.69     | 1.63        | 19     | 1     |
| 1:A:168:VAL:HG22 | 1:A:198:LEU:CB   | 0.69     | 2.16        | 19     | 2     |
| 1:A:139:LEU:N    | 1:A:139:LEU:HD23 | 0.69     | 2.02        | 19     | 1     |
| 1:A:89:PHE:O     | 1:A:89:PHE:CD1   | 0.69     | 2.46        | 7      | 7     |
| 1:A:138:THR:HG21 | 1:A:153:VAL:CG1  | 0.69     | 2.18        | 8      | 4     |
| 1:A:55:VAL:HG23  | 1:A:59:PHE:CE2   | 0.69     | 2.22        | 13     | 4     |
| 1:A:145:LEU:CD2  | 1:A:186:ALA:HB1  | 0.69     | 2.18        | 5      | 3     |
| 1:A:145:LEU:HD22 | 1:A:146:LEU:N    | 0.69     | 2.02        | 5      | 16    |
| 1:A:162:MET:HB3  | 1:A:168:VAL:HG11 | 0.69     | 1.64        | 5      | 3     |
| 1:A:19:VAL:HG23  | 1:A:22:ALA:CB    | 0.69     | 2.14        | 15     | 6     |
| 1:A:117:ARG:HG3  | 1:A:157:TRP:CH2  | 0.69     | 2.22        | 12     | 1     |
| 1:A:166:TRP:N    | 1:A:166:TRP:CD1  | 0.69     | 2.60        | 12     | 11    |
| 1:A:103:PHE:CD1  | 1:A:200:ARG:NH2  | 0.69     | 2.60        | 15     | 1     |
| 1:A:99:HIS:N     | 1:A:129:PRO:HB3  | 0.69     | 2.02        | 16     | 20    |
| 1:A:12:TYR:HE2   | 1:A:171:VAL:HG21 | 0.69     | 1.46        | 12     | 2     |
| 1:A:139:LEU:N    | 1:A:139:LEU:HD22 | 0.69     | 2.01        | 2      | 3     |
| 1:A:121:VAL:HG22 | 1:A:162:MET:HE2  | 0.69     | 1.64        | 17     | 1     |
| 1:A:51:SER:O     | 1:A:55:VAL:CG1   | 0.69     | 2.41        | 17     | 7     |
| 1:A:136:LEU:HB3  | 1:A:196:TYR:CE2  | 0.69     | 2.23        | 18     | 1     |
| 1:A:26:VAL:O     | 1:A:26:VAL:HG22  | 0.69     | 1.85        | 17     | 1     |
| 1:A:168:VAL:CG2  | 1:A:196:TYR:CZ   | 0.68     | 2.76        | 15     | 1     |
| 1:A:137:ILE:CD1  | 1:A:195:VAL:HG22 | 0.68     | 2.17        | 1      | 5     |
| 1:A:158:LEU:HD23 | 1:A:162:MET:CE   | 0.68     | 2.18        | 10     | 1     |
| 1:A:198:LEU:H    | 1:A:198:LEU:HD12 | 0.68     | 1.49        | 20     | 6     |
| 1:A:22:ALA:HB1   | 1:A:101:ALA:HA   | 0.68     | 1.65        | 7      | 20    |
| 1:A:74:PHE:CG    | 1:A:88:ASP:CB    | 0.68     | 2.77        | 8      | 15    |
| 1:A:196:TYR:CZ   | 1:A:198:LEU:CD2  | 0.68     | 2.76        | 20     | 2     |
| 1:A:97:ILE:O     | 1:A:99:HIS:CE1   | 0.68     | 2.46        | 7      | 1     |
| 1:A:50:LEU:HD21  | 1:A:89:PHE:CB    | 0.68     | 2.18        | 15     | 5     |
| 1:A:136:LEU:HD12 | 1:A:162:MET:HE1  | 0.68     | 1.64        | 3      | 2     |
| 1:A:146:LEU:HD12 | 1:A:146:LEU:C    | 0.68     | 2.08        | 3      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:125:GLU:CG   | 1:A:166:TRP:CE2  | 0.68     | 2.77        | 11     | 5     |
| 1:A:177:LEU:C    | 1:A:177:LEU:HD22 | 0.68     | 2.07        | 15     | 2     |
| 1:A:28:LEU:HD22  | 1:A:50:LEU:HD23  | 0.68     | 1.65        | 11     | 1     |
| 1:A:28:LEU:CD1   | 1:A:28:LEU:N     | 0.68     | 2.56        | 3      | 5     |
| 1:A:176:THR:O    | 1:A:176:THR:HG23 | 0.68     | 1.87        | 14     | 7     |
| 1:A:24:VAL:HG21  | 1:A:38:LEU:HD13  | 0.68     | 1.64        | 9      | 1     |
| 1:A:26:VAL:HG12  | 1:A:104:TYR:HB3  | 0.68     | 1.64        | 4      | 5     |
| 1:A:6:ASN:ND2    | 1:A:137:ILE:HD12 | 0.68     | 2.03        | 1      | 1     |
| 1:A:157:TRP:CE2  | 1:A:161:VAL:HG11 | 0.68     | 2.24        | 13     | 19    |
| 1:A:59:PHE:CD1   | 1:A:59:PHE:N     | 0.68     | 2.60        | 17     | 9     |
| 1:A:142:ASP:HB3  | 1:A:188:LEU:HD11 | 0.68     | 1.64        | 15     | 12    |
| 1:A:5:VAL:HG21   | 1:A:37:TRP:CB    | 0.68     | 2.19        | 4      | 11    |
| 1:A:135:LEU:CD1  | 1:A:197:VAL:HG22 | 0.68     | 2.19        | 13     | 4     |
| 1:A:168:VAL:HG12 | 1:A:198:LEU:HD23 | 0.68     | 1.65        | 6      | 5     |
| 1:A:104:TYR:CE1  | 1:A:135:LEU:CB   | 0.68     | 2.77        | 10     | 1     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:HG23  | 0.68     | 1.65        | 4      | 1     |
| 1:A:12:TYR:CZ    | 1:A:197:VAL:HG21 | 0.67     | 2.24        | 18     | 1     |
| 1:A:171:VAL:O    | 1:A:195:VAL:O    | 0.67     | 2.11        | 14     | 19    |
| 1:A:26:VAL:CG1   | 1:A:26:VAL:O     | 0.67     | 2.42        | 1      | 2     |
| 1:A:28:LEU:N     | 1:A:28:LEU:CD1   | 0.67     | 2.55        | 17     | 6     |
| 1:A:165:ASN:OD1  | 1:A:166:TRP:CD1  | 0.67     | 2.47        | 3      | 1     |
| 1:A:46:VAL:HG11  | 1:A:97:ILE:CD1   | 0.67     | 2.19        | 19     | 2     |
| 1:A:51:SER:HB3   | 1:A:54:ALA:HB3   | 0.67     | 1.66        | 9      | 7     |
| 1:A:45:VAL:CG1   | 1:A:82:ILE:HD11  | 0.67     | 2.18        | 9      | 4     |
| 1:A:77:TYR:O     | 1:A:77:TYR:CD1   | 0.67     | 2.48        | 10     | 2     |
| 1:A:92:LEU:HD22  | 1:A:97:ILE:HD13  | 0.67     | 1.67        | 20     | 1     |
| 1:A:25:LEU:CD2   | 1:A:128:MET:CE   | 0.67     | 2.72        | 10     | 5     |
| 1:A:48:ALA:HB2   | 1:A:85:TRP:CD2   | 0.67     | 2.23        | 20     | 12    |
| 1:A:46:VAL:CG1   | 1:A:97:ILE:HD12  | 0.67     | 2.20        | 17     | 2     |
| 1:A:162:MET:SD   | 1:A:166:TRP:CZ2  | 0.67     | 2.88        | 17     | 7     |
| 1:A:109:MET:HE1  | 1:A:136:LEU:HD11 | 0.67     | 1.66        | 1      | 4     |
| 1:A:26:VAL:HG23  | 1:A:29:CYS:CB    | 0.67     | 2.20        | 17     | 2     |
| 1:A:92:LEU:HD22  | 1:A:92:LEU:C     | 0.67     | 2.10        | 11     | 4     |
| 1:A:136:LEU:HD21 | 1:A:138:THR:CG2  | 0.67     | 2.19        | 18     | 2     |
| 1:A:117:ARG:HB3  | 1:A:157:TRP:CH2  | 0.67     | 2.25        | 13     | 18    |
| 1:A:177:LEU:O    | 1:A:177:LEU:HD13 | 0.67     | 1.88        | 1      | 2     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:HG12 | 0.67     | 1.67        | 6      | 2     |
| 1:A:46:VAL:HG21  | 1:A:97:ILE:HD12  | 0.67     | 1.64        | 12     | 3     |
| 1:A:27:PRO:CD    | 1:A:104:TYR:O    | 0.67     | 2.43        | 20     | 1     |
| 1:A:103:PHE:CG   | 1:A:103:PHE:O    | 0.67     | 2.47        | 5      | 6     |
| 1:A:167:GLU:O    | 1:A:198:LEU:HA   | 0.67     | 1.90        | 19     | 7     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:97:ILE:C     | 1:A:97:ILE:HD13  | 0.67     | 2.10        | 19     | 2     |
| 1:A:171:VAL:HG22 | 1:A:172:GLY:N    | 0.67     | 2.04        | 12     | 3     |
| 1:A:158:LEU:HD23 | 1:A:162:MET:CG   | 0.67     | 2.20        | 4      | 1     |
| 1:A:178:HIS:CD2  | 1:A:184:LEU:CD2  | 0.67     | 2.77        | 15     | 1     |
| 1:A:195:VAL:O    | 1:A:196:TYR:CD1  | 0.67     | 2.48        | 13     | 14    |
| 1:A:18:VAL:HG12  | 1:A:22:ALA:CB    | 0.67     | 2.20        | 9      | 6     |
| 1:A:92:LEU:HD22  | 1:A:93:THR:N     | 0.67     | 2.05        | 9      | 7     |
| 1:A:124:LEU:HD13 | 1:A:128:MET:SD   | 0.67     | 2.29        | 4      | 3     |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:HD21 | 0.67     | 1.65        | 19     | 1     |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:CD2  | 0.66     | 2.19        | 9      | 3     |
| 1:A:171:VAL:HG11 | 1:A:197:VAL:CG2  | 0.66     | 2.20        | 18     | 1     |
| 1:A:117:ARG:NH1  | 1:A:157:TRP:CZ3  | 0.66     | 2.62        | 17     | 2     |
| 1:A:104:TYR:CE1  | 1:A:137:ILE:HD11 | 0.66     | 2.26        | 2      | 1     |
| 1:A:89:PHE:O     | 1:A:89:PHE:CD2   | 0.66     | 2.47        | 18     | 4     |
| 1:A:136:LEU:HD22 | 1:A:137:ILE:H    | 0.66     | 1.48        | 20     | 1     |
| 1:A:160:ARG:HG3  | 1:A:161:VAL:N    | 0.66     | 2.05        | 1      | 15    |
| 1:A:26:VAL:HG13  | 1:A:29:CYS:SG    | 0.66     | 2.30        | 1      | 1     |
| 1:A:168:VAL:HG12 | 1:A:198:LEU:HB3  | 0.66     | 1.66        | 3      | 12    |
| 1:A:154:PRO:HB2  | 1:A:156:THR:HG22 | 0.66     | 1.66        | 13     | 6     |
| 1:A:24:VAL:CG1   | 1:A:38:LEU:HD13  | 0.66     | 2.16        | 14     | 3     |
| 1:A:46:VAL:HG21  | 1:A:97:ILE:HG13  | 0.66     | 1.67        | 4      | 1     |
| 1:A:29:CYS:SG    | 1:A:104:TYR:CD1  | 0.66     | 2.89        | 5      | 1     |
| 1:A:162:MET:CE   | 1:A:166:TRP:CH2  | 0.66     | 2.79        | 19     | 5     |
| 1:A:19:VAL:HG13  | 1:A:22:ALA:CB    | 0.66     | 2.13        | 20     | 3     |
| 1:A:117:ARG:CZ   | 1:A:153:VAL:HG21 | 0.66     | 2.21        | 17     | 1     |
| 1:A:168:VAL:CB   | 1:A:196:TYR:CE1  | 0.66     | 2.79        | 20     | 1     |
| 1:A:158:LEU:HD22 | 1:A:196:TYR:CE2  | 0.66     | 2.26        | 20     | 1     |
| 1:A:89:PHE:CG    | 1:A:89:PHE:O     | 0.66     | 2.47        | 11     | 3     |
| 1:A:94:ALA:HB3   | 1:A:127:LEU:HD12 | 0.66     | 1.67        | 4      | 1     |
| 1:A:9:LEU:HD23   | 1:A:135:LEU:HD23 | 0.66     | 1.66        | 13     | 2     |
| 1:A:85:TRP:CZ3   | 1:A:88:ASP:O     | 0.66     | 2.49        | 17     | 18    |
| 1:A:19:VAL:HG23  | 1:A:20:PRO:HD2   | 0.66     | 1.68        | 18     | 7     |
| 1:A:107:ALA:HB1  | 1:A:139:LEU:HD11 | 0.66     | 1.68        | 16     | 1     |
| 1:A:137:ILE:HD13 | 1:A:195:VAL:HG22 | 0.66     | 1.67        | 11     | 3     |
| 1:A:107:ALA:HB1  | 1:A:139:LEU:HD21 | 0.66     | 1.68        | 4      | 1     |
| 1:A:50:LEU:CD1   | 1:A:74:PHE:CZ    | 0.66     | 2.78        | 20     | 1     |
| 1:A:127:LEU:C    | 1:A:127:LEU:CD1  | 0.66     | 2.64        | 16     | 13    |
| 1:A:12:TYR:CD1   | 1:A:197:VAL:HG21 | 0.66     | 2.26        | 15     | 4     |
| 1:A:98:GLY:O     | 1:A:99:HIS:CD2   | 0.66     | 2.50        | 7      | 1     |
| 1:A:90:PHE:O     | 1:A:90:PHE:CG    | 0.66     | 2.48        | 11     | 1     |
| 1:A:158:LEU:O    | 1:A:162:MET:N    | 0.65     | 2.29        | 10     | 11    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:HD11 | 0.65     | 1.69        | 16     | 3     |
| 1:A:26:VAL:HG22  | 1:A:26:VAL:O     | 0.65     | 1.90        | 6      | 3     |
| 1:A:24:VAL:HG11  | 1:A:38:LEU:HD23  | 0.65     | 1.67        | 6      | 3     |
| 1:A:136:LEU:C    | 1:A:137:ILE:HD13 | 0.65     | 2.11        | 13     | 4     |
| 1:A:25:LEU:HD12  | 1:A:97:ILE:HD11  | 0.65     | 1.67        | 15     | 2     |
| 1:A:164:GLY:O    | 1:A:165:ASN:CB   | 0.65     | 2.43        | 15     | 18    |
| 1:A:27:PRO:O     | 1:A:28:LEU:C     | 0.65     | 2.34        | 14     | 16    |
| 1:A:189:GLU:O    | 1:A:190:ARG:HB3  | 0.65     | 1.91        | 20     | 7     |
| 1:A:89:PHE:O     | 1:A:90:PHE:CD1   | 0.65     | 2.49        | 14     | 2     |
| 1:A:109:MET:HB3  | 1:A:117:ARG:CZ   | 0.65     | 2.21        | 16     | 3     |
| 1:A:121:VAL:HG22 | 1:A:162:MET:CE   | 0.65     | 2.21        | 17     | 1     |
| 1:A:117:ARG:NE   | 1:A:153:VAL:HG21 | 0.65     | 2.06        | 17     | 1     |
| 1:A:92:LEU:CD2   | 1:A:97:ILE:CG2   | 0.65     | 2.75        | 16     | 5     |
| 1:A:74:PHE:CD1   | 1:A:88:ASP:CG    | 0.65     | 2.70        | 4      | 8     |
| 1:A:28:LEU:HB3   | 1:A:50:LEU:HD23  | 0.65     | 1.67        | 5      | 5     |
| 1:A:103:PHE:CZ   | 1:A:134:GLY:HA3  | 0.65     | 2.27        | 12     | 6     |
| 1:A:158:LEU:HD22 | 1:A:196:TYR:CD2  | 0.65     | 2.27        | 14     | 1     |
| 1:A:172:GLY:CA   | 1:A:195:VAL:HG22 | 0.65     | 2.22        | 14     | 2     |
| 1:A:157:TRP:CZ2  | 1:A:161:VAL:HG11 | 0.65     | 2.26        | 13     | 18    |
| 1:A:95:ARG:N     | 1:A:127:LEU:O    | 0.65     | 2.30        | 13     | 19    |
| 1:A:158:LEU:HD22 | 1:A:196:TYR:CZ   | 0.65     | 2.27        | 18     | 1     |
| 1:A:46:VAL:HG11  | 1:A:97:ILE:CG1   | 0.65     | 2.21        | 4      | 5     |
| 1:A:138:THR:C    | 1:A:139:LEU:HD12 | 0.65     | 2.12        | 7      | 2     |
| 1:A:142:ASP:HB3  | 1:A:146:LEU:HD12 | 0.65     | 1.67        | 18     | 9     |
| 1:A:198:LEU:N    | 1:A:198:LEU:CD2  | 0.65     | 2.56        | 14     | 3     |
| 1:A:89:PHE:O     | 1:A:90:PHE:CG    | 0.65     | 2.50        | 8      | 7     |
| 1:A:196:TYR:O    | 1:A:196:TYR:CG   | 0.65     | 2.50        | 18     | 1     |
| 1:A:49:GLU:O     | 1:A:51:SER:N     | 0.64     | 2.31        | 20     | 4     |
| 1:A:177:LEU:C    | 1:A:177:LEU:HD12 | 0.64     | 2.13        | 4      | 4     |
| 1:A:55:VAL:O     | 1:A:59:PHE:CE1   | 0.64     | 2.50        | 13     | 2     |
| 1:A:59:PHE:CE2   | 1:A:68:ILE:HG21  | 0.64     | 2.27        | 3      | 3     |
| 1:A:172:GLY:N    | 1:A:195:VAL:HG22 | 0.64     | 2.07        | 14     | 2     |
| 1:A:35:MET:HA    | 1:A:38:LEU:HD12  | 0.64     | 1.67        | 13     | 2     |
| 1:A:89:PHE:O     | 1:A:89:PHE:CG    | 0.64     | 2.50        | 20     | 5     |
| 1:A:173:GLY:O    | 1:A:193:GLU:O    | 0.64     | 2.16        | 19     | 20    |
| 1:A:128:MET:HB3  | 1:A:129:PRO:HD2  | 0.64     | 1.70        | 16     | 18    |
| 1:A:158:LEU:CD1  | 1:A:196:TYR:CD2  | 0.64     | 2.81        | 2      | 2     |
| 1:A:171:VAL:HG13 | 1:A:195:VAL:C    | 0.64     | 2.13        | 15     | 1     |
| 1:A:109:MET:HB3  | 1:A:117:ARG:NE   | 0.64     | 2.08        | 18     | 2     |
| 1:A:59:PHE:CE1   | 1:A:77:TYR:CD2   | 0.64     | 2.85        | 17     | 7     |
| 1:A:145:LEU:CD2  | 1:A:145:LEU:C    | 0.64     | 2.64        | 5      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:92:LEU:C     | 1:A:92:LEU:HD22  | 0.64     | 2.13        | 16     | 5     |
| 1:A:49:GLU:CD    | 1:A:84:ILE:HD12  | 0.64     | 2.14        | 19     | 1     |
| 1:A:198:LEU:HD12 | 1:A:198:LEU:H    | 0.64     | 1.53        | 17     | 3     |
| 1:A:188:LEU:N    | 1:A:188:LEU:HD12 | 0.63     | 2.07        | 20     | 6     |
| 1:A:196:TYR:CZ   | 1:A:198:LEU:HG   | 0.63     | 2.29        | 20     | 1     |
| 1:A:117:ARG:HG2  | 1:A:157:TRP:CH2  | 0.63     | 2.28        | 12     | 1     |
| 1:A:77:TYR:O     | 1:A:85:TRP:HA    | 0.63     | 1.93        | 7      | 19    |
| 1:A:109:MET:HE1  | 1:A:158:LEU:HD11 | 0.63     | 1.68        | 5      | 1     |
| 1:A:98:GLY:O     | 1:A:99:HIS:CG    | 0.63     | 2.51        | 18     | 2     |
| 1:A:136:LEU:C    | 1:A:137:ILE:HD12 | 0.63     | 2.13        | 16     | 4     |
| 1:A:26:VAL:HG23  | 1:A:29:CYS:HB3   | 0.63     | 1.68        | 17     | 2     |
| 1:A:23:ARG:H     | 1:A:101:ALA:HB2  | 0.63     | 1.51        | 17     | 20    |
| 1:A:160:ARG:HG2  | 1:A:161:VAL:HG12 | 0.63     | 1.70        | 5      | 13    |
| 1:A:28:LEU:CD2   | 1:A:89:PHE:CD1   | 0.63     | 2.80        | 7      | 1     |
| 1:A:52:GLU:O     | 1:A:55:VAL:HG22  | 0.63     | 1.93        | 16     | 3     |
| 1:A:197:VAL:HG13 | 1:A:197:VAL:O    | 0.63     | 1.93        | 17     | 5     |
| 1:A:183:GLY:HA2  | 1:A:188:LEU:HD13 | 0.63     | 1.71        | 14     | 3     |
| 1:A:125:GLU:HG2  | 1:A:166:TRP:CE2  | 0.63     | 2.28        | 11     | 4     |
| 1:A:127:LEU:CD1  | 1:A:127:LEU:C    | 0.63     | 2.67        | 1      | 7     |
| 1:A:10:GLN:O     | 1:A:14:SER:CB    | 0.63     | 2.47        | 10     | 20    |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:CD2  | 0.63     | 2.24        | 15     | 3     |
| 1:A:109:MET:HG3  | 1:A:117:ARG:CZ   | 0.63     | 2.23        | 12     | 2     |
| 1:A:124:LEU:HD22 | 1:A:128:MET:SD   | 0.63     | 2.32        | 4      | 1     |
| 1:A:34:ASP:OD1   | 1:A:104:TYR:CE2  | 0.63     | 2.51        | 7      | 2     |
| 1:A:26:VAL:HG12  | 1:A:26:VAL:O     | 0.63     | 1.93        | 15     | 1     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:HD21 | 0.63     | 1.71        | 5      | 4     |
| 1:A:33:GLN:HG2   | 1:A:181:ALA:HB2  | 0.63     | 1.71        | 7      | 1     |
| 1:A:107:ALA:CB   | 1:A:139:LEU:HD21 | 0.63     | 2.24        | 4      | 1     |
| 1:A:49:GLU:O     | 1:A:87:GLY:C     | 0.62     | 2.37        | 17     | 14    |
| 1:A:103:PHE:O    | 1:A:134:GLY:HA2  | 0.62     | 1.93        | 10     | 8     |
| 1:A:117:ARG:NH2  | 1:A:120:TYR:CG   | 0.62     | 2.68        | 5      | 1     |
| 1:A:145:LEU:CD1  | 1:A:145:LEU:N    | 0.62     | 2.62        | 11     | 3     |
| 1:A:100:CYS:HA   | 1:A:132:CYS:SG   | 0.62     | 2.33        | 6      | 5     |
| 1:A:196:TYR:CZ   | 1:A:198:LEU:CG   | 0.62     | 2.82        | 20     | 1     |
| 1:A:51:SER:OG    | 1:A:54:ALA:HB2   | 0.62     | 1.93        | 11     | 3     |
| 1:A:124:LEU:CD2  | 1:A:127:LEU:HD11 | 0.62     | 2.24        | 8      | 9     |
| 1:A:176:THR:CG2  | 1:A:176:THR:O    | 0.62     | 2.47        | 19     | 10    |
| 1:A:12:TYR:CE2   | 1:A:171:VAL:HG13 | 0.62     | 2.29        | 6      | 1     |
| 1:A:109:MET:SD   | 1:A:120:TYR:CD1  | 0.62     | 2.92        | 19     | 1     |
| 1:A:51:SER:HB2   | 1:A:54:ALA:HB3   | 0.62     | 1.70        | 15     | 2     |
| 1:A:103:PHE:CD1  | 1:A:104:TYR:N    | 0.62     | 2.67        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:55:VAL:HG23  | 1:A:59:PHE:CZ    | 0.62     | 2.28        | 13     | 2     |
| 1:A:136:LEU:HD11 | 1:A:138:THR:HG23 | 0.62     | 1.71        | 20     | 1     |
| 1:A:171:VAL:CG2  | 1:A:172:GLY:N    | 0.62     | 2.62        | 20     | 18    |
| 1:A:37:TRP:CH2   | 1:A:41:GLN:NE2   | 0.62     | 2.67        | 4      | 1     |
| 1:A:125:GLU:CD   | 1:A:166:TRP:CD1  | 0.62     | 2.72        | 19     | 1     |
| 1:A:168:VAL:HG12 | 1:A:196:TYR:HB3  | 0.62     | 1.70        | 9      | 2     |
| 1:A:26:VAL:CG1   | 1:A:29:CYS:HB3   | 0.62     | 2.23        | 3      | 1     |
| 1:A:103:PHE:O    | 1:A:103:PHE:CD1  | 0.62     | 2.52        | 10     | 2     |
| 1:A:162:MET:SD   | 1:A:198:LEU:CD2  | 0.62     | 2.88        | 11     | 4     |
| 1:A:94:ALA:O     | 1:A:98:GLY:HA3   | 0.62     | 1.95        | 16     | 2     |
| 1:A:168:VAL:HG13 | 1:A:198:LEU:CG   | 0.62     | 2.23        | 17     | 2     |
| 1:A:162:MET:O    | 1:A:166:TRP:NE1  | 0.62     | 2.33        | 15     | 14    |
| 1:A:12:TYR:CE2   | 1:A:171:VAL:CG1  | 0.62     | 2.83        | 6      | 1     |
| 1:A:65:GLN:N     | 1:A:66:PRO:CD    | 0.62     | 2.62        | 14     | 17    |
| 1:A:66:PRO:CG    | 1:A:77:TYR:CE1   | 0.62     | 2.83        | 19     | 11    |
| 1:A:59:PHE:N     | 1:A:59:PHE:CD1   | 0.62     | 2.64        | 13     | 11    |
| 1:A:135:LEU:HD13 | 1:A:197:VAL:HG23 | 0.62     | 1.72        | 11     | 2     |
| 1:A:125:GLU:HG3  | 1:A:166:TRP:CE2  | 0.62     | 2.30        | 6      | 6     |
| 1:A:124:LEU:O    | 1:A:127:LEU:HD12 | 0.61     | 1.95        | 5      | 3     |
| 1:A:25:LEU:HD22  | 1:A:26:VAL:H     | 0.61     | 1.54        | 5      | 2     |
| 1:A:165:ASN:C    | 1:A:201:VAL:HG22 | 0.61     | 2.14        | 13     | 2     |
| 1:A:103:PHE:CE1  | 1:A:105:ASP:CG   | 0.61     | 2.74        | 2      | 1     |
| 1:A:50:LEU:CD2   | 1:A:89:PHE:HB3   | 0.61     | 2.25        | 11     | 13    |
| 1:A:29:CYS:SG    | 1:A:29:CYS:O     | 0.61     | 2.58        | 16     | 2     |
| 1:A:117:ARG:HD2  | 1:A:157:TRP:CH2  | 0.61     | 2.30        | 7      | 1     |
| 1:A:22:ALA:CB    | 1:A:101:ALA:CB   | 0.61     | 2.75        | 18     | 20    |
| 1:A:177:LEU:HD22 | 1:A:177:LEU:C    | 0.61     | 2.14        | 5      | 2     |
| 1:A:89:PHE:O     | 1:A:90:PHE:CB    | 0.61     | 2.47        | 8      | 10    |
| 1:A:136:LEU:HB3  | 1:A:196:TYR:CD2  | 0.61     | 2.30        | 18     | 1     |
| 1:A:158:LEU:HD22 | 1:A:196:TYR:HE2  | 0.61     | 1.54        | 20     | 1     |
| 1:A:89:PHE:O     | 1:A:90:PHE:HB3   | 0.61     | 1.94        | 17     | 2     |
| 1:A:136:LEU:HD11 | 1:A:138:THR:CG2  | 0.61     | 2.25        | 20     | 1     |
| 1:A:46:VAL:CG1   | 1:A:97:ILE:HD11  | 0.61     | 2.26        | 4      | 1     |
| 1:A:158:LEU:O    | 1:A:162:MET:HB2  | 0.61     | 1.95        | 17     | 19    |
| 1:A:103:PHE:CE2  | 1:A:134:GLY:HA3  | 0.61     | 2.31        | 16     | 11    |
| 1:A:74:PHE:CE1   | 1:A:88:ASP:OD2   | 0.61     | 2.54        | 7      | 4     |
| 1:A:59:PHE:CZ    | 1:A:68:ILE:HD12  | 0.61     | 2.31        | 14     | 9     |
| 1:A:74:PHE:CE1   | 1:A:88:ASP:OD1   | 0.61     | 2.54        | 10     | 7     |
| 1:A:177:LEU:HD13 | 1:A:177:LEU:C    | 0.61     | 2.16        | 6      | 4     |
| 1:A:23:ARG:CG    | 1:A:97:ILE:O     | 0.61     | 2.49        | 20     | 16    |
| 1:A:74:PHE:CE2   | 1:A:88:ASP:OD2   | 0.61     | 2.53        | 10     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:178:HIS:HA   | 1:A:184:LEU:HD21 | 0.61     | 1.73        | 3      | 1     |
| 1:A:26:VAL:HG13  | 1:A:47:GLY:CA    | 0.61     | 2.25        | 17     | 3     |
| 1:A:136:LEU:HD22 | 1:A:138:THR:HG23 | 0.61     | 1.70        | 14     | 1     |
| 1:A:162:MET:HE1  | 1:A:166:TRP:CH2  | 0.61     | 2.30        | 19     | 1     |
| 1:A:27:PRO:C     | 1:A:28:LEU:HD23  | 0.61     | 2.16        | 9      | 1     |
| 1:A:23:ARG:CB    | 1:A:97:ILE:O     | 0.61     | 2.48        | 7      | 15    |
| 1:A:50:LEU:HD13  | 1:A:74:PHE:CZ    | 0.61     | 2.31        | 20     | 1     |
| 1:A:104:TYR:CZ   | 1:A:135:LEU:CB   | 0.61     | 2.84        | 10     | 1     |
| 1:A:130:GLN:O    | 1:A:201:VAL:C    | 0.60     | 2.39        | 15     | 15    |
| 1:A:85:TRP:CZ2   | 1:A:92:LEU:HG    | 0.60     | 2.31        | 20     | 12    |
| 1:A:198:LEU:CD2  | 1:A:198:LEU:N    | 0.60     | 2.57        | 10     | 2     |
| 1:A:24:VAL:HG21  | 1:A:38:LEU:HG    | 0.60     | 1.72        | 19     | 1     |
| 1:A:23:ARG:NH1   | 1:A:44:HIS:CG    | 0.60     | 2.69        | 11     | 2     |
| 1:A:142:ASP:CB   | 1:A:146:LEU:HD12 | 0.60     | 2.26        | 1      | 8     |
| 1:A:139:LEU:HD12 | 1:A:146:LEU:CD2  | 0.60     | 2.26        | 14     | 1     |
| 1:A:139:LEU:CD2  | 1:A:191:MET:CE   | 0.60     | 2.79        | 7      | 1     |
| 1:A:59:PHE:CE1   | 1:A:77:TYR:HB2   | 0.60     | 2.31        | 6      | 12    |
| 1:A:77:TYR:O     | 1:A:84:ILE:O     | 0.60     | 2.19        | 20     | 13    |
| 1:A:162:MET:HE2  | 1:A:166:TRP:CH2  | 0.60     | 2.31        | 14     | 7     |
| 1:A:76:VAL:CG2   | 1:A:76:VAL:O     | 0.60     | 2.48        | 17     | 4     |
| 1:A:124:LEU:HD22 | 1:A:128:MET:HG2  | 0.60     | 1.73        | 19     | 1     |
| 1:A:158:LEU:HD23 | 1:A:168:VAL:HG11 | 0.60     | 1.72        | 19     | 2     |
| 1:A:102:ALA:CB   | 1:A:133:SER:O    | 0.60     | 2.45        | 1      | 14    |
| 1:A:28:LEU:CD1   | 1:A:89:PHE:CD1   | 0.60     | 2.84        | 1      | 1     |
| 1:A:27:PRO:C     | 1:A:28:LEU:HD13  | 0.60     | 2.16        | 1      | 6     |
| 1:A:27:PRO:HD2   | 1:A:104:TYR:O    | 0.60     | 1.97        | 7      | 11    |
| 1:A:85:TRP:CZ3   | 1:A:89:PHE:HA    | 0.60     | 2.32        | 14     | 12    |
| 1:A:94:ALA:CB    | 1:A:127:LEU:CD1  | 0.60     | 2.79        | 4      | 1     |
| 1:A:125:GLU:HG2  | 1:A:166:TRP:CD2  | 0.60     | 2.32        | 12     | 3     |
| 1:A:9:LEU:C      | 1:A:9:LEU:CD1    | 0.60     | 2.67        | 10     | 5     |
| 1:A:177:LEU:HD13 | 1:A:177:LEU:O    | 0.60     | 1.97        | 14     | 2     |
| 1:A:124:LEU:HD22 | 1:A:127:LEU:HD11 | 0.60     | 1.72        | 1      | 8     |
| 1:A:25:LEU:CD2   | 1:A:128:MET:HE1  | 0.60     | 2.27        | 17     | 4     |
| 1:A:48:ALA:CB    | 1:A:85:TRP:CE2   | 0.59     | 2.81        | 8      | 2     |
| 1:A:188:LEU:HD13 | 1:A:191:MET:SD   | 0.59     | 2.36        | 14     | 1     |
| 1:A:125:GLU:CG   | 1:A:166:TRP:CD2  | 0.59     | 2.84        | 11     | 5     |
| 1:A:98:GLY:C     | 1:A:99:HIS:CG    | 0.59     | 2.75        | 7      | 2     |
| 1:A:137:ILE:HD12 | 1:A:195:VAL:HG22 | 0.59     | 1.74        | 7      | 2     |
| 1:A:168:VAL:HA   | 1:A:196:TYR:HE1  | 0.59     | 1.57        | 20     | 1     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:HD11 | 0.59     | 1.73        | 13     | 7     |
| 1:A:32:SER:HB3   | 1:A:181:ALA:HB2  | 0.59     | 1.73        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:49:GLU:O     | 1:A:87:GLY:O     | 0.59     | 2.19        | 11     | 17    |
| 1:A:141:TYR:O    | 1:A:142:ASP:C    | 0.59     | 2.41        | 2      | 20    |
| 1:A:154:PRO:O    | 1:A:157:TRP:N    | 0.59     | 2.34        | 16     | 13    |
| 1:A:184:LEU:HD22 | 1:A:184:LEU:N    | 0.59     | 2.12        | 2      | 2     |
| 1:A:55:VAL:HG11  | 1:A:75:LYS:HD2   | 0.59     | 1.74        | 4      | 2     |
| 1:A:55:VAL:HG23  | 1:A:86:CYS:SG    | 0.59     | 2.38        | 14     | 7     |
| 1:A:89:PHE:O     | 1:A:90:PHE:CD2   | 0.59     | 2.55        | 8      | 7     |
| 1:A:145:LEU:CD2  | 1:A:188:LEU:HG   | 0.59     | 2.25        | 7      | 4     |
| 1:A:25:LEU:CD1   | 1:A:25:LEU:C     | 0.59     | 2.71        | 8      | 5     |
| 1:A:161:VAL:HG22 | 1:A:162:MET:N    | 0.59     | 2.11        | 12     | 8     |
| 1:A:145:LEU:HD21 | 1:A:188:LEU:HD22 | 0.59     | 1.75        | 15     | 1     |
| 1:A:127:LEU:HD12 | 1:A:128:MET:N    | 0.59     | 2.13        | 17     | 13    |
| 1:A:50:LEU:CD2   | 1:A:50:LEU:N     | 0.59     | 2.65        | 16     | 1     |
| 1:A:188:LEU:HD22 | 1:A:191:MET:HG3  | 0.59     | 1.75        | 20     | 1     |
| 1:A:104:TYR:CZ   | 1:A:137:ILE:HD11 | 0.59     | 2.33        | 2      | 1     |
| 1:A:117:ARG:HH11 | 1:A:153:VAL:HG23 | 0.59     | 1.56        | 11     | 1     |
| 1:A:104:TYR:CZ   | 1:A:137:ILE:CD1  | 0.59     | 2.82        | 16     | 3     |
| 1:A:197:VAL:O    | 1:A:197:VAL:CG1  | 0.59     | 2.50        | 9      | 3     |
| 1:A:26:VAL:O     | 1:A:26:VAL:CG2   | 0.59     | 2.51        | 17     | 2     |
| 1:A:161:VAL:C    | 1:A:163:SER:H    | 0.59     | 2.00        | 19     | 15    |
| 1:A:9:LEU:O      | 1:A:13:TRP:HB2   | 0.59     | 1.97        | 10     | 16    |
| 1:A:124:LEU:O    | 1:A:128:MET:CG   | 0.59     | 2.50        | 5      | 10    |
| 1:A:69:THR:HG22  | 1:A:76:VAL:HG13  | 0.59     | 1.74        | 5      | 7     |
| 1:A:72:GLY:O     | 1:A:73:ASP:CB    | 0.59     | 2.51        | 20     | 1     |
| 1:A:162:MET:SD   | 1:A:198:LEU:HD23 | 0.59     | 2.38        | 1      | 3     |
| 1:A:142:ASP:OD2  | 1:A:146:LEU:HD23 | 0.59     | 1.97        | 20     | 4     |
| 1:A:74:PHE:CZ    | 1:A:88:ASP:OD2   | 0.59     | 2.56        | 18     | 3     |
| 1:A:74:PHE:CD2   | 1:A:88:ASP:CG    | 0.59     | 2.75        | 2      | 2     |
| 1:A:45:VAL:HG12  | 1:A:82:ILE:CD1   | 0.59     | 2.27        | 8      | 5     |
| 1:A:108:ALA:N    | 1:A:110:ILE:CD1  | 0.59     | 2.66        | 10     | 2     |
| 1:A:138:THR:OG1  | 1:A:196:TYR:CE2  | 0.59     | 2.56        | 19     | 1     |
| 1:A:139:LEU:CD2  | 1:A:139:LEU:N    | 0.59     | 2.66        | 9      | 3     |
| 1:A:139:LEU:H    | 1:A:139:LEU:HD22 | 0.59     | 1.55        | 4      | 1     |
| 1:A:168:VAL:HA   | 1:A:196:TYR:CE1  | 0.59     | 2.33        | 20     | 1     |
| 1:A:190:ARG:O    | 1:A:191:MET:CE   | 0.59     | 2.51        | 20     | 1     |
| 1:A:74:PHE:CZ    | 1:A:88:ASP:OD1   | 0.59     | 2.56        | 2      | 2     |
| 1:A:145:LEU:CD2  | 1:A:188:LEU:HD22 | 0.59     | 2.27        | 15     | 1     |
| 1:A:112:LEU:HD23 | 1:A:116:MET:HG3  | 0.59     | 1.72        | 16     | 1     |
| 1:A:196:TYR:OH   | 1:A:198:LEU:CD1  | 0.59     | 2.47        | 18     | 1     |
| 1:A:136:LEU:HD13 | 1:A:158:LEU:HD21 | 0.58     | 1.75        | 16     | 2     |
| 1:A:166:TRP:CE3  | 1:A:198:LEU:HD12 | 0.58     | 2.33        | 2      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:136:LEU:CD2  | 1:A:138:THR:HG23 | 0.58     | 2.28        | 18     | 2     |
| 1:A:28:LEU:HD23  | 1:A:89:PHE:CD1   | 0.58     | 2.32        | 7      | 1     |
| 1:A:117:ARG:O    | 1:A:121:VAL:HB   | 0.58     | 1.97        | 17     | 1     |
| 1:A:29:CYS:SG    | 1:A:106:ARG:N    | 0.58     | 2.76        | 20     | 1     |
| 1:A:104:TYR:CE1  | 1:A:135:LEU:HB2  | 0.58     | 2.32        | 10     | 1     |
| 1:A:100:CYS:SG   | 1:A:131:ALA:HB3  | 0.58     | 2.38        | 14     | 1     |
| 1:A:74:PHE:CE1   | 1:A:87:GLY:O     | 0.58     | 2.56        | 20     | 1     |
| 1:A:34:ASP:OD1   | 1:A:104:TYR:CG   | 0.58     | 2.56        | 1      | 1     |
| 1:A:5:VAL:O      | 1:A:6:ASN:O      | 0.58     | 2.21        | 16     | 15    |
| 1:A:117:ARG:HB3  | 1:A:157:TRP:CZ2  | 0.58     | 2.34        | 13     | 6     |
| 1:A:55:VAL:HG11  | 1:A:87:GLY:HA2   | 0.58     | 1.74        | 16     | 5     |
| 1:A:140:GLU:O    | 1:A:141:TYR:C    | 0.58     | 2.42        | 16     | 18    |
| 1:A:34:ASP:CG    | 1:A:104:TYR:CG   | 0.58     | 2.76        | 8      | 3     |
| 1:A:116:MET:O    | 1:A:119:ARG:HG3  | 0.58     | 1.98        | 12     | 2     |
| 1:A:94:ALA:H     | 1:A:127:LEU:HD13 | 0.58     | 1.59        | 4      | 1     |
| 1:A:118:GLU:HG2  | 1:A:161:VAL:HG21 | 0.58     | 1.75        | 16     | 11    |
| 1:A:170:LYS:C    | 1:A:171:VAL:HG12 | 0.58     | 2.17        | 18     | 7     |
| 1:A:74:PHE:CD2   | 1:A:88:ASP:OD2   | 0.58     | 2.56        | 3      | 2     |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:CD2  | 0.58     | 2.33        | 10     | 2     |
| 1:A:66:PRO:HG3   | 1:A:77:TYR:CE2   | 0.58     | 2.32        | 20     | 3     |
| 1:A:132:CYS:O    | 1:A:200:ARG:HB3  | 0.58     | 1.98        | 16     | 9     |
| 1:A:26:VAL:HG23  | 1:A:47:GLY:HA3   | 0.58     | 1.73        | 10     | 5     |
| 1:A:66:PRO:HG2   | 1:A:77:TYR:CD2   | 0.58     | 2.33        | 13     | 3     |
| 1:A:13:TRP:CZ3   | 1:A:104:TYR:CE1  | 0.58     | 2.92        | 10     | 1     |
| 1:A:55:VAL:HG13  | 1:A:59:PHE:CE2   | 0.58     | 2.34        | 2      | 9     |
| 1:A:177:LEU:HD12 | 1:A:189:GLU:HA   | 0.58     | 1.73        | 5      | 2     |
| 1:A:50:LEU:N     | 1:A:50:LEU:CD2   | 0.58     | 2.65        | 8      | 1     |
| 1:A:109:MET:HB3  | 1:A:117:ARG:CG   | 0.58     | 2.29        | 18     | 1     |
| 1:A:34:ASP:CG    | 1:A:104:TYR:CD1  | 0.58     | 2.77        | 13     | 1     |
| 1:A:136:LEU:HD22 | 1:A:158:LEU:HD21 | 0.58     | 1.74        | 13     | 1     |
| 1:A:171:VAL:CG2  | 1:A:172:GLY:H    | 0.58     | 2.11        | 12     | 3     |
| 1:A:198:LEU:HD12 | 1:A:198:LEU:N    | 0.58     | 2.11        | 20     | 2     |
| 1:A:135:LEU:HG   | 1:A:197:VAL:HG22 | 0.58     | 1.74        | 2      | 1     |
| 1:A:75:LYS:O     | 1:A:87:GLY:HA3   | 0.58     | 1.98        | 19     | 13    |
| 1:A:109:MET:SD   | 1:A:136:LEU:CD2  | 0.58     | 2.92        | 16     | 2     |
| 1:A:7:LYS:O      | 1:A:11:GLN:CB    | 0.58     | 2.52        | 10     | 11    |
| 1:A:165:ASN:OD1  | 1:A:166:TRP:CG   | 0.58     | 2.57        | 3      | 1     |
| 1:A:97:ILE:C     | 1:A:97:ILE:CD1   | 0.58     | 2.71        | 10     | 2     |
| 1:A:159:HIS:O    | 1:A:163:SER:HB3  | 0.58     | 1.98        | 20     | 19    |
| 1:A:139:LEU:H    | 1:A:139:LEU:HD12 | 0.58     | 1.58        | 16     | 1     |
| 1:A:125:GLU:CD   | 1:A:166:TRP:CG   | 0.58     | 2.77        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:94:ALA:CB    | 1:A:127:LEU:HD13 | 0.58     | 2.25        | 9      | 3     |
| 1:A:49:GLU:OE2   | 1:A:84:ILE:HG23  | 0.58     | 1.99        | 7      | 1     |
| 1:A:28:LEU:HD22  | 1:A:50:LEU:CD2   | 0.58     | 2.29        | 11     | 1     |
| 1:A:104:TYR:CZ   | 1:A:135:LEU:HB3  | 0.58     | 2.34        | 10     | 1     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:HD13 | 0.58     | 1.76        | 4      | 5     |
| 1:A:169:THR:C    | 1:A:196:TYR:CD1  | 0.58     | 2.77        | 3      | 2     |
| 1:A:103:PHE:CD2  | 1:A:134:GLY:CA   | 0.58     | 2.87        | 6      | 4     |
| 1:A:139:LEU:CD1  | 1:A:146:LEU:HD23 | 0.58     | 2.28        | 19     | 1     |
| 1:A:155:GLN:HB3  | 1:A:196:TYR:CE1  | 0.57     | 2.33        | 16     | 2     |
| 1:A:88:ASP:OD1   | 1:A:90:PHE:CD1   | 0.57     | 2.57        | 18     | 2     |
| 1:A:46:VAL:HG11  | 1:A:97:ILE:HG12  | 0.57     | 1.75        | 13     | 1     |
| 1:A:66:PRO:HG2   | 1:A:77:TYR:CE2   | 0.57     | 2.34        | 13     | 3     |
| 1:A:55:VAL:CG1   | 1:A:59:PHE:CZ    | 0.57     | 2.85        | 12     | 1     |
| 1:A:26:VAL:HG21  | 1:A:35:MET:CE    | 0.57     | 2.30        | 14     | 1     |
| 1:A:125:GLU:HG3  | 1:A:166:TRP:CD2  | 0.57     | 2.33        | 19     | 2     |
| 1:A:103:PHE:CD1  | 1:A:134:GLY:CA   | 0.57     | 2.87        | 7      | 2     |
| 1:A:197:VAL:O    | 1:A:197:VAL:HG13 | 0.57     | 1.98        | 9      | 2     |
| 1:A:26:VAL:CG2   | 1:A:29:CYS:SG    | 0.57     | 2.92        | 11     | 2     |
| 1:A:28:LEU:HD12  | 1:A:50:LEU:HG    | 0.57     | 1.76        | 8      | 2     |
| 1:A:124:LEU:HD12 | 1:A:166:TRP:CZ3  | 0.57     | 2.34        | 15     | 2     |
| 1:A:162:MET:SD   | 1:A:166:TRP:CD2  | 0.57     | 2.97        | 12     | 1     |
| 1:A:9:LEU:O      | 1:A:13:TRP:CB    | 0.57     | 2.53        | 15     | 8     |
| 1:A:142:ASP:O    | 1:A:143:GLN:CB   | 0.57     | 2.52        | 7      | 5     |
| 1:A:125:GLU:CD   | 1:A:166:TRP:CE2  | 0.57     | 2.78        | 19     | 1     |
| 1:A:128:MET:SD   | 1:A:129:PRO:CD   | 0.57     | 2.92        | 16     | 19    |
| 1:A:155:GLN:HG2  | 1:A:196:TYR:CE1  | 0.57     | 2.34        | 16     | 2     |
| 1:A:74:PHE:CE1   | 1:A:88:ASP:CG    | 0.57     | 2.78        | 5      | 6     |
| 1:A:109:MET:CE   | 1:A:117:ARG:NH2  | 0.57     | 2.67        | 12     | 1     |
| 1:A:74:PHE:CG    | 1:A:88:ASP:HB3   | 0.57     | 2.34        | 19     | 10    |
| 1:A:13:TRP:CD1   | 1:A:37:TRP:CZ3   | 0.57     | 2.92        | 10     | 4     |
| 1:A:107:ALA:CB   | 1:A:139:LEU:CD1  | 0.57     | 2.82        | 13     | 5     |
| 1:A:145:LEU:C    | 1:A:145:LEU:CD2  | 0.57     | 2.73        | 6      | 10    |
| 1:A:26:VAL:HA    | 1:A:104:TYR:O    | 0.57     | 2.00        | 10     | 3     |
| 1:A:188:LEU:HD22 | 1:A:191:MET:SD   | 0.57     | 2.40        | 14     | 1     |
| 1:A:171:VAL:HG22 | 1:A:195:VAL:CG1  | 0.57     | 2.29        | 20     | 4     |
| 1:A:55:VAL:HG11  | 1:A:75:LYS:CD    | 0.57     | 2.30        | 12     | 2     |
| 1:A:106:ARG:O    | 1:A:106:ARG:NH1  | 0.57     | 2.37        | 11     | 1     |
| 1:A:197:VAL:CG1  | 1:A:197:VAL:O    | 0.57     | 2.52        | 17     | 3     |
| 1:A:109:MET:CE   | 1:A:136:LEU:HD11 | 0.57     | 2.29        | 16     | 6     |
| 1:A:145:LEU:N    | 1:A:145:LEU:CD1  | 0.57     | 2.63        | 20     | 1     |
| 1:A:135:LEU:HD12 | 1:A:196:TYR:O    | 0.56     | 2.00        | 13     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:162:MET:CE   | 1:A:166:TRP:CZ2  | 0.56     | 2.88        | 7      | 1     |
| 1:A:27:PRO:O     | 1:A:29:CYS:N     | 0.56     | 2.39        | 14     | 14    |
| 1:A:107:ALA:C    | 1:A:110:ILE:CD1  | 0.56     | 2.72        | 6      | 12    |
| 1:A:159:HIS:O    | 1:A:163:SER:HB2  | 0.56     | 2.00        | 18     | 18    |
| 1:A:76:VAL:O     | 1:A:76:VAL:CG2   | 0.56     | 2.53        | 16     | 1     |
| 1:A:119:ARG:O    | 1:A:123:HIS:CD2  | 0.56     | 2.59        | 20     | 2     |
| 1:A:162:MET:HE2  | 1:A:166:TRP:CZ3  | 0.56     | 2.36        | 14     | 3     |
| 1:A:171:VAL:HG12 | 1:A:196:TYR:CA   | 0.56     | 2.27        | 14     | 1     |
| 1:A:125:GLU:CD   | 1:A:166:TRP:CD2  | 0.56     | 2.78        | 19     | 1     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:H    | 0.56     | 1.61        | 9      | 1     |
| 1:A:97:ILE:C     | 1:A:99:HIS:CE1   | 0.56     | 2.79        | 7      | 1     |
| 1:A:184:LEU:N    | 1:A:184:LEU:HD22 | 0.56     | 2.15        | 9      | 5     |
| 1:A:188:LEU:HB3  | 1:A:191:MET:HG3  | 0.56     | 1.77        | 15     | 1     |
| 1:A:104:TYR:CE1  | 1:A:135:LEU:HB3  | 0.56     | 2.35        | 10     | 1     |
| 1:A:157:TRP:O    | 1:A:160:ARG:HG2  | 0.56     | 2.00        | 4      | 17    |
| 1:A:119:ARG:O    | 1:A:123:HIS:CG   | 0.56     | 2.59        | 20     | 5     |
| 1:A:50:LEU:N     | 1:A:50:LEU:HD23  | 0.56     | 2.16        | 16     | 1     |
| 1:A:28:LEU:HD22  | 1:A:50:LEU:HG    | 0.56     | 1.77        | 9      | 1     |
| 1:A:151:PHE:O    | 1:A:152:SER:C    | 0.56     | 2.43        | 18     | 14    |
| 1:A:51:SER:HG    | 1:A:54:ALA:HB3   | 0.56     | 1.58        | 3      | 1     |
| 1:A:162:MET:HG2  | 1:A:166:TRP:CZ2  | 0.56     | 2.36        | 13     | 7     |
| 1:A:164:GLY:O    | 1:A:165:ASN:CG   | 0.56     | 2.44        | 19     | 13    |
| 1:A:136:LEU:CD2  | 1:A:138:THR:CG2  | 0.56     | 2.83        | 8      | 2     |
| 1:A:177:LEU:HD23 | 1:A:191:MET:CE   | 0.56     | 2.30        | 18     | 1     |
| 1:A:27:PRO:CG    | 1:A:104:TYR:O    | 0.56     | 2.53        | 20     | 1     |
| 1:A:192:ASP:OD1  | 1:A:193:GLU:N    | 0.56     | 2.39        | 14     | 3     |
| 1:A:139:LEU:CB   | 1:A:142:ASP:OD2  | 0.56     | 2.54        | 2      | 5     |
| 1:A:121:VAL:HG12 | 1:A:122:GLN:N    | 0.56     | 2.16        | 17     | 1     |
| 1:A:129:PRO:O    | 1:A:200:ARG:NE   | 0.56     | 2.38        | 9      | 6     |
| 1:A:110:ILE:HG21 | 1:A:138:THR:HB   | 0.56     | 1.78        | 18     | 4     |
| 1:A:105:ASP:OD2  | 1:A:136:LEU:HD12 | 0.56     | 2.01        | 6      | 1     |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:HE1  | 0.56     | 1.61        | 6      | 1     |
| 1:A:109:MET:HA   | 1:A:117:ARG:HD3  | 0.56     | 1.78        | 9      | 1     |
| 1:A:117:ARG:HH21 | 1:A:121:VAL:HG12 | 0.56     | 1.61        | 12     | 1     |
| 1:A:162:MET:CE   | 1:A:198:LEU:CD1  | 0.56     | 2.84        | 14     | 3     |
| 1:A:146:LEU:C    | 1:A:146:LEU:HD12 | 0.56     | 2.21        | 15     | 1     |
| 1:A:124:LEU:O    | 1:A:128:MET:N    | 0.55     | 2.39        | 9      | 15    |
| 1:A:128:MET:SD   | 1:A:129:PRO:HD2  | 0.55     | 2.41        | 5      | 18    |
| 1:A:144:ALA:O    | 1:A:145:LEU:HB3  | 0.55     | 2.01        | 15     | 16    |
| 1:A:12:TYR:CE2   | 1:A:171:VAL:CG2  | 0.55     | 2.89        | 4      | 3     |
| 1:A:160:ARG:CG   | 1:A:161:VAL:HG12 | 0.55     | 2.31        | 13     | 17    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:122:GLN:CG   | 1:A:123:HIS:N    | 0.55     | 2.69        | 6      | 20    |
| 1:A:89:PHE:HZ    | 1:A:127:LEU:HD21 | 0.55     | 1.59        | 8      | 1     |
| 1:A:109:MET:O    | 1:A:117:ARG:CD   | 0.55     | 2.54        | 15     | 5     |
| 1:A:92:LEU:HD22  | 1:A:93:THR:H     | 0.55     | 1.60        | 4      | 1     |
| 1:A:103:PHE:N    | 1:A:103:PHE:CD1  | 0.55     | 2.74        | 12     | 3     |
| 1:A:142:ASP:N    | 1:A:142:ASP:OD1  | 0.55     | 2.38        | 18     | 6     |
| 1:A:158:LEU:CD2  | 1:A:162:MET:CE   | 0.55     | 2.84        | 10     | 1     |
| 1:A:77:TYR:CG    | 1:A:77:TYR:O     | 0.55     | 2.59        | 6      | 9     |
| 1:A:50:LEU:HA    | 1:A:87:GLY:O     | 0.55     | 2.02        | 16     | 6     |
| 1:A:188:LEU:O    | 1:A:190:ARG:N    | 0.55     | 2.40        | 7      | 4     |
| 1:A:119:ARG:C    | 1:A:119:ARG:CD   | 0.55     | 2.75        | 12     | 1     |
| 1:A:12:TYR:CD2   | 1:A:197:VAL:HG21 | 0.55     | 2.37        | 1      | 2     |
| 1:A:139:LEU:HD23 | 1:A:142:ASP:OD1  | 0.55     | 2.00        | 3      | 1     |
| 1:A:95:ARG:CD    | 1:A:128:MET:O    | 0.55     | 2.55        | 5      | 5     |
| 1:A:124:LEU:HD22 | 1:A:128:MET:CG   | 0.55     | 2.32        | 19     | 1     |
| 1:A:74:PHE:CG    | 1:A:88:ASP:HB2   | 0.55     | 2.37        | 20     | 6     |
| 1:A:32:SER:O     | 1:A:36:SER:CB    | 0.55     | 2.55        | 6      | 4     |
| 1:A:4:GLU:CG     | 1:A:4:GLU:O      | 0.55     | 2.55        | 11     | 6     |
| 1:A:73:ASP:O     | 1:A:74:PHE:CD1   | 0.55     | 2.59        | 5      | 3     |
| 1:A:158:LEU:CD1  | 1:A:196:TYR:CE2  | 0.55     | 2.89        | 2      | 1     |
| 1:A:71:GLN:O     | 1:A:71:GLN:CG    | 0.55     | 2.54        | 12     | 2     |
| 1:A:64:GLU:O     | 1:A:65:GLN:CB    | 0.55     | 2.54        | 14     | 17    |
| 1:A:109:MET:SD   | 1:A:136:LEU:CD1  | 0.55     | 2.95        | 16     | 3     |
| 1:A:134:GLY:O    | 1:A:198:LEU:HD12 | 0.55     | 2.01        | 9      | 3     |
| 1:A:34:ASP:CG    | 1:A:104:TYR:CD2  | 0.55     | 2.80        | 14     | 4     |
| 1:A:124:LEU:O    | 1:A:128:MET:HG2  | 0.55     | 2.01        | 15     | 10    |
| 1:A:103:PHE:CE1  | 1:A:105:ASP:HB2  | 0.55     | 2.36        | 9      | 5     |
| 1:A:49:GLU:OE2   | 1:A:84:ILE:HD12  | 0.55     | 2.02        | 19     | 1     |
| 1:A:124:LEU:HD12 | 1:A:166:TRP:HZ3  | 0.55     | 1.61        | 13     | 2     |
| 1:A:158:LEU:HD23 | 1:A:162:MET:HE3  | 0.55     | 1.79        | 10     | 1     |
| 1:A:77:TYR:O     | 1:A:77:TYR:CG    | 0.55     | 2.59        | 14     | 5     |
| 1:A:34:ASP:HB3   | 1:A:104:TYR:CE2  | 0.55     | 2.37        | 9      | 3     |
| 1:A:169:THR:O    | 1:A:196:TYR:HA   | 0.54     | 2.01        | 19     | 11    |
| 1:A:141:TYR:O    | 1:A:142:ASP:O    | 0.54     | 2.25        | 18     | 17    |
| 1:A:109:MET:HG3  | 1:A:153:VAL:HG21 | 0.54     | 1.78        | 16     | 1     |
| 1:A:135:LEU:HD21 | 1:A:195:VAL:CG1  | 0.54     | 2.32        | 10     | 2     |
| 1:A:48:ALA:HB2   | 1:A:85:TRP:NE1   | 0.54     | 2.16        | 8      | 2     |
| 1:A:26:VAL:HG23  | 1:A:26:VAL:O     | 0.54     | 2.02        | 18     | 5     |
| 1:A:132:CYS:HB2  | 1:A:200:ARG:CZ   | 0.54     | 2.32        | 6      | 1     |
| 1:A:124:LEU:CD1  | 1:A:128:MET:SD   | 0.54     | 2.95        | 4      | 1     |
| 1:A:136:LEU:CD1  | 1:A:138:THR:HG23 | 0.54     | 2.31        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:ASN:OD1    | 1:A:137:ILE:HG21 | 0.54     | 2.03        | 15     | 1     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:HB   | 0.54     | 1.80        | 15     | 1     |
| 1:A:29:CYS:O     | 1:A:30:GLY:C     | 0.54     | 2.45        | 20     | 7     |
| 1:A:34:ASP:CG    | 1:A:104:TYR:CZ   | 0.54     | 2.80        | 4      | 1     |
| 1:A:28:LEU:CD2   | 1:A:50:LEU:HD23  | 0.54     | 2.31        | 11     | 1     |
| 1:A:157:TRP:O    | 1:A:161:VAL:HG12 | 0.54     | 2.02        | 10     | 7     |
| 1:A:188:LEU:O    | 1:A:189:GLU:CG   | 0.54     | 2.55        | 1      | 8     |
| 1:A:34:ASP:HB2   | 1:A:104:TYR:CE2  | 0.54     | 2.37        | 8      | 2     |
| 1:A:103:PHE:N    | 1:A:200:ARG:HH22 | 0.54     | 2.00        | 6      | 1     |
| 1:A:125:GLU:OE2  | 1:A:166:TRP:CD1  | 0.54     | 2.59        | 19     | 1     |
| 1:A:92:LEU:CD2   | 1:A:97:ILE:CD1   | 0.54     | 2.85        | 20     | 1     |
| 1:A:74:PHE:CB    | 1:A:88:ASP:HB3   | 0.54     | 2.32        | 6      | 5     |
| 1:A:51:SER:OG    | 1:A:54:ALA:CB    | 0.54     | 2.56        | 11     | 3     |
| 1:A:161:VAL:C    | 1:A:163:SER:N    | 0.54     | 2.61        | 20     | 17    |
| 1:A:26:VAL:O     | 1:A:26:VAL:HG23  | 0.54     | 2.02        | 12     | 3     |
| 1:A:95:ARG:CB    | 1:A:127:LEU:O    | 0.54     | 2.56        | 3      | 1     |
| 1:A:50:LEU:HD23  | 1:A:50:LEU:N     | 0.54     | 2.17        | 8      | 1     |
| 1:A:146:LEU:HA   | 1:A:186:ALA:HB1  | 0.54     | 1.80        | 4      | 5     |
| 1:A:13:TRP:HH2   | 1:A:102:ALA:HB3  | 0.54     | 1.55        | 10     | 2     |
| 1:A:103:PHE:C    | 1:A:103:PHE:CD1  | 0.54     | 2.81        | 9      | 2     |
| 1:A:145:LEU:CG   | 1:A:188:LEU:HD13 | 0.54     | 2.33        | 4      | 10    |
| 1:A:25:LEU:HD22  | 1:A:26:VAL:N     | 0.54     | 2.16        | 7      | 3     |
| 1:A:29:CYS:O     | 1:A:31:LYS:N     | 0.54     | 2.41        | 20     | 4     |
| 1:A:103:PHE:CD2  | 1:A:134:GLY:HA3  | 0.54     | 2.38        | 6      | 4     |
| 1:A:177:LEU:CD2  | 1:A:191:MET:SD   | 0.54     | 2.96        | 14     | 1     |
| 1:A:157:TRP:HE3  | 1:A:158:LEU:HD12 | 0.54     | 1.62        | 13     | 2     |
| 1:A:140:GLU:OE2  | 1:A:194:HIS:CD2  | 0.54     | 2.61        | 7      | 1     |
| 1:A:103:PHE:CE1  | 1:A:134:GLY:N    | 0.54     | 2.76        | 12     | 2     |
| 1:A:8:ASP:O      | 1:A:12:TYR:N     | 0.54     | 2.38        | 3      | 11    |
| 1:A:145:LEU:CD1  | 1:A:188:LEU:CD1  | 0.54     | 2.82        | 13     | 10    |
| 1:A:117:ARG:NH2  | 1:A:120:TYR:CD1  | 0.54     | 2.75        | 5      | 2     |
| 1:A:26:VAL:O     | 1:A:47:GLY:CA    | 0.54     | 2.55        | 5      | 1     |
| 1:A:107:ALA:HB1  | 1:A:110:ILE:HG12 | 0.54     | 1.78        | 9      | 1     |
| 1:A:13:TRP:CE3   | 1:A:104:TYR:CE1  | 0.54     | 2.95        | 10     | 1     |
| 1:A:114:ALA:O    | 1:A:117:ARG:N    | 0.54     | 2.41        | 16     | 6     |
| 1:A:109:MET:HE1  | 1:A:136:LEU:HD21 | 0.54     | 1.79        | 3      | 1     |
| 1:A:101:ALA:O    | 1:A:132:CYS:HA   | 0.54     | 2.02        | 15     | 11    |
| 1:A:69:THR:HG22  | 1:A:76:VAL:HB    | 0.54     | 1.77        | 10     | 4     |
| 1:A:104:TYR:CE2  | 1:A:137:ILE:CD1  | 0.54     | 2.90        | 18     | 1     |
| 1:A:125:GLU:OE1  | 1:A:166:TRP:NE1  | 0.54     | 2.41        | 19     | 1     |
| 1:A:139:LEU:CD1  | 1:A:146:LEU:CD2  | 0.54     | 2.85        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:168:VAL:HB   | 1:A:196:TYR:CE2  | 0.54     | 2.38        | 4      | 1     |
| 1:A:74:PHE:CD2   | 1:A:88:ASP:HB3   | 0.54     | 2.37        | 12     | 1     |
| 1:A:85:TRP:CD1   | 1:A:85:TRP:N     | 0.54     | 2.75        | 20     | 8     |
| 1:A:157:TRP:CE3  | 1:A:158:LEU:HD12 | 0.54     | 2.38        | 6      | 3     |
| 1:A:66:PRO:HG3   | 1:A:77:TYR:CE1   | 0.54     | 2.37        | 19     | 6     |
| 1:A:104:TYR:CE1  | 1:A:137:ILE:HD13 | 0.54     | 2.38        | 5      | 2     |
| 1:A:13:TRP:CH2   | 1:A:24:VAL:HG13  | 0.54     | 2.38        | 18     | 4     |
| 1:A:25:LEU:C     | 1:A:25:LEU:CD1   | 0.54     | 2.74        | 12     | 3     |
| 1:A:196:TYR:CE1  | 1:A:198:LEU:CG   | 0.54     | 2.89        | 20     | 1     |
| 1:A:139:LEU:HD23 | 1:A:191:MET:SD   | 0.54     | 2.43        | 13     | 2     |
| 1:A:99:HIS:N     | 1:A:129:PRO:HG3  | 0.54     | 2.18        | 15     | 1     |
| 1:A:85:TRP:N     | 1:A:85:TRP:CD1   | 0.54     | 2.74        | 13     | 11    |
| 1:A:171:VAL:HG12 | 1:A:172:GLY:N    | 0.54     | 2.18        | 6      | 1     |
| 1:A:125:GLU:OE2  | 1:A:165:ASN:CB   | 0.54     | 2.55        | 19     | 1     |
| 1:A:12:TYR:CE2   | 1:A:197:VAL:HG21 | 0.53     | 2.38        | 1      | 2     |
| 1:A:158:LEU:CD2  | 1:A:162:MET:SD   | 0.53     | 2.96        | 3      | 8     |
| 1:A:5:VAL:O      | 1:A:6:ASN:C      | 0.53     | 2.45        | 17     | 20    |
| 1:A:26:VAL:HB    | 1:A:29:CYS:CB    | 0.53     | 2.33        | 18     | 1     |
| 1:A:109:MET:HB2  | 1:A:117:ARG:NH2  | 0.53     | 2.17        | 19     | 2     |
| 1:A:109:MET:HA   | 1:A:117:ARG:CD   | 0.53     | 2.32        | 9      | 1     |
| 1:A:162:MET:HE3  | 1:A:166:TRP:CH2  | 0.53     | 2.38        | 7      | 1     |
| 1:A:71:GLN:CA    | 1:A:71:GLN:OE1   | 0.53     | 2.55        | 15     | 2     |
| 1:A:5:VAL:HG22   | 1:A:5:VAL:O      | 0.53     | 2.03        | 16     | 10    |
| 1:A:161:VAL:O    | 1:A:163:SER:N    | 0.53     | 2.42        | 20     | 18    |
| 1:A:95:ARG:CG    | 1:A:128:MET:O    | 0.53     | 2.57        | 5      | 4     |
| 1:A:158:LEU:HD23 | 1:A:162:MET:SD   | 0.53     | 2.43        | 4      | 2     |
| 1:A:135:LEU:CD2  | 1:A:195:VAL:CG1  | 0.53     | 2.87        | 6      | 3     |
| 1:A:71:GLN:NE2   | 1:A:91:ALA:HB2   | 0.53     | 2.18        | 4      | 2     |
| 1:A:121:VAL:HG21 | 1:A:161:VAL:CG2  | 0.53     | 2.34        | 10     | 1     |
| 1:A:146:LEU:HD23 | 1:A:147:GLU:H    | 0.53     | 1.64        | 6      | 6     |
| 1:A:25:LEU:HD23  | 1:A:103:PHE:HB2  | 0.53     | 1.80        | 17     | 2     |
| 1:A:103:PHE:CZ   | 1:A:105:ASP:HB2  | 0.53     | 2.38        | 9      | 2     |
| 1:A:13:TRP:HH2   | 1:A:24:VAL:HG13  | 0.53     | 1.63        | 18     | 2     |
| 1:A:162:MET:HE1  | 1:A:166:TRP:CZ3  | 0.53     | 2.38        | 19     | 3     |
| 1:A:9:LEU:HD22   | 1:A:13:TRP:CD1   | 0.53     | 2.39        | 1      | 1     |
| 1:A:121:VAL:HG21 | 1:A:161:VAL:HG22 | 0.53     | 1.80        | 3      | 4     |
| 1:A:121:VAL:O    | 1:A:166:TRP:CZ2  | 0.53     | 2.61        | 8      | 7     |
| 1:A:139:LEU:CD2  | 1:A:142:ASP:OD2  | 0.53     | 2.56        | 8      | 2     |
| 1:A:9:LEU:CD2    | 1:A:104:TYR:CE1  | 0.53     | 2.89        | 6      | 2     |
| 1:A:50:LEU:HD21  | 1:A:89:PHE:H     | 0.53     | 1.63        | 7      | 2     |
| 1:A:25:LEU:HD22  | 1:A:94:ALA:HB1   | 0.53     | 1.80        | 10     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:117:ARG:CB   | 1:A:157:TRP:CZ2  | 0.53     | 2.92        | 16     | 1     |
| 1:A:103:PHE:CE1  | 1:A:105:ASP:CB   | 0.53     | 2.91        | 9      | 1     |
| 1:A:110:ILE:C    | 1:A:110:ILE:HD12 | 0.53     | 2.23        | 9      | 1     |
| 1:A:46:VAL:CG2   | 1:A:97:ILE:HD13  | 0.53     | 2.33        | 9      | 2     |
| 1:A:125:GLU:HG2  | 1:A:166:TRP:CE3  | 0.53     | 2.38        | 12     | 1     |
| 1:A:200:ARG:HH11 | 1:A:201:VAL:N    | 0.53     | 2.02        | 10     | 2     |
| 1:A:103:PHE:CD1  | 1:A:103:PHE:C    | 0.53     | 2.82        | 20     | 2     |
| 1:A:64:GLU:O     | 1:A:65:GLN:CG    | 0.53     | 2.57        | 14     | 9     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:HD12  | 0.53     | 1.79        | 5      | 1     |
| 1:A:104:TYR:CE1  | 1:A:137:ILE:HG13 | 0.53     | 2.39        | 15     | 3     |
| 1:A:28:LEU:HD13  | 1:A:28:LEU:H     | 0.53     | 1.58        | 8      | 2     |
| 1:A:51:SER:O     | 1:A:55:VAL:HG23  | 0.53     | 2.04        | 12     | 2     |
| 1:A:121:VAL:O    | 1:A:125:GLU:CG   | 0.53     | 2.57        | 16     | 7     |
| 1:A:57:ARG:CD    | 1:A:57:ARG:C     | 0.53     | 2.77        | 19     | 2     |
| 1:A:136:LEU:HB2  | 1:A:198:LEU:HD21 | 0.53     | 1.80        | 3      | 2     |
| 1:A:125:GLU:CB   | 1:A:200:ARG:NH2  | 0.53     | 2.72        | 5      | 1     |
| 1:A:123:HIS:O    | 1:A:126:ALA:HB3  | 0.53     | 2.04        | 15     | 4     |
| 1:A:46:VAL:HG13  | 1:A:97:ILE:HD11  | 0.53     | 1.79        | 4      | 1     |
| 1:A:8:ASP:OD1    | 1:A:171:VAL:HG22 | 0.53     | 2.03        | 12     | 1     |
| 1:A:26:VAL:CG2   | 1:A:47:GLY:HA3   | 0.53     | 2.34        | 8      | 9     |
| 1:A:168:VAL:HG22 | 1:A:198:LEU:HD22 | 0.53     | 1.79        | 14     | 2     |
| 1:A:5:VAL:O      | 1:A:5:VAL:HG22   | 0.53     | 2.04        | 6      | 6     |
| 1:A:135:LEU:CD1  | 1:A:197:VAL:CG2  | 0.53     | 2.87        | 13     | 1     |
| 1:A:113:PRO:HD2  | 1:A:116:MET:CB   | 0.53     | 2.34        | 16     | 11    |
| 1:A:95:ARG:CB    | 1:A:128:MET:O    | 0.53     | 2.57        | 19     | 4     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:CG2   | 0.53     | 2.34        | 19     | 2     |
| 1:A:71:GLN:CG    | 1:A:71:GLN:O     | 0.53     | 2.56        | 4      | 1     |
| 1:A:74:PHE:CB    | 1:A:88:ASP:CG    | 0.53     | 2.78        | 13     | 1     |
| 1:A:69:THR:CG2   | 1:A:71:GLN:OE1   | 0.53     | 2.57        | 15     | 1     |
| 1:A:177:LEU:CD2  | 1:A:188:LEU:HB2  | 0.52     | 2.34        | 20     | 4     |
| 1:A:128:MET:HB3  | 1:A:129:PRO:CD   | 0.52     | 2.32        | 16     | 16    |
| 1:A:18:VAL:CG1   | 1:A:22:ALA:CB    | 0.52     | 2.86        | 9      | 3     |
| 1:A:145:LEU:HD11 | 1:A:188:LEU:HD23 | 0.52     | 1.81        | 7      | 3     |
| 1:A:139:LEU:N    | 1:A:139:LEU:CD2  | 0.52     | 2.71        | 2      | 1     |
| 1:A:105:ASP:OD1  | 1:A:106:ARG:CZ   | 0.52     | 2.57        | 11     | 1     |
| 1:A:74:PHE:CG    | 1:A:88:ASP:CG    | 0.52     | 2.83        | 10     | 6     |
| 1:A:55:VAL:HG21  | 1:A:87:GLY:CA    | 0.52     | 2.34        | 6      | 5     |
| 1:A:22:ALA:CB    | 1:A:101:ALA:HB2  | 0.52     | 2.33        | 18     | 6     |
| 1:A:103:PHE:CZ   | 1:A:105:ASP:CB   | 0.52     | 2.92        | 9      | 1     |
| 1:A:177:LEU:HD21 | 1:A:189:GLU:N    | 0.52     | 2.19        | 20     | 1     |
| 1:A:109:MET:HE3  | 1:A:120:TYR:CE1  | 0.52     | 2.40        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:122:GLN:HG3  | 1:A:123:HIS:N    | 0.52     | 2.18        | 19     | 18    |
| 1:A:174:GLN:O    | 1:A:175:ASP:CB   | 0.52     | 2.56        | 18     | 3     |
| 1:A:50:LEU:HD21  | 1:A:89:PHE:N     | 0.52     | 2.19        | 7      | 2     |
| 1:A:124:LEU:CD2  | 1:A:128:MET:SD   | 0.52     | 2.97        | 4      | 1     |
| 1:A:74:PHE:CB    | 1:A:88:ASP:CB    | 0.52     | 2.88        | 1      | 3     |
| 1:A:102:ALA:N    | 1:A:132:CYS:HB2  | 0.52     | 2.19        | 16     | 8     |
| 1:A:196:TYR:O    | 1:A:198:LEU:CD2  | 0.52     | 2.57        | 3      | 2     |
| 1:A:165:ASN:CA   | 1:A:201:VAL:HG22 | 0.52     | 2.34        | 13     | 2     |
| 1:A:125:GLU:HB2  | 1:A:166:TRP:CZ2  | 0.52     | 2.40        | 8      | 1     |
| 1:A:128:MET:SD   | 1:A:200:ARG:NE   | 0.52     | 2.82        | 15     | 1     |
| 1:A:9:LEU:CD1    | 1:A:10:GLN:N     | 0.52     | 2.72        | 10     | 1     |
| 1:A:118:GLU:HG2  | 1:A:157:TRP:CZ2  | 0.52     | 2.40        | 17     | 13    |
| 1:A:25:LEU:O     | 1:A:103:PHE:HA   | 0.52     | 2.03        | 16     | 8     |
| 1:A:117:ARG:HA   | 1:A:117:ARG:NH1  | 0.52     | 2.19        | 16     | 1     |
| 1:A:59:PHE:CZ    | 1:A:77:TYR:HB2   | 0.52     | 2.39        | 6      | 11    |
| 1:A:145:LEU:HD13 | 1:A:146:LEU:H    | 0.52     | 1.64        | 18     | 4     |
| 1:A:109:MET:CE   | 1:A:120:TYR:CD1  | 0.52     | 2.92        | 19     | 1     |
| 1:A:145:LEU:CD2  | 1:A:186:ALA:CB   | 0.52     | 2.87        | 5      | 3     |
| 1:A:173:GLY:O    | 1:A:176:THR:HG22 | 0.52     | 2.04        | 8      | 3     |
| 1:A:155:GLN:HB2  | 1:A:196:TYR:CE1  | 0.52     | 2.40        | 9      | 7     |
| 1:A:135:LEU:HD11 | 1:A:195:VAL:CG1  | 0.52     | 2.35        | 19     | 3     |
| 1:A:49:GLU:CD    | 1:A:84:ILE:CD1   | 0.52     | 2.78        | 19     | 1     |
| 1:A:158:LEU:HD23 | 1:A:162:MET:HG3  | 0.52     | 1.81        | 4      | 2     |
| 1:A:190:ARG:O    | 1:A:190:ARG:CG   | 0.52     | 2.56        | 20     | 1     |
| 1:A:157:TRP:CH2  | 1:A:161:VAL:HG11 | 0.52     | 2.40        | 12     | 1     |
| 1:A:74:PHE:CD1   | 1:A:88:ASP:CB    | 0.52     | 2.93        | 16     | 6     |
| 1:A:155:GLN:CB   | 1:A:196:TYR:CE1  | 0.52     | 2.93        | 4      | 2     |
| 1:A:175:ASP:HA   | 1:A:191:MET:O    | 0.52     | 2.03        | 4      | 2     |
| 1:A:158:LEU:HD22 | 1:A:162:MET:SD   | 0.52     | 2.44        | 2      | 2     |
| 1:A:177:LEU:CD1  | 1:A:177:LEU:C    | 0.52     | 2.77        | 1      | 2     |
| 1:A:141:TYR:CD2  | 1:A:191:MET:HA   | 0.52     | 2.40        | 5      | 5     |
| 1:A:171:VAL:CG1  | 1:A:197:VAL:HG23 | 0.52     | 2.30        | 18     | 1     |
| 1:A:118:GLU:O    | 1:A:121:VAL:HG22 | 0.52     | 2.04        | 10     | 2     |
| 1:A:18:VAL:O     | 1:A:19:VAL:C     | 0.52     | 2.48        | 15     | 16    |
| 1:A:184:LEU:H    | 1:A:184:LEU:HD22 | 0.52     | 1.63        | 16     | 4     |
| 1:A:103:PHE:CZ   | 1:A:134:GLY:CA   | 0.52     | 2.93        | 3      | 5     |
| 1:A:26:VAL:HG22  | 1:A:47:GLY:HA3   | 0.52     | 1.81        | 12     | 4     |
| 1:A:178:HIS:CG   | 1:A:184:LEU:HD21 | 0.52     | 2.40        | 15     | 1     |
| 1:A:107:ALA:HB1  | 1:A:110:ILE:HD12 | 0.52     | 1.83        | 1      | 4     |
| 1:A:197:VAL:C    | 1:A:198:LEU:CD2  | 0.52     | 2.77        | 18     | 1     |
| 1:A:142:ASP:OD2  | 1:A:150:PRO:CG   | 0.52     | 2.58        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:146:LEU:HB2  | 1:A:188:LEU:HD21 | 0.52     | 1.81        | 11     | 2     |
| 1:A:117:ARG:HB2  | 1:A:157:TRP:CZ2  | 0.51     | 2.40        | 16     | 1     |
| 1:A:169:THR:CG2  | 1:A:197:VAL:CG1  | 0.51     | 2.88        | 16     | 7     |
| 1:A:28:LEU:HD12  | 1:A:50:LEU:CD2   | 0.51     | 2.36        | 16     | 3     |
| 1:A:113:PRO:O    | 1:A:117:ARG:HB2  | 0.51     | 2.05        | 5      | 4     |
| 1:A:130:GLN:CG   | 1:A:131:ALA:N    | 0.51     | 2.74        | 5      | 1     |
| 1:A:57:ARG:C     | 1:A:57:ARG:CD    | 0.51     | 2.78        | 8      | 1     |
| 1:A:26:VAL:HG21  | 1:A:35:MET:SD    | 0.51     | 2.45        | 19     | 1     |
| 1:A:162:MET:HE3  | 1:A:166:TRP:CZ2  | 0.51     | 2.40        | 7      | 1     |
| 1:A:106:ARG:CG   | 1:A:107:ALA:N    | 0.51     | 2.73        | 2      | 4     |
| 1:A:46:VAL:HG21  | 1:A:97:ILE:HD11  | 0.51     | 1.78        | 8      | 1     |
| 1:A:28:LEU:HA    | 1:A:48:ALA:O     | 0.51     | 2.05        | 10     | 2     |
| 1:A:137:ILE:CD1  | 1:A:195:VAL:CG2  | 0.51     | 2.87        | 11     | 1     |
| 1:A:12:TYR:CG    | 1:A:197:VAL:HG21 | 0.51     | 2.40        | 12     | 2     |
| 1:A:55:VAL:HG12  | 1:A:86:CYS:SG    | 0.51     | 2.45        | 16     | 2     |
| 1:A:13:TRP:CE2   | 1:A:38:LEU:HD11  | 0.51     | 2.41        | 19     | 4     |
| 1:A:74:PHE:CD1   | 1:A:88:ASP:HB3   | 0.51     | 2.40        | 3      | 1     |
| 1:A:145:LEU:HD22 | 1:A:186:ALA:HB1  | 0.51     | 1.81        | 7      | 3     |
| 1:A:23:ARG:NE    | 1:A:97:ILE:O     | 0.51     | 2.43        | 14     | 1     |
| 1:A:59:PHE:CE1   | 1:A:77:TYR:CB    | 0.51     | 2.92        | 6      | 1     |
| 1:A:28:LEU:HD22  | 1:A:50:LEU:HB2   | 0.51     | 1.82        | 20     | 1     |
| 1:A:55:VAL:CG2   | 1:A:86:CYS:O     | 0.51     | 2.58        | 20     | 1     |
| 1:A:109:MET:CA   | 1:A:117:ARG:HD3  | 0.51     | 2.35        | 13     | 1     |
| 1:A:117:ARG:NH2  | 1:A:121:VAL:HG12 | 0.51     | 2.20        | 12     | 1     |
| 1:A:101:ALA:C    | 1:A:132:CYS:HB2  | 0.51     | 2.26        | 19     | 4     |
| 1:A:97:ILE:CG1   | 1:A:98:GLY:N     | 0.51     | 2.73        | 15     | 6     |
| 1:A:103:PHE:CD1  | 1:A:103:PHE:N    | 0.51     | 2.78        | 3      | 2     |
| 1:A:135:LEU:CD2  | 1:A:196:TYR:O    | 0.51     | 2.59        | 10     | 1     |
| 1:A:97:ILE:CD1   | 1:A:97:ILE:C     | 0.51     | 2.79        | 19     | 3     |
| 1:A:155:GLN:HB3  | 1:A:196:TYR:CZ   | 0.51     | 2.41        | 4      | 2     |
| 1:A:136:LEU:HD12 | 1:A:162:MET:CE   | 0.51     | 2.36        | 3      | 2     |
| 1:A:109:MET:CE   | 1:A:136:LEU:CD1  | 0.51     | 2.89        | 5      | 1     |
| 1:A:155:GLN:HG3  | 1:A:196:TYR:CE1  | 0.51     | 2.40        | 19     | 2     |
| 1:A:184:LEU:HD22 | 1:A:184:LEU:H    | 0.51     | 1.65        | 13     | 5     |
| 1:A:107:ALA:HB1  | 1:A:110:ILE:CG1  | 0.51     | 2.36        | 9      | 1     |
| 1:A:125:GLU:HB3  | 1:A:166:TRP:CZ2  | 0.51     | 2.40        | 4      | 1     |
| 1:A:64:GLU:O     | 1:A:66:PRO:N     | 0.51     | 2.42        | 17     | 1     |
| 1:A:93:THR:C     | 1:A:95:ARG:N     | 0.51     | 2.64        | 4      | 13    |
| 1:A:162:MET:SD   | 1:A:198:LEU:CD1  | 0.51     | 2.99        | 14     | 1     |
| 1:A:103:PHE:CE1  | 1:A:124:LEU:HD11 | 0.51     | 2.41        | 19     | 1     |
| 1:A:92:LEU:HD21  | 1:A:97:ILE:HG21  | 0.51     | 1.82        | 19     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:55:VAL:CG2   | 1:A:86:CYS:C     | 0.51     | 2.78        | 20     | 1     |
| 1:A:12:TYR:CE1   | 1:A:171:VAL:HG21 | 0.51     | 2.40        | 1      | 1     |
| 1:A:109:MET:HA   | 1:A:117:ARG:CZ   | 0.51     | 2.36        | 16     | 1     |
| 1:A:100:CYS:CA   | 1:A:132:CYS:SG   | 0.51     | 2.98        | 6      | 2     |
| 1:A:12:TYR:CZ    | 1:A:171:VAL:HG13 | 0.51     | 2.40        | 6      | 1     |
| 1:A:100:CYS:CA   | 1:A:131:ALA:O    | 0.51     | 2.58        | 19     | 1     |
| 1:A:46:VAL:HG13  | 1:A:83:GLU:CG    | 0.51     | 2.36        | 9      | 1     |
| 1:A:26:VAL:CG1   | 1:A:30:GLY:N     | 0.51     | 2.73        | 20     | 1     |
| 1:A:109:MET:HB2  | 1:A:117:ARG:CG   | 0.51     | 2.36        | 5      | 1     |
| 1:A:44:HIS:O     | 1:A:46:VAL:HG12  | 0.51     | 2.05        | 8      | 2     |
| 1:A:34:ASP:CB    | 1:A:104:TYR:CE2  | 0.51     | 2.93        | 9      | 3     |
| 1:A:92:LEU:HD21  | 1:A:97:ILE:HG12  | 0.51     | 1.83        | 7      | 1     |
| 1:A:50:LEU:HD22  | 1:A:89:PHE:N     | 0.51     | 2.21        | 20     | 1     |
| 1:A:189:GLU:O    | 1:A:190:ARG:CD   | 0.51     | 2.58        | 20     | 1     |
| 1:A:146:LEU:HD13 | 1:A:186:ALA:CB   | 0.51     | 2.35        | 16     | 2     |
| 1:A:164:GLY:O    | 1:A:165:ASN:HB3  | 0.51     | 2.05        | 3      | 1     |
| 1:A:104:TYR:CZ   | 1:A:137:ILE:HG13 | 0.51     | 2.40        | 14     | 8     |
| 1:A:103:PHE:CD1  | 1:A:134:GLY:HA3  | 0.51     | 2.41        | 7      | 2     |
| 1:A:27:PRO:C     | 1:A:28:LEU:HG    | 0.51     | 2.26        | 7      | 4     |
| 1:A:71:GLN:OE1   | 1:A:71:GLN:CA    | 0.51     | 2.59        | 17     | 2     |
| 1:A:162:MET:HB2  | 1:A:168:VAL:HG11 | 0.51     | 1.83        | 10     | 1     |
| 1:A:146:LEU:HG   | 1:A:186:ALA:HB3  | 0.51     | 1.82        | 9      | 5     |
| 1:A:109:MET:O    | 1:A:117:ARG:CG   | 0.51     | 2.59        | 3      | 4     |
| 1:A:183:GLY:CA   | 1:A:191:MET:CE   | 0.51     | 2.89        | 9      | 1     |
| 1:A:30:GLY:O     | 1:A:31:LYS:CB    | 0.51     | 2.59        | 2      | 1     |
| 1:A:4:GLU:O      | 1:A:4:GLU:CG     | 0.50     | 2.59        | 2      | 5     |
| 1:A:28:LEU:CB    | 1:A:50:LEU:HB2   | 0.50     | 2.35        | 12     | 6     |
| 1:A:16:LEU:HD13  | 1:A:133:SER:CB   | 0.50     | 2.36        | 15     | 2     |
| 1:A:117:ARG:NE   | 1:A:153:VAL:CG2  | 0.50     | 2.75        | 17     | 1     |
| 1:A:141:TYR:CD1  | 1:A:191:MET:SD   | 0.50     | 3.03        | 15     | 1     |
| 1:A:117:ARG:HG2  | 1:A:157:TRP:CZ2  | 0.50     | 2.41        | 12     | 1     |
| 1:A:107:ALA:N    | 1:A:137:ILE:O    | 0.50     | 2.43        | 5      | 4     |
| 1:A:109:MET:CA   | 1:A:117:ARG:CZ   | 0.50     | 2.90        | 16     | 1     |
| 1:A:110:ILE:O    | 1:A:151:PHE:N    | 0.50     | 2.43        | 9      | 7     |
| 1:A:125:GLU:HG2  | 1:A:166:TRP:CZ2  | 0.50     | 2.41        | 11     | 2     |
| 1:A:23:ARG:HG3   | 1:A:99:HIS:CE1   | 0.50     | 2.41        | 7      | 1     |
| 1:A:25:LEU:HG    | 1:A:26:VAL:N     | 0.50     | 2.21        | 16     | 4     |
| 1:A:183:GLY:CA   | 1:A:188:LEU:HD23 | 0.50     | 2.36        | 3      | 2     |
| 1:A:188:LEU:O    | 1:A:189:GLU:C    | 0.50     | 2.48        | 15     | 6     |
| 1:A:25:LEU:HD13  | 1:A:27:PRO:CD    | 0.50     | 2.33        | 7      | 1     |
| 1:A:76:VAL:HG23  | 1:A:85:TRP:HB3   | 0.50     | 1.81        | 2      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:9:LEU:CD1    | 1:A:9:LEU:C      | 0.50     | 2.80        | 4      | 6     |
| 1:A:57:ARG:HG3   | 1:A:58:TYR:N     | 0.50     | 2.21        | 19     | 3     |
| 1:A:74:PHE:CD1   | 1:A:88:ASP:HB2   | 0.50     | 2.41        | 2      | 5     |
| 1:A:176:THR:O    | 1:A:176:THR:CG2  | 0.50     | 2.57        | 14     | 4     |
| 1:A:97:ILE:HD13  | 1:A:98:GLY:H     | 0.50     | 1.57        | 5      | 1     |
| 1:A:41:GLN:HB3   | 1:A:43:TYR:CE1   | 0.50     | 2.42        | 8      | 1     |
| 1:A:52:GLU:HG3   | 1:A:74:PHE:CE1   | 0.50     | 2.41        | 20     | 1     |
| 1:A:65:GLN:N     | 1:A:66:PRO:HD2   | 0.50     | 2.22        | 14     | 15    |
| 1:A:177:LEU:CD2  | 1:A:191:MET:HG3  | 0.50     | 2.36        | 19     | 1     |
| 1:A:155:GLN:CG   | 1:A:196:TYR:CD1  | 0.50     | 2.94        | 4      | 1     |
| 1:A:152:SER:O    | 1:A:152:SER:OG   | 0.50     | 2.28        | 16     | 2     |
| 1:A:139:LEU:HD23 | 1:A:191:MET:HE2  | 0.50     | 1.79        | 5      | 2     |
| 1:A:117:ARG:NH1  | 1:A:157:TRP:CE2  | 0.50     | 2.79        | 14     | 1     |
| 1:A:89:PHE:C     | 1:A:89:PHE:CD1   | 0.50     | 2.84        | 8      | 2     |
| 1:A:175:ASP:CA   | 1:A:191:MET:O    | 0.50     | 2.60        | 13     | 2     |
| 1:A:109:MET:O    | 1:A:117:ARG:HD3  | 0.50     | 2.07        | 13     | 1     |
| 1:A:12:TYR:CE2   | 1:A:197:VAL:CG2  | 0.50     | 2.94        | 12     | 1     |
| 1:A:135:LEU:CD2  | 1:A:195:VAL:HG13 | 0.50     | 2.36        | 7      | 2     |
| 1:A:109:MET:HE1  | 1:A:136:LEU:CD1  | 0.50     | 2.37        | 5      | 1     |
| 1:A:106:ARG:HG3  | 1:A:107:ALA:N    | 0.50     | 2.21        | 12     | 2     |
| 1:A:37:TRP:CH2   | 1:A:41:GLN:HG3   | 0.50     | 2.41        | 8      | 2     |
| 1:A:117:ARG:HD2  | 1:A:121:VAL:CG1  | 0.50     | 2.37        | 18     | 1     |
| 1:A:110:ILE:CD1  | 1:A:110:ILE:C    | 0.50     | 2.80        | 9      | 1     |
| 1:A:168:VAL:HB   | 1:A:196:TYR:CD2  | 0.50     | 2.42        | 4      | 1     |
| 1:A:175:ASP:CB   | 1:A:191:MET:C    | 0.50     | 2.79        | 13     | 2     |
| 1:A:46:VAL:HG22  | 1:A:97:ILE:CD1   | 0.50     | 2.28        | 2      | 1     |
| 1:A:117:ARG:HH11 | 1:A:153:VAL:HG11 | 0.50     | 1.66        | 12     | 1     |
| 1:A:97:ILE:CD1   | 1:A:98:GLY:N     | 0.50     | 2.65        | 5      | 1     |
| 1:A:140:GLU:OE2  | 1:A:194:HIS:CE1  | 0.50     | 2.65        | 14     | 2     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:CG1  | 0.50     | 2.36        | 15     | 5     |
| 1:A:23:ARG:HG3   | 1:A:99:HIS:NE2   | 0.50     | 2.22        | 18     | 2     |
| 1:A:117:ARG:NE   | 1:A:117:ARG:HA   | 0.50     | 2.19        | 9      | 1     |
| 1:A:18:VAL:HG12  | 1:A:19:VAL:N     | 0.50     | 2.22        | 1      | 1     |
| 1:A:124:LEU:HD13 | 1:A:128:MET:HG3  | 0.50     | 1.84        | 20     | 8     |
| 1:A:6:ASN:ND2    | 1:A:8:ASP:OD2    | 0.50     | 2.45        | 12     | 2     |
| 1:A:138:THR:OG1  | 1:A:194:HIS:O    | 0.50     | 2.27        | 18     | 5     |
| 1:A:137:ILE:HD12 | 1:A:137:ILE:N    | 0.50     | 2.22        | 6      | 1     |
| 1:A:177:LEU:HD12 | 1:A:178:HIS:N    | 0.50     | 2.22        | 11     | 2     |
| 1:A:139:LEU:C    | 1:A:139:LEU:HD22 | 0.49     | 2.27        | 3      | 1     |
| 1:A:146:LEU:C    | 1:A:146:LEU:CD1  | 0.49     | 2.80        | 3      | 1     |
| 1:A:6:ASN:O      | 1:A:9:LEU:N      | 0.49     | 2.45        | 20     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:101:ALA:N    | 1:A:132:CYS:SG   | 0.49     | 2.85        | 8      | 6     |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:HD22 | 0.49     | 1.84        | 6      | 1     |
| 1:A:24:VAL:CG2   | 1:A:38:LEU:HD13  | 0.49     | 2.37        | 9      | 1     |
| 1:A:196:TYR:CE2  | 1:A:198:LEU:HD23 | 0.49     | 2.42        | 20     | 1     |
| 1:A:169:THR:CB   | 1:A:197:VAL:HG12 | 0.49     | 2.36        | 17     | 6     |
| 1:A:170:LYS:HA   | 1:A:196:TYR:CD1  | 0.49     | 2.42        | 16     | 1     |
| 1:A:30:GLY:O     | 1:A:31:LYS:O     | 0.49     | 2.29        | 19     | 3     |
| 1:A:186:ALA:HB3  | 1:A:188:LEU:CD2  | 0.49     | 2.37        | 3      | 1     |
| 1:A:110:ILE:HD13 | 1:A:150:PRO:HB3  | 0.49     | 1.84        | 14     | 1     |
| 1:A:195:VAL:C    | 1:A:196:TYR:CD1  | 0.49     | 2.86        | 14     | 3     |
| 1:A:106:ARG:O    | 1:A:108:ALA:N    | 0.49     | 2.45        | 12     | 1     |
| 1:A:164:GLY:O    | 1:A:165:ASN:ND2  | 0.49     | 2.43        | 3      | 3     |
| 1:A:177:LEU:HD11 | 1:A:184:LEU:CD1  | 0.49     | 2.38        | 9      | 3     |
| 1:A:18:VAL:HG13  | 1:A:43:TYR:CE2   | 0.49     | 2.42        | 19     | 1     |
| 1:A:49:GLU:HG3   | 1:A:86:CYS:HA    | 0.49     | 1.82        | 7      | 1     |
| 1:A:25:LEU:CD1   | 1:A:27:PRO:HD3   | 0.49     | 2.37        | 11     | 6     |
| 1:A:35:MET:HG3   | 1:A:45:VAL:HG11  | 0.49     | 1.83        | 9      | 2     |
| 1:A:19:VAL:CG2   | 1:A:20:PRO:HD2   | 0.49     | 2.37        | 1      | 6     |
| 1:A:158:LEU:CA   | 1:A:162:MET:HB2  | 0.49     | 2.38        | 20     | 4     |
| 1:A:13:TRP:CZ2   | 1:A:38:LEU:HD11  | 0.49     | 2.43        | 19     | 3     |
| 1:A:176:THR:HG1  | 1:A:178:HIS:CD2  | 0.49     | 2.26        | 13     | 1     |
| 1:A:188:LEU:O    | 1:A:190:ARG:CG   | 0.49     | 2.60        | 11     | 1     |
| 1:A:125:GLU:OE2  | 1:A:200:ARG:CZ   | 0.49     | 2.60        | 12     | 2     |
| 1:A:28:LEU:HB3   | 1:A:50:LEU:HB2   | 0.49     | 1.83        | 11     | 9     |
| 1:A:107:ALA:C    | 1:A:110:ILE:HD12 | 0.49     | 2.27        | 6      | 4     |
| 1:A:132:CYS:O    | 1:A:200:ARG:HB2  | 0.49     | 2.07        | 15     | 2     |
| 1:A:177:LEU:HD12 | 1:A:177:LEU:O    | 0.49     | 2.07        | 4      | 1     |
| 1:A:178:HIS:CG   | 1:A:178:HIS:O    | 0.49     | 2.65        | 2      | 1     |
| 1:A:178:HIS:O    | 1:A:179:SER:C    | 0.49     | 2.50        | 15     | 2     |
| 1:A:38:LEU:HB3   | 1:A:45:VAL:HG22  | 0.49     | 1.85        | 19     | 1     |
| 1:A:103:PHE:CZ   | 1:A:105:ASP:OD2  | 0.49     | 2.65        | 2      | 1     |
| 1:A:6:ASN:ND2    | 1:A:137:ILE:CD1  | 0.49     | 2.76        | 1      | 1     |
| 1:A:158:LEU:O    | 1:A:162:MET:CA   | 0.49     | 2.61        | 2      | 11    |
| 1:A:12:TYR:CE1   | 1:A:197:VAL:HG11 | 0.49     | 2.43        | 8      | 2     |
| 1:A:134:GLY:C    | 1:A:198:LEU:HD12 | 0.49     | 2.27        | 6      | 5     |
| 1:A:109:MET:CB   | 1:A:117:ARG:CG   | 0.49     | 2.91        | 18     | 1     |
| 1:A:176:THR:OG1  | 1:A:178:HIS:CD2  | 0.49     | 2.65        | 13     | 1     |
| 1:A:128:MET:CB   | 1:A:129:PRO:CD   | 0.49     | 2.90        | 16     | 17    |
| 1:A:85:TRP:CZ2   | 1:A:92:LEU:CB    | 0.49     | 2.89        | 16     | 2     |
| 1:A:35:MET:CE    | 1:A:39:SER:OG    | 0.49     | 2.61        | 9      | 1     |
| 1:A:177:LEU:HD23 | 1:A:188:LEU:HB2  | 0.49     | 1.85        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:26:VAL:N     | 1:A:46:VAL:O     | 0.49     | 2.46        | 15     | 1     |
| 1:A:62:ARG:CZ    | 1:A:77:TYR:OH    | 0.49     | 2.61        | 12     | 1     |
| 1:A:109:MET:CA   | 1:A:117:ARG:NE   | 0.49     | 2.76        | 16     | 1     |
| 1:A:128:MET:SD   | 1:A:129:PRO:HD3  | 0.49     | 2.48        | 6      | 4     |
| 1:A:129:PRO:CG   | 1:A:132:CYS:SG   | 0.49     | 3.01        | 3      | 4     |
| 1:A:129:PRO:CB   | 1:A:132:CYS:SG   | 0.49     | 3.01        | 3      | 4     |
| 1:A:49:GLU:OE1   | 1:A:50:LEU:N     | 0.49     | 2.46        | 12     | 6     |
| 1:A:141:TYR:O    | 1:A:143:GLN:CG   | 0.49     | 2.60        | 7      | 3     |
| 1:A:153:VAL:HG13 | 1:A:153:VAL:O    | 0.49     | 2.07        | 14     | 2     |
| 1:A:142:ASP:OD2  | 1:A:146:LEU:CD1  | 0.49     | 2.60        | 6      | 3     |
| 1:A:137:ILE:CG2  | 1:A:193:GLU:OE2  | 0.49     | 2.61        | 6      | 1     |
| 1:A:30:GLY:HA2   | 1:A:84:ILE:HD12  | 0.49     | 1.83        | 7      | 1     |
| 1:A:168:VAL:HB   | 1:A:196:TYR:CZ   | 0.49     | 2.43        | 20     | 1     |
| 1:A:196:TYR:HH   | 1:A:198:LEU:HD23 | 0.49     | 1.65        | 20     | 1     |
| 1:A:18:VAL:CG1   | 1:A:19:VAL:N     | 0.48     | 2.76        | 1      | 1     |
| 1:A:170:LYS:HA   | 1:A:196:TYR:CE1  | 0.48     | 2.43        | 16     | 1     |
| 1:A:27:PRO:CG    | 1:A:105:ASP:OD1  | 0.48     | 2.61        | 16     | 2     |
| 1:A:145:LEU:HD13 | 1:A:146:LEU:N    | 0.48     | 2.22        | 18     | 4     |
| 1:A:168:VAL:HA   | 1:A:197:VAL:O    | 0.48     | 2.07        | 18     | 1     |
| 1:A:102:ALA:HA   | 1:A:133:SER:N    | 0.48     | 2.23        | 15     | 3     |
| 1:A:146:LEU:HD13 | 1:A:186:ALA:HB2  | 0.48     | 1.84        | 12     | 2     |
| 1:A:117:ARG:NH2  | 1:A:153:VAL:HG13 | 0.48     | 2.23        | 10     | 1     |
| 1:A:157:TRP:O    | 1:A:161:VAL:CG1  | 0.48     | 2.61        | 10     | 7     |
| 1:A:145:LEU:CD1  | 1:A:188:LEU:HD13 | 0.48     | 2.38        | 4      | 5     |
| 1:A:84:ILE:O     | 1:A:84:ILE:HG22  | 0.48     | 2.08        | 8      | 2     |
| 1:A:157:TRP:O    | 1:A:160:ARG:N    | 0.48     | 2.47        | 20     | 7     |
| 1:A:6:ASN:ND2    | 1:A:104:TYR:OH   | 0.48     | 2.46        | 9      | 4     |
| 1:A:105:ASP:CG   | 1:A:136:LEU:CD2  | 0.48     | 2.81        | 19     | 1     |
| 1:A:147:GLU:O    | 1:A:147:GLU:CG   | 0.48     | 2.60        | 9      | 1     |
| 1:A:106:ARG:C    | 1:A:106:ARG:HD2  | 0.48     | 2.29        | 11     | 1     |
| 1:A:5:VAL:HG13   | 1:A:10:GLN:OE1   | 0.48     | 2.08        | 15     | 1     |
| 1:A:137:ILE:HD13 | 1:A:195:VAL:CB   | 0.48     | 2.38        | 12     | 1     |
| 1:A:92:LEU:O     | 1:A:92:LEU:CD2   | 0.48     | 2.49        | 1      | 1     |
| 1:A:48:ALA:CB    | 1:A:85:TRP:CZ2   | 0.48     | 2.95        | 16     | 2     |
| 1:A:24:VAL:CG2   | 1:A:45:VAL:HA    | 0.48     | 2.35        | 2      | 2     |
| 1:A:105:ASP:OD1  | 1:A:105:ASP:C    | 0.48     | 2.51        | 9      | 1     |
| 1:A:55:VAL:CG2   | 1:A:56:GLU:N     | 0.48     | 2.76        | 17     | 2     |
| 1:A:183:GLY:O    | 1:A:188:LEU:HD12 | 0.48     | 2.07        | 11     | 2     |
| 1:A:110:ILE:HG22 | 1:A:153:VAL:CB   | 0.48     | 2.39        | 15     | 1     |
| 1:A:136:LEU:N    | 1:A:198:LEU:HD11 | 0.48     | 2.23        | 1      | 2     |
| 1:A:176:THR:OG1  | 1:A:179:SER:CB   | 0.48     | 2.62        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:127:LEU:O    | 1:A:127:LEU:HD13 | 0.48     | 2.09        | 5      | 1     |
| 1:A:195:VAL:CG1  | 1:A:196:TYR:N    | 0.48     | 2.76        | 5      | 4     |
| 1:A:103:PHE:CD1  | 1:A:134:GLY:HA2  | 0.48     | 2.43        | 7      | 3     |
| 1:A:26:VAL:HG13  | 1:A:29:CYS:HB3   | 0.48     | 1.85        | 7      | 1     |
| 1:A:117:ARG:HA   | 1:A:117:ARG:NE   | 0.48     | 2.23        | 13     | 1     |
| 1:A:25:LEU:O     | 1:A:26:VAL:HG13  | 0.48     | 2.08        | 10     | 1     |
| 1:A:110:ILE:HB   | 1:A:153:VAL:HG23 | 0.48     | 1.85        | 12     | 1     |
| 1:A:183:GLY:O    | 1:A:187:GLY:N    | 0.48     | 2.46        | 7      | 4     |
| 1:A:85:TRP:CZ2   | 1:A:92:LEU:CG    | 0.48     | 2.96        | 3      | 3     |
| 1:A:95:ARG:CD    | 1:A:96:ASP:N     | 0.48     | 2.76        | 3      | 1     |
| 1:A:35:MET:O     | 1:A:38:LEU:N     | 0.48     | 2.46        | 10     | 4     |
| 1:A:92:LEU:CD2   | 1:A:92:LEU:O     | 0.48     | 2.55        | 19     | 2     |
| 1:A:28:LEU:O     | 1:A:106:ARG:NH1  | 0.48     | 2.46        | 4      | 1     |
| 1:A:25:LEU:CD1   | 1:A:97:ILE:HD11  | 0.48     | 2.36        | 15     | 1     |
| 1:A:177:LEU:HG   | 1:A:190:ARG:N    | 0.48     | 2.24        | 14     | 2     |
| 1:A:10:GLN:O     | 1:A:14:SER:HB2   | 0.48     | 2.08        | 10     | 8     |
| 1:A:129:PRO:HB2  | 1:A:132:CYS:SG   | 0.48     | 2.48        | 8      | 3     |
| 1:A:165:ASN:O    | 1:A:201:VAL:CG2  | 0.48     | 2.56        | 13     | 2     |
| 1:A:168:VAL:CA   | 1:A:198:LEU:HB3  | 0.48     | 2.39        | 19     | 1     |
| 1:A:46:VAL:CG1   | 1:A:97:ILE:CD1   | 0.48     | 2.89        | 7      | 1     |
| 1:A:177:LEU:C    | 1:A:177:LEU:CD2  | 0.48     | 2.79        | 15     | 1     |
| 1:A:142:ASP:OD1  | 1:A:191:MET:SD   | 0.48     | 2.71        | 19     | 5     |
| 1:A:38:LEU:O     | 1:A:41:GLN:N     | 0.48     | 2.43        | 12     | 7     |
| 1:A:183:GLY:HA2  | 1:A:191:MET:HE1  | 0.48     | 1.85        | 9      | 1     |
| 1:A:23:ARG:CD    | 1:A:97:ILE:O     | 0.48     | 2.61        | 20     | 1     |
| 1:A:109:MET:CB   | 1:A:117:ARG:NE   | 0.48     | 2.76        | 16     | 1     |
| 1:A:25:LEU:HA    | 1:A:46:VAL:O     | 0.48     | 2.09        | 4      | 6     |
| 1:A:55:VAL:HG21  | 1:A:87:GLY:HA2   | 0.48     | 1.86        | 3      | 6     |
| 1:A:27:PRO:HB2   | 1:A:28:LEU:CD1   | 0.48     | 2.32        | 5      | 1     |
| 1:A:105:ASP:OD2  | 1:A:136:LEU:CD1  | 0.48     | 2.61        | 6      | 1     |
| 1:A:171:VAL:CG1  | 1:A:172:GLY:N    | 0.48     | 2.77        | 6      | 2     |
| 1:A:35:MET:CG    | 1:A:36:SER:N     | 0.48     | 2.76        | 6      | 2     |
| 1:A:169:THR:HG22 | 1:A:197:VAL:CG1  | 0.48     | 2.35        | 17     | 3     |
| 1:A:117:ARG:HD2  | 1:A:157:TRP:CZ3  | 0.48     | 2.43        | 7      | 1     |
| 1:A:168:VAL:CG2  | 1:A:196:TYR:CE1  | 0.48     | 2.94        | 15     | 1     |
| 1:A:12:TYR:CD2   | 1:A:197:VAL:CG2  | 0.48     | 2.97        | 12     | 1     |
| 1:A:95:ARG:CG    | 1:A:96:ASP:N     | 0.48     | 2.77        | 8      | 4     |
| 1:A:34:ASP:CB    | 1:A:104:TYR:CD2  | 0.48     | 2.97        | 2      | 2     |
| 1:A:107:ALA:CB   | 1:A:139:LEU:CD2  | 0.48     | 2.91        | 6      | 3     |
| 1:A:64:GLU:O     | 1:A:65:GLN:C     | 0.48     | 2.52        | 17     | 1     |
| 1:A:146:LEU:CD2  | 1:A:191:MET:HE1  | 0.48     | 2.38        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:159:HIS:O    | 1:A:159:HIS:CD2  | 0.48     | 2.66        | 10     | 1     |
| 1:A:28:LEU:CD1   | 1:A:89:PHE:CE1   | 0.48     | 2.97        | 1      | 1     |
| 1:A:109:MET:HB2  | 1:A:117:ARG:CZ   | 0.48     | 2.38        | 16     | 1     |
| 1:A:168:VAL:CG2  | 1:A:196:TYR:CE2  | 0.48     | 2.97        | 16     | 1     |
| 1:A:84:ILE:O     | 1:A:84:ILE:CG2   | 0.48     | 2.62        | 14     | 3     |
| 1:A:168:VAL:HG22 | 1:A:198:LEU:CG   | 0.48     | 2.39        | 14     | 2     |
| 1:A:106:ARG:NH2  | 1:A:182:ARG:NH2  | 0.48     | 2.61        | 6      | 1     |
| 1:A:26:VAL:HB    | 1:A:29:CYS:HB3   | 0.48     | 1.86        | 18     | 1     |
| 1:A:177:LEU:CD2  | 1:A:190:ARG:H    | 0.48     | 2.21        | 19     | 3     |
| 1:A:32:SER:N     | 1:A:35:MET:SD    | 0.48     | 2.87        | 4      | 1     |
| 1:A:110:ILE:HD13 | 1:A:111:ALA:N    | 0.48     | 2.23        | 12     | 2     |
| 1:A:92:LEU:CD2   | 1:A:92:LEU:C     | 0.48     | 2.83        | 11     | 1     |
| 1:A:162:MET:O    | 1:A:164:GLY:N    | 0.48     | 2.47        | 15     | 1     |
| 1:A:25:LEU:CD2   | 1:A:94:ALA:HB1   | 0.48     | 2.38        | 10     | 1     |
| 1:A:6:ASN:CG     | 1:A:104:TYR:OH   | 0.47     | 2.53        | 2      | 4     |
| 1:A:9:LEU:HD13   | 1:A:10:GLN:N     | 0.47     | 2.23        | 10     | 6     |
| 1:A:109:MET:HA   | 1:A:117:ARG:NE   | 0.47     | 2.24        | 16     | 1     |
| 1:A:12:TYR:OH    | 1:A:171:VAL:HG13 | 0.47     | 2.09        | 6      | 1     |
| 1:A:16:LEU:HD21  | 1:A:133:SER:OG   | 0.47     | 2.09        | 6      | 1     |
| 1:A:29:CYS:O     | 1:A:29:CYS:SG    | 0.47     | 2.72        | 6      | 2     |
| 1:A:46:VAL:CG2   | 1:A:83:GLU:HB3   | 0.47     | 2.34        | 20     | 2     |
| 1:A:169:THR:O    | 1:A:196:TYR:CD1  | 0.47     | 2.67        | 4      | 1     |
| 1:A:29:CYS:SG    | 1:A:104:TYR:O    | 0.47     | 2.67        | 15     | 2     |
| 1:A:35:MET:SD    | 1:A:36:SER:N     | 0.47     | 2.86        | 1      | 2     |
| 1:A:128:MET:SD   | 1:A:200:ARG:CD   | 0.47     | 3.02        | 6      | 1     |
| 1:A:135:LEU:O    | 1:A:137:ILE:CD1  | 0.47     | 2.62        | 6      | 1     |
| 1:A:92:LEU:HD22  | 1:A:97:ILE:HG21  | 0.47     | 1.83        | 19     | 2     |
| 1:A:76:VAL:CG1   | 1:A:85:TRP:CB    | 0.47     | 2.92        | 4      | 4     |
| 1:A:151:PHE:O    | 1:A:152:SER:O    | 0.47     | 2.32        | 12     | 2     |
| 1:A:142:ASP:O    | 1:A:150:PRO:CG   | 0.47     | 2.63        | 4      | 1     |
| 1:A:103:PHE:CE1  | 1:A:134:GLY:HA2  | 0.47     | 2.42        | 15     | 1     |
| 1:A:27:PRO:O     | 1:A:29:CYS:SG    | 0.47     | 2.72        | 15     | 1     |
| 1:A:174:GLN:CB   | 1:A:192:ASP:CG   | 0.47     | 2.82        | 10     | 1     |
| 1:A:162:MET:CE   | 1:A:198:LEU:HD13 | 0.47     | 2.39        | 3      | 2     |
| 1:A:146:LEU:HD13 | 1:A:186:ALA:HB3  | 0.47     | 1.86        | 13     | 2     |
| 1:A:142:ASP:O    | 1:A:143:GLN:HB3  | 0.47     | 2.09        | 5      | 10    |
| 1:A:168:VAL:CG2  | 1:A:198:LEU:HD22 | 0.47     | 2.40        | 14     | 1     |
| 1:A:115:ASP:O    | 1:A:118:GLU:HB2  | 0.47     | 2.09        | 18     | 1     |
| 1:A:152:SER:O    | 1:A:153:VAL:C    | 0.47     | 2.52        | 15     | 10    |
| 1:A:77:TYR:CD2   | 1:A:86:CYS:HB2   | 0.47     | 2.43        | 8      | 1     |
| 1:A:168:VAL:HA   | 1:A:198:LEU:HA   | 0.47     | 1.85        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:94:ALA:HA    | 1:A:97:ILE:HG22  | 0.47     | 1.86        | 19     | 1     |
| 1:A:177:LEU:C    | 1:A:179:SER:N    | 0.47     | 2.68        | 7      | 2     |
| 1:A:177:LEU:CD2  | 1:A:189:GLU:C    | 0.47     | 2.83        | 13     | 2     |
| 1:A:188:LEU:C    | 1:A:189:GLU:OE1  | 0.47     | 2.53        | 11     | 1     |
| 1:A:146:LEU:HD12 | 1:A:147:GLU:H    | 0.47     | 1.66        | 12     | 1     |
| 1:A:27:PRO:C     | 1:A:29:CYS:N     | 0.47     | 2.65        | 20     | 8     |
| 1:A:158:LEU:HA   | 1:A:162:MET:HB2  | 0.47     | 1.85        | 16     | 5     |
| 1:A:128:MET:HB3  | 1:A:200:ARG:NE   | 0.47     | 2.24        | 16     | 1     |
| 1:A:188:LEU:C    | 1:A:190:ARG:N    | 0.47     | 2.68        | 5      | 6     |
| 1:A:171:VAL:CG1  | 1:A:195:VAL:HG23 | 0.47     | 2.33        | 14     | 2     |
| 1:A:129:PRO:O    | 1:A:200:ARG:NH1  | 0.47     | 2.48        | 8      | 3     |
| 1:A:171:VAL:HG23 | 1:A:172:GLY:N    | 0.47     | 2.23        | 18     | 6     |
| 1:A:30:GLY:O     | 1:A:31:LYS:C     | 0.47     | 2.53        | 19     | 1     |
| 1:A:135:LEU:HD23 | 1:A:196:TYR:O    | 0.47     | 2.09        | 10     | 1     |
| 1:A:74:PHE:HB3   | 1:A:88:ASP:CB    | 0.47     | 2.39        | 1      | 14    |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:CD1  | 0.47     | 2.44        | 17     | 6     |
| 1:A:108:ALA:O    | 1:A:112:LEU:HD21 | 0.47     | 2.09        | 1      | 1     |
| 1:A:69:THR:CG2   | 1:A:76:VAL:CG1   | 0.47     | 2.91        | 8      | 5     |
| 1:A:69:THR:CG2   | 1:A:76:VAL:HG13  | 0.47     | 2.39        | 18     | 3     |
| 1:A:41:GLN:HB3   | 1:A:43:TYR:CD1   | 0.47     | 2.44        | 8      | 1     |
| 1:A:116:MET:CE   | 1:A:116:MET:HA   | 0.47     | 2.40        | 18     | 1     |
| 1:A:103:PHE:CZ   | 1:A:124:LEU:CD1  | 0.47     | 2.98        | 19     | 1     |
| 1:A:49:GLU:OE2   | 1:A:84:ILE:CG2   | 0.47     | 2.62        | 7      | 1     |
| 1:A:68:ILE:HG22  | 1:A:75:LYS:HE3   | 0.47     | 1.85        | 7      | 1     |
| 1:A:155:GLN:O    | 1:A:158:LEU:N    | 0.47     | 2.48        | 13     | 1     |
| 1:A:66:PRO:CB    | 1:A:77:TYR:CE1   | 0.47     | 2.97        | 1      | 5     |
| 1:A:129:PRO:HG2  | 1:A:132:CYS:SG   | 0.47     | 2.50        | 18     | 7     |
| 1:A:79:ALA:O     | 1:A:82:ILE:O     | 0.47     | 2.32        | 18     | 5     |
| 1:A:98:GLY:C     | 1:A:129:PRO:HB3  | 0.47     | 2.29        | 5      | 3     |
| 1:A:109:MET:HG3  | 1:A:153:VAL:HG11 | 0.47     | 1.86        | 9      | 2     |
| 1:A:30:GLY:CA    | 1:A:49:GLU:CD    | 0.47     | 2.83        | 8      | 2     |
| 1:A:6:ASN:ND2    | 1:A:179:SER:O    | 0.47     | 2.48        | 8      | 3     |
| 1:A:125:GLU:HA   | 1:A:128:MET:HB2  | 0.47     | 1.87        | 6      | 6     |
| 1:A:105:ASP:CG   | 1:A:136:LEU:CD1  | 0.47     | 2.83        | 9      | 2     |
| 1:A:147:GLU:CG   | 1:A:147:GLU:O    | 0.47     | 2.62        | 18     | 2     |
| 1:A:117:ARG:NH2  | 1:A:158:LEU:HD11 | 0.47     | 2.24        | 7      | 2     |
| 1:A:35:MET:SD    | 1:A:35:MET:C     | 0.47     | 2.93        | 17     | 1     |
| 1:A:102:ALA:N    | 1:A:132:CYS:SG   | 0.47     | 2.87        | 15     | 1     |
| 1:A:166:TRP:HD1  | 1:A:166:TRP:N    | 0.47     | 2.01        | 10     | 1     |
| 1:A:27:PRO:CG    | 1:A:105:ASP:OD2  | 0.47     | 2.63        | 10     | 1     |
| 1:A:112:LEU:HD12 | 1:A:117:ARG:HA   | 0.47     | 1.87        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:145:LEU:CD2  | 1:A:188:LEU:CD1  | 0.47     | 2.87        | 13     | 4     |
| 1:A:11:GLN:O     | 1:A:14:SER:N     | 0.47     | 2.48        | 2      | 2     |
| 1:A:142:ASP:HB3  | 1:A:188:LEU:CD1  | 0.47     | 2.39        | 9      | 8     |
| 1:A:125:GLU:OE2  | 1:A:166:TRP:CD2  | 0.47     | 2.68        | 6      | 2     |
| 1:A:117:ARG:NH2  | 1:A:151:PHE:CG   | 0.47     | 2.83        | 6      | 1     |
| 1:A:37:TRP:CE3   | 1:A:38:LEU:HD12  | 0.47     | 2.44        | 17     | 2     |
| 1:A:69:THR:CG2   | 1:A:70:SER:N     | 0.47     | 2.78        | 20     | 1     |
| 1:A:170:LYS:O    | 1:A:171:VAL:HG23 | 0.47     | 2.09        | 13     | 1     |
| 1:A:47:GLY:O     | 1:A:84:ILE:HA    | 0.47     | 2.10        | 13     | 8     |
| 1:A:55:VAL:HG11  | 1:A:87:GLY:CA    | 0.47     | 2.40        | 16     | 2     |
| 1:A:55:VAL:O     | 1:A:59:PHE:CG    | 0.47     | 2.68        | 11     | 4     |
| 1:A:164:GLY:O    | 1:A:165:ASN:HB2  | 0.47     | 2.10        | 12     | 9     |
| 1:A:21:GLY:O     | 1:A:44:HIS:ND1   | 0.47     | 2.48        | 14     | 1     |
| 1:A:153:VAL:O    | 1:A:196:TYR:OH   | 0.47     | 2.28        | 8      | 1     |
| 1:A:119:ARG:O    | 1:A:123:HIS:ND1  | 0.47     | 2.48        | 6      | 2     |
| 1:A:105:ASP:HB3  | 1:A:136:LEU:CD1  | 0.47     | 2.40        | 18     | 3     |
| 1:A:109:MET:HE2  | 1:A:136:LEU:HD11 | 0.47     | 1.86        | 7      | 1     |
| 1:A:28:LEU:CD2   | 1:A:89:PHE:CE1   | 0.47     | 2.98        | 7      | 1     |
| 1:A:177:LEU:HD23 | 1:A:191:MET:CG   | 0.47     | 2.39        | 20     | 2     |
| 1:A:128:MET:SD   | 1:A:200:ARG:NH2  | 0.47     | 2.87        | 15     | 1     |
| 1:A:145:LEU:CD2  | 1:A:188:LEU:CD2  | 0.47     | 2.91        | 15     | 1     |
| 1:A:190:ARG:CG   | 1:A:190:ARG:O    | 0.47     | 2.62        | 10     | 1     |
| 1:A:139:LEU:H    | 1:A:139:LEU:HD13 | 0.47     | 1.69        | 3      | 1     |
| 1:A:170:LYS:O    | 1:A:171:VAL:CG2  | 0.47     | 2.63        | 6      | 1     |
| 1:A:34:ASP:OD1   | 1:A:104:TYR:CZ   | 0.47     | 2.68        | 4      | 1     |
| 1:A:128:MET:HB3  | 1:A:200:ARG:CD   | 0.47     | 2.39        | 17     | 1     |
| 1:A:77:TYR:CD1   | 1:A:86:CYS:HB2   | 0.47     | 2.45        | 17     | 1     |
| 1:A:55:VAL:HG12  | 1:A:56:GLU:N     | 0.47     | 2.25        | 2      | 2     |
| 1:A:168:VAL:HG23 | 1:A:196:TYR:OH   | 0.47     | 2.08        | 15     | 1     |
| 1:A:4:GLU:HB2    | 1:A:178:HIS:CD2  | 0.47     | 2.45        | 15     | 1     |
| 1:A:121:VAL:CG2  | 1:A:122:GLN:N    | 0.46     | 2.78        | 14     | 6     |
| 1:A:162:MET:SD   | 1:A:196:TYR:OH   | 0.46     | 2.74        | 18     | 1     |
| 1:A:25:LEU:HD12  | 1:A:128:MET:CE   | 0.46     | 2.40        | 7      | 1     |
| 1:A:63:GLY:O     | 1:A:64:GLU:CB    | 0.46     | 2.62        | 7      | 2     |
| 1:A:107:ALA:HB2  | 1:A:139:LEU:HD13 | 0.46     | 1.87        | 7      | 1     |
| 1:A:13:TRP:O     | 1:A:16:LEU:N     | 0.46     | 2.48        | 11     | 1     |
| 1:A:90:PHE:CE1   | 1:A:123:HIS:CE1  | 0.46     | 3.02        | 15     | 1     |
| 1:A:76:VAL:O     | 1:A:76:VAL:HG22  | 0.46     | 2.09        | 16     | 2     |
| 1:A:154:PRO:O    | 1:A:155:GLN:C    | 0.46     | 2.53        | 13     | 4     |
| 1:A:198:LEU:H    | 1:A:198:LEU:HD23 | 0.46     | 1.67        | 5      | 2     |
| 1:A:35:MET:CE    | 1:A:84:ILE:CG1   | 0.46     | 2.93        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:142:ASP:HB3  | 1:A:188:LEU:CD2  | 0.46     | 2.39        | 14     | 4     |
| 1:A:25:LEU:O     | 1:A:103:PHE:CA   | 0.46     | 2.64        | 12     | 3     |
| 1:A:69:THR:CB    | 1:A:76:VAL:HG13  | 0.46     | 2.39        | 18     | 2     |
| 1:A:62:ARG:NE    | 1:A:77:TYR:OH    | 0.46     | 2.49        | 9      | 2     |
| 1:A:69:THR:HG22  | 1:A:76:VAL:CG2   | 0.46     | 2.39        | 20     | 2     |
| 1:A:177:LEU:HD23 | 1:A:190:ARG:N    | 0.46     | 2.25        | 9      | 1     |
| 1:A:155:GLN:HG3  | 1:A:196:TYR:CD1  | 0.46     | 2.45        | 4      | 1     |
| 1:A:26:VAL:O     | 1:A:26:VAL:CG1   | 0.46     | 2.63        | 15     | 1     |
| 1:A:6:ASN:ND2    | 1:A:6:ASN:H      | 0.46     | 2.07        | 15     | 1     |
| 1:A:125:GLU:OE1  | 1:A:200:ARG:CZ   | 0.46     | 2.63        | 10     | 1     |
| 1:A:159:HIS:O    | 1:A:163:SER:OG   | 0.46     | 2.32        | 10     | 1     |
| 1:A:74:PHE:CE2   | 1:A:88:ASP:OD1   | 0.46     | 2.68        | 12     | 1     |
| 1:A:146:LEU:HG   | 1:A:186:ALA:CB   | 0.46     | 2.41        | 4      | 6     |
| 1:A:31:LYS:HA    | 1:A:35:MET:CB    | 0.46     | 2.40        | 9      | 2     |
| 1:A:177:LEU:HD23 | 1:A:190:ARG:H    | 0.46     | 1.70        | 9      | 2     |
| 1:A:15:SER:O     | 1:A:16:LEU:C     | 0.46     | 2.53        | 9      | 10    |
| 1:A:59:PHE:CE2   | 1:A:68:ILE:CG2   | 0.46     | 2.98        | 3      | 1     |
| 1:A:142:ASP:CG   | 1:A:191:MET:SD   | 0.46     | 2.94        | 3      | 2     |
| 1:A:89:PHE:CD1   | 1:A:90:PHE:N     | 0.46     | 2.84        | 19     | 1     |
| 1:A:177:LEU:O    | 1:A:179:SER:N    | 0.46     | 2.49        | 7      | 3     |
| 1:A:155:GLN:HE21 | 1:A:170:LYS:N    | 0.46     | 2.08        | 9      | 1     |
| 1:A:142:ASP:O    | 1:A:150:PRO:CD   | 0.46     | 2.63        | 4      | 1     |
| 1:A:57:ARG:O     | 1:A:61:GLU:CG    | 0.46     | 2.64        | 20     | 3     |
| 1:A:121:VAL:HB   | 1:A:162:MET:HG2  | 0.46     | 1.87        | 20     | 1     |
| 1:A:107:ALA:CA   | 1:A:110:ILE:HD12 | 0.46     | 2.40        | 6      | 5     |
| 1:A:10:GLN:O     | 1:A:14:SER:OG    | 0.46     | 2.33        | 7      | 7     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:CD1   | 0.46     | 2.40        | 5      | 1     |
| 1:A:129:PRO:HD2  | 1:A:200:ARG:CD   | 0.46     | 2.40        | 2      | 3     |
| 1:A:168:VAL:HA   | 1:A:198:LEU:HB3  | 0.46     | 1.87        | 19     | 1     |
| 1:A:10:GLN:O     | 1:A:14:SER:HB3   | 0.46     | 2.11        | 10     | 2     |
| 1:A:188:LEU:N    | 1:A:188:LEU:CD1  | 0.46     | 2.78        | 20     | 1     |
| 1:A:125:GLU:O    | 1:A:200:ARG:NH2  | 0.46     | 2.49        | 2      | 1     |
| 1:A:118:GLU:CG   | 1:A:161:VAL:HG21 | 0.46     | 2.40        | 14     | 5     |
| 1:A:189:GLU:C    | 1:A:190:ARG:CG   | 0.46     | 2.83        | 1      | 1     |
| 1:A:9:LEU:HD23   | 1:A:104:TYR:HD2  | 0.46     | 1.71        | 16     | 1     |
| 1:A:93:THR:O     | 1:A:97:ILE:CG2   | 0.46     | 2.64        | 4      | 2     |
| 1:A:105:ASP:HB2  | 1:A:136:LEU:CD1  | 0.46     | 2.40        | 8      | 1     |
| 1:A:18:VAL:HG12  | 1:A:22:ALA:HB2   | 0.46     | 1.88        | 9      | 1     |
| 1:A:77:TYR:HB3   | 1:A:86:CYS:CB    | 0.46     | 2.40        | 20     | 2     |
| 1:A:169:THR:HG22 | 1:A:197:VAL:HB   | 0.46     | 1.87        | 10     | 2     |
| 1:A:140:GLU:HG3  | 1:A:141:TYR:N    | 0.46     | 2.26        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:184:LEU:N    | 1:A:184:LEU:HD13 | 0.46     | 2.24        | 12     | 1     |
| 1:A:117:ARG:CZ   | 1:A:153:VAL:HG11 | 0.46     | 2.40        | 19     | 1     |
| 1:A:108:ALA:O    | 1:A:111:ALA:HB3  | 0.46     | 2.11        | 19     | 1     |
| 1:A:168:VAL:CA   | 1:A:196:TYR:CE1  | 0.46     | 2.99        | 20     | 1     |
| 1:A:109:MET:O    | 1:A:117:ARG:NE   | 0.46     | 2.49        | 15     | 1     |
| 1:A:125:GLU:OE2  | 1:A:200:ARG:NH1  | 0.46     | 2.49        | 10     | 1     |
| 1:A:108:ALA:O    | 1:A:112:LEU:CD2  | 0.46     | 2.64        | 1      | 1     |
| 1:A:51:SER:HB3   | 1:A:54:ALA:CB    | 0.46     | 2.41        | 16     | 1     |
| 1:A:27:PRO:O     | 1:A:28:LEU:O     | 0.46     | 2.34        | 3      | 1     |
| 1:A:171:VAL:CG1  | 1:A:196:TYR:HA   | 0.46     | 2.41        | 15     | 2     |
| 1:A:7:LYS:O      | 1:A:11:GLN:HB2   | 0.46     | 2.11        | 10     | 2     |
| 1:A:170:LYS:C    | 1:A:171:VAL:CG1  | 0.46     | 2.84        | 18     | 1     |
| 1:A:13:TRP:CZ2   | 1:A:24:VAL:HG22  | 0.46     | 2.45        | 19     | 1     |
| 1:A:142:ASP:O    | 1:A:143:GLN:CG   | 0.46     | 2.64        | 7      | 1     |
| 1:A:174:GLN:O    | 1:A:176:THR:N    | 0.46     | 2.43        | 4      | 2     |
| 1:A:112:LEU:CD2  | 1:A:116:MET:CG   | 0.46     | 2.94        | 13     | 1     |
| 1:A:199:GLU:O    | 1:A:201:VAL:HG13 | 0.46     | 2.11        | 15     | 1     |
| 1:A:108:ALA:N    | 1:A:110:ILE:HD12 | 0.46     | 2.25        | 10     | 1     |
| 1:A:188:LEU:N    | 1:A:188:LEU:HD22 | 0.46     | 2.25        | 1      | 6     |
| 1:A:35:MET:CE    | 1:A:84:ILE:HG13  | 0.46     | 2.40        | 14     | 1     |
| 1:A:140:GLU:N    | 1:A:142:ASP:OD1  | 0.46     | 2.49        | 14     | 1     |
| 1:A:157:TRP:O    | 1:A:160:ARG:CG   | 0.46     | 2.64        | 10     | 2     |
| 1:A:125:GLU:HG3  | 1:A:166:TRP:CE3  | 0.46     | 2.46        | 19     | 1     |
| 1:A:125:GLU:OE1  | 1:A:126:ALA:N    | 0.46     | 2.49        | 15     | 2     |
| 1:A:139:LEU:CD2  | 1:A:191:MET:HE3  | 0.46     | 2.41        | 7      | 1     |
| 1:A:196:TYR:CE2  | 1:A:198:LEU:CD2  | 0.46     | 2.99        | 20     | 1     |
| 1:A:175:ASP:N    | 1:A:175:ASP:OD1  | 0.46     | 2.49        | 13     | 1     |
| 1:A:103:PHE:CD1  | 1:A:103:PHE:O    | 0.46     | 2.68        | 16     | 1     |
| 1:A:122:GLN:O    | 1:A:125:GLU:HG3  | 0.46     | 2.11        | 5      | 8     |
| 1:A:93:THR:O     | 1:A:95:ARG:N     | 0.46     | 2.49        | 14     | 3     |
| 1:A:177:LEU:CD2  | 1:A:183:GLY:HA3  | 0.46     | 2.41        | 17     | 2     |
| 1:A:32:SER:OG    | 1:A:181:ALA:CB   | 0.46     | 2.64        | 14     | 1     |
| 1:A:196:TYR:CD1  | 1:A:198:LEU:HD22 | 0.46     | 2.39        | 18     | 1     |
| 1:A:97:ILE:O     | 1:A:99:HIS:NE2   | 0.46     | 2.49        | 18     | 1     |
| 1:A:117:ARG:HH21 | 1:A:153:VAL:HG11 | 0.46     | 1.70        | 17     | 1     |
| 1:A:28:LEU:HB3   | 1:A:50:LEU:CB    | 0.46     | 2.41        | 20     | 1     |
| 1:A:34:ASP:CG    | 1:A:104:TYR:CE2  | 0.46     | 2.89        | 15     | 1     |
| 1:A:165:ASN:O    | 1:A:200:ARG:NH1  | 0.45     | 2.49        | 1      | 2     |
| 1:A:46:VAL:CB    | 1:A:83:GLU:HB3   | 0.45     | 2.41        | 13     | 7     |
| 1:A:177:LEU:O    | 1:A:180:SER:N    | 0.45     | 2.49        | 11     | 2     |
| 1:A:121:VAL:CG1  | 1:A:122:GLN:N    | 0.45     | 2.79        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:25:LEU:CD2   | 1:A:128:MET:HE3  | 0.45     | 2.40        | 16     | 2     |
| 1:A:134:GLY:N    | 1:A:200:ARG:HH21 | 0.45     | 2.10        | 6      | 1     |
| 1:A:152:SER:OG   | 1:A:152:SER:O    | 0.45     | 2.31        | 4      | 4     |
| 1:A:26:VAL:HG11  | 1:A:84:ILE:HD11  | 0.45     | 1.89        | 7      | 1     |
| 1:A:188:LEU:O    | 1:A:189:GLU:HG2  | 0.45     | 2.11        | 11     | 2     |
| 1:A:6:ASN:ND2    | 1:A:179:SER:OG   | 0.45     | 2.48        | 13     | 2     |
| 1:A:24:VAL:CG1   | 1:A:38:LEU:HD23  | 0.45     | 2.42        | 17     | 1     |
| 1:A:171:VAL:HG13 | 1:A:195:VAL:HG12 | 0.45     | 1.88        | 20     | 1     |
| 1:A:177:LEU:CG   | 1:A:188:LEU:HB2  | 0.45     | 2.41        | 15     | 1     |
| 1:A:198:LEU:HD23 | 1:A:198:LEU:H    | 0.45     | 1.72        | 3      | 2     |
| 1:A:33:GLN:NE2   | 1:A:181:ALA:HB2  | 0.45     | 2.26        | 16     | 1     |
| 1:A:127:LEU:C    | 1:A:127:LEU:HD13 | 0.45     | 2.32        | 5      | 1     |
| 1:A:112:LEU:HD13 | 1:A:116:MET:HG3  | 0.45     | 1.89        | 14     | 1     |
| 1:A:105:ASP:OD1  | 1:A:106:ARG:O    | 0.45     | 2.33        | 17     | 2     |
| 1:A:177:LEU:CD1  | 1:A:184:LEU:HD11 | 0.45     | 2.41        | 9      | 1     |
| 1:A:194:HIS:CD2  | 1:A:194:HIS:N    | 0.45     | 2.84        | 4      | 1     |
| 1:A:59:PHE:CZ    | 1:A:68:ILE:CD1   | 0.45     | 2.99        | 13     | 2     |
| 1:A:49:GLU:CB    | 1:A:86:CYS:SG    | 0.45     | 3.04        | 20     | 1     |
| 1:A:7:LYS:HG2    | 1:A:8:ASP:N      | 0.45     | 2.25        | 11     | 2     |
| 1:A:180:SER:N    | 1:A:193:GLU:OE2  | 0.45     | 2.49        | 15     | 1     |
| 1:A:190:ARG:O    | 1:A:191:MET:HG2  | 0.45     | 2.11        | 15     | 1     |
| 1:A:30:GLY:O     | 1:A:106:ARG:NH2  | 0.45     | 2.49        | 1      | 1     |
| 1:A:142:ASP:OD2  | 1:A:191:MET:SD   | 0.45     | 2.75        | 4      | 5     |
| 1:A:139:LEU:N    | 1:A:139:LEU:CD1  | 0.45     | 2.73        | 10     | 4     |
| 1:A:76:VAL:HG22  | 1:A:76:VAL:O     | 0.45     | 2.11        | 17     | 3     |
| 1:A:59:PHE:HE1   | 1:A:77:TYR:CD2   | 0.45     | 2.26        | 17     | 4     |
| 1:A:105:ASP:OD1  | 1:A:106:ARG:NH2  | 0.45     | 2.49        | 11     | 1     |
| 1:A:95:ARG:NH1   | 1:A:126:ALA:O    | 0.45     | 2.50        | 10     | 1     |
| 1:A:122:GLN:HA   | 1:A:125:GLU:CG   | 0.45     | 2.42        | 3      | 7     |
| 1:A:141:TYR:O    | 1:A:143:GLN:NE2  | 0.45     | 2.49        | 16     | 1     |
| 1:A:46:VAL:HB    | 1:A:83:GLU:CB    | 0.45     | 2.41        | 8      | 4     |
| 1:A:109:MET:CB   | 1:A:117:ARG:CD   | 0.45     | 2.95        | 5      | 1     |
| 1:A:6:ASN:CB     | 1:A:104:TYR:OH   | 0.45     | 2.64        | 6      | 2     |
| 1:A:71:GLN:HG3   | 1:A:91:ALA:CB    | 0.45     | 2.42        | 9      | 1     |
| 1:A:125:GLU:OE1  | 1:A:165:ASN:ND2  | 0.45     | 2.49        | 7      | 1     |
| 1:A:112:LEU:HD12 | 1:A:117:ARG:N    | 0.45     | 2.27        | 15     | 1     |
| 1:A:171:VAL:HG13 | 1:A:196:TYR:N    | 0.45     | 2.25        | 15     | 1     |
| 1:A:71:GLN:HA    | 1:A:71:GLN:OE1   | 0.45     | 2.11        | 10     | 2     |
| 1:A:107:ALA:CB   | 1:A:110:ILE:CD1  | 0.45     | 2.94        | 1      | 1     |
| 1:A:160:ARG:HG2  | 1:A:161:VAL:N    | 0.45     | 2.27        | 16     | 1     |
| 1:A:26:VAL:HG22  | 1:A:104:TYR:HB3  | 0.45     | 1.89        | 3      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:160:ARG:CG  | 1:A:161:VAL:N    | 0.45     | 2.80        | 7      | 8     |
| 1:A:146:LEU:CD1 | 1:A:147:GLU:N    | 0.45     | 2.77        | 3      | 1     |
| 1:A:35:MET:CE   | 1:A:39:SER:HB3   | 0.45     | 2.42        | 9      | 1     |
| 1:A:140:GLU:CD  | 1:A:194:HIS:ND1  | 0.45     | 2.70        | 2      | 1     |
| 1:A:7:LYS:O     | 1:A:10:GLN:NE2   | 0.45     | 2.50        | 1      | 1     |
| 1:A:27:PRO:CD   | 1:A:105:ASP:OD1  | 0.45     | 2.65        | 16     | 1     |
| 1:A:103:PHE:CD2 | 1:A:134:GLY:HA2  | 0.45     | 2.47        | 5      | 3     |
| 1:A:8:ASP:CG    | 1:A:195:VAL:HG21 | 0.45     | 2.31        | 14     | 1     |
| 1:A:27:PRO:HD3  | 1:A:103:PHE:CE1  | 0.45     | 2.46        | 9      | 1     |
| 1:A:71:GLN:HG3  | 1:A:71:GLN:O     | 0.45     | 2.12        | 12     | 2     |
| 1:A:6:ASN:OD1   | 1:A:9:LEU:CB     | 0.45     | 2.65        | 20     | 1     |
| 1:A:5:VAL:O     | 1:A:7:LYS:N      | 0.45     | 2.50        | 15     | 1     |
| 1:A:74:PHE:CD1  | 1:A:88:ASP:OD1   | 0.45     | 2.70        | 10     | 1     |
| 1:A:140:GLU:O   | 1:A:142:ASP:O    | 0.45     | 2.34        | 11     | 5     |
| 1:A:116:MET:O   | 1:A:120:TYR:HB2  | 0.45     | 2.12        | 12     | 2     |
| 1:A:85:TRP:CZ2  | 1:A:92:LEU:HD12  | 0.45     | 2.47        | 3      | 1     |
| 1:A:137:ILE:N   | 1:A:137:ILE:HD12 | 0.45     | 2.27        | 5      | 1     |
| 1:A:180:SER:CB  | 1:A:193:GLU:OE2  | 0.45     | 2.65        | 14     | 1     |
| 1:A:95:ARG:HB3  | 1:A:128:MET:O    | 0.45     | 2.12        | 8      | 1     |
| 1:A:125:GLU:HG3 | 1:A:166:TRP:CZ2  | 0.45     | 2.47        | 19     | 1     |
| 1:A:30:GLY:N    | 1:A:49:GLU:OE1   | 0.45     | 2.44        | 19     | 1     |
| 1:A:48:ALA:O    | 1:A:49:GLU:OE1   | 0.45     | 2.35        | 13     | 2     |
| 1:A:137:ILE:CG2 | 1:A:193:GLU:CD   | 0.45     | 2.85        | 7      | 2     |
| 1:A:23:ARG:HD2  | 1:A:46:VAL:HG11  | 0.45     | 1.88        | 7      | 1     |
| 1:A:26:VAL:HG13 | 1:A:29:CYS:CB    | 0.45     | 2.32        | 15     | 2     |
| 1:A:24:VAL:CG1  | 1:A:38:LEU:CD2   | 0.45     | 2.93        | 17     | 1     |
| 1:A:140:GLU:CD  | 1:A:192:ASP:OD2  | 0.45     | 2.55        | 2      | 1     |
| 1:A:200:ARG:NH1 | 1:A:201:VAL:C    | 0.45     | 2.71        | 1      | 3     |
| 1:A:28:LEU:HD12 | 1:A:50:LEU:CG    | 0.45     | 2.41        | 8      | 2     |
| 1:A:26:VAL:O    | 1:A:47:GLY:HA2   | 0.45     | 2.12        | 5      | 2     |
| 1:A:139:LEU:CG  | 1:A:142:ASP:OD2  | 0.45     | 2.65        | 3      | 1     |
| 1:A:13:TRP:CZ2  | 1:A:38:LEU:HD22  | 0.45     | 2.46        | 14     | 1     |
| 1:A:146:LEU:CD2 | 1:A:191:MET:HE3  | 0.45     | 2.41        | 14     | 1     |
| 1:A:195:VAL:C   | 1:A:196:TYR:CG   | 0.45     | 2.90        | 6      | 2     |
| 1:A:97:ILE:O    | 1:A:97:ILE:HD12  | 0.45     | 2.12        | 9      | 1     |
| 1:A:142:ASP:C   | 1:A:143:GLN:CG   | 0.45     | 2.85        | 7      | 1     |
| 1:A:95:ARG:NH1  | 1:A:129:PRO:O    | 0.45     | 2.49        | 2      | 2     |
| 1:A:164:GLY:O   | 1:A:165:ASN:OD1  | 0.45     | 2.35        | 4      | 3     |
| 1:A:182:ARG:HB3 | 1:A:182:ARG:CZ   | 0.45     | 2.42        | 20     | 1     |
| 1:A:191:MET:SD  | 1:A:191:MET:O    | 0.45     | 2.75        | 13     | 1     |
| 1:A:46:VAL:CG1  | 1:A:97:ILE:HG12  | 0.45     | 2.42        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:TRP:HZ3   | 1:A:43:TYR:CE2   | 0.45     | 2.30        | 1      | 1     |
| 1:A:109:MET:HA   | 1:A:117:ARG:NH2  | 0.45     | 2.26        | 16     | 1     |
| 1:A:38:LEU:O     | 1:A:42:GLY:N     | 0.45     | 2.47        | 16     | 1     |
| 1:A:112:LEU:HB2  | 1:A:116:MET:HB3  | 0.45     | 1.88        | 2      | 2     |
| 1:A:12:TYR:CZ    | 1:A:197:VAL:CG2  | 0.45     | 3.00        | 18     | 1     |
| 1:A:177:LEU:O    | 1:A:177:LEU:CD2  | 0.45     | 2.51        | 18     | 1     |
| 1:A:97:ILE:O     | 1:A:99:HIS:CD2   | 0.45     | 2.70        | 18     | 1     |
| 1:A:105:ASP:OD1  | 1:A:106:ARG:N    | 0.45     | 2.50        | 17     | 1     |
| 1:A:49:GLU:HB3   | 1:A:86:CYS:SG    | 0.45     | 2.52        | 20     | 1     |
| 1:A:151:PHE:CD1  | 1:A:151:PHE:O    | 0.45     | 2.69        | 20     | 1     |
| 1:A:188:LEU:O    | 1:A:191:MET:CG   | 0.45     | 2.65        | 15     | 1     |
| 1:A:104:TYR:CZ   | 1:A:135:LEU:CD1  | 0.45     | 2.95        | 10     | 1     |
| 1:A:125:GLU:HG2  | 1:A:166:TRP:CZ3  | 0.45     | 2.47        | 12     | 1     |
| 1:A:181:ALA:O    | 1:A:184:LEU:N    | 0.44     | 2.50        | 7      | 2     |
| 1:A:117:ARG:O    | 1:A:120:TYR:N    | 0.44     | 2.50        | 5      | 1     |
| 1:A:26:VAL:CG2   | 1:A:35:MET:HE1   | 0.44     | 2.42        | 14     | 1     |
| 1:A:9:LEU:HA     | 1:A:135:LEU:CD2  | 0.44     | 2.41        | 11     | 2     |
| 1:A:109:MET:CB   | 1:A:117:ARG:NH2  | 0.44     | 2.80        | 17     | 2     |
| 1:A:112:LEU:HB2  | 1:A:113:PRO:HD2  | 0.44     | 1.89        | 12     | 2     |
| 1:A:192:ASP:C    | 1:A:192:ASP:OD1  | 0.44     | 2.55        | 2      | 3     |
| 1:A:171:VAL:HG13 | 1:A:195:VAL:HG22 | 0.44     | 1.86        | 14     | 2     |
| 1:A:84:ILE:HG22  | 1:A:84:ILE:O     | 0.44     | 2.12        | 14     | 3     |
| 1:A:153:VAL:CG1  | 1:A:157:TRP:CE3  | 0.44     | 3.00        | 4      | 1     |
| 1:A:110:ILE:CD1  | 1:A:139:LEU:HD12 | 0.44     | 2.42        | 17     | 1     |
| 1:A:110:ILE:HD12 | 1:A:150:PRO:CB   | 0.44     | 2.42        | 17     | 1     |
| 1:A:69:THR:HG23  | 1:A:70:SER:N     | 0.44     | 2.27        | 20     | 1     |
| 1:A:112:LEU:HB2  | 1:A:117:ARG:NE   | 0.44     | 2.27        | 13     | 1     |
| 1:A:71:GLN:O     | 1:A:73:ASP:N     | 0.44     | 2.51        | 10     | 1     |
| 1:A:168:VAL:HG23 | 1:A:196:TYR:CE2  | 0.44     | 2.48        | 16     | 1     |
| 1:A:181:ALA:O    | 1:A:183:GLY:N    | 0.44     | 2.51        | 12     | 4     |
| 1:A:13:TRP:CE2   | 1:A:38:LEU:CD2   | 0.44     | 3.00        | 14     | 1     |
| 1:A:28:LEU:CD1   | 1:A:50:LEU:HG    | 0.44     | 2.42        | 8      | 1     |
| 1:A:113:PRO:O    | 1:A:117:ARG:CG   | 0.44     | 2.66        | 8      | 2     |
| 1:A:168:VAL:CG1  | 1:A:196:TYR:HB3  | 0.44     | 2.41        | 19     | 1     |
| 1:A:117:ARG:CZ   | 1:A:158:LEU:HD11 | 0.44     | 2.42        | 7      | 1     |
| 1:A:31:LYS:HE3   | 1:A:58:TYR:CZ    | 0.44     | 2.47        | 17     | 1     |
| 1:A:28:LEU:CD2   | 1:A:89:PHE:CD2   | 0.44     | 3.00        | 20     | 1     |
| 1:A:179:SER:CB   | 1:A:193:GLU:OE2  | 0.44     | 2.65        | 20     | 2     |
| 1:A:113:PRO:O    | 1:A:117:ARG:N    | 0.44     | 2.47        | 16     | 1     |
| 1:A:121:VAL:O    | 1:A:125:GLU:HG3  | 0.44     | 2.13        | 18     | 5     |
| 1:A:188:LEU:HD22 | 1:A:188:LEU:N    | 0.44     | 2.28        | 8      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:34:ASP:O     | 1:A:38:LEU:CD2   | 0.44     | 2.56        | 6      | 2     |
| 1:A:37:TRP:O     | 1:A:41:GLN:N     | 0.44     | 2.50        | 6      | 1     |
| 1:A:113:PRO:HD2  | 1:A:116:MET:HB3  | 0.44     | 1.88        | 9      | 4     |
| 1:A:6:ASN:HA     | 1:A:179:SER:CB   | 0.44     | 2.43        | 19     | 1     |
| 1:A:156:THR:CG2  | 1:A:157:TRP:N    | 0.44     | 2.80        | 4      | 1     |
| 1:A:70:SER:C     | 1:A:71:GLN:OE1   | 0.44     | 2.56        | 17     | 1     |
| 1:A:21:GLY:O     | 1:A:22:ALA:C     | 0.44     | 2.55        | 16     | 9     |
| 1:A:51:SER:CB    | 1:A:54:ALA:HB3   | 0.44     | 2.40        | 15     | 2     |
| 1:A:154:PRO:O    | 1:A:156:THR:N    | 0.44     | 2.50        | 19     | 2     |
| 1:A:191:MET:SD   | 1:A:191:MET:C    | 0.44     | 2.96        | 19     | 2     |
| 1:A:168:VAL:HA   | 1:A:198:LEU:CA   | 0.44     | 2.42        | 19     | 1     |
| 1:A:50:LEU:HD13  | 1:A:88:ASP:HA    | 0.44     | 1.88        | 7      | 1     |
| 1:A:47:GLY:O     | 1:A:85:TRP:NE1   | 0.44     | 2.51        | 4      | 1     |
| 1:A:177:LEU:CD1  | 1:A:184:LEU:CD1  | 0.44     | 2.96        | 12     | 1     |
| 1:A:189:GLU:CD   | 1:A:189:GLU:O    | 0.44     | 2.56        | 12     | 1     |
| 1:A:198:LEU:N    | 1:A:198:LEU:HD12 | 0.44     | 2.27        | 1      | 1     |
| 1:A:103:PHE:CE2  | 1:A:105:ASP:HB2  | 0.44     | 2.47        | 7      | 2     |
| 1:A:174:GLN:C    | 1:A:176:THR:N    | 0.44     | 2.71        | 14     | 2     |
| 1:A:69:THR:CG2   | 1:A:76:VAL:HB    | 0.44     | 2.42        | 20     | 4     |
| 1:A:135:LEU:HD13 | 1:A:197:VAL:CG2  | 0.44     | 2.37        | 18     | 2     |
| 1:A:109:MET:HA   | 1:A:117:ARG:CG   | 0.44     | 2.43        | 9      | 1     |
| 1:A:183:GLY:HA2  | 1:A:191:MET:CE   | 0.44     | 2.43        | 9      | 1     |
| 1:A:173:GLY:O    | 1:A:174:GLN:C    | 0.44     | 2.56        | 4      | 2     |
| 1:A:110:ILE:HD12 | 1:A:150:PRO:HB3  | 0.44     | 1.88        | 17     | 1     |
| 1:A:129:PRO:CD   | 1:A:200:ARG:HD3  | 0.44     | 2.43        | 20     | 1     |
| 1:A:99:HIS:CA    | 1:A:129:PRO:CB   | 0.44     | 2.96        | 15     | 1     |
| 1:A:132:CYS:CB   | 1:A:200:ARG:NH1  | 0.44     | 2.81        | 15     | 1     |
| 1:A:18:VAL:O     | 1:A:43:TYR:OH    | 0.44     | 2.35        | 1      | 1     |
| 1:A:129:PRO:HD2  | 1:A:200:ARG:HD3  | 0.44     | 1.90        | 16     | 2     |
| 1:A:168:VAL:HG22 | 1:A:198:LEU:CD2  | 0.44     | 2.43        | 14     | 1     |
| 1:A:145:LEU:HD22 | 1:A:188:LEU:CG   | 0.44     | 2.42        | 14     | 3     |
| 1:A:110:ILE:N    | 1:A:110:ILE:HD13 | 0.44     | 2.27        | 18     | 3     |
| 1:A:125:GLU:OE2  | 1:A:165:ASN:HB3  | 0.44     | 2.12        | 19     | 1     |
| 1:A:153:VAL:O    | 1:A:153:VAL:HG13 | 0.44     | 2.12        | 9      | 2     |
| 1:A:28:LEU:HD22  | 1:A:50:LEU:CB    | 0.44     | 2.42        | 20     | 1     |
| 1:A:46:VAL:HA    | 1:A:83:GLU:O     | 0.44     | 2.13        | 2      | 1     |
| 1:A:99:HIS:HA    | 1:A:129:PRO:HB3  | 0.44     | 1.90        | 15     | 1     |
| 1:A:136:LEU:HD21 | 1:A:138:THR:HG23 | 0.44     | 1.89        | 15     | 1     |
| 1:A:161:VAL:CG2  | 1:A:162:MET:N    | 0.44     | 2.80        | 12     | 2     |
| 1:A:166:TRP:H    | 1:A:166:TRP:HD1  | 0.44     | 1.55        | 10     | 1     |
| 1:A:104:TYR:CD1  | 1:A:105:ASP:N    | 0.44     | 2.86        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:125:GLU:HA   | 1:A:128:MET:HG3  | 0.44     | 1.90        | 16     | 1     |
| 1:A:139:LEU:CD1  | 1:A:139:LEU:N    | 0.44     | 2.69        | 16     | 2     |
| 1:A:39:SER:O     | 1:A:42:GLY:N     | 0.44     | 2.49        | 20     | 2     |
| 1:A:186:ALA:HB3  | 1:A:188:LEU:CD1  | 0.44     | 2.40        | 14     | 4     |
| 1:A:35:MET:CE    | 1:A:39:SER:CB    | 0.44     | 2.96        | 9      | 1     |
| 1:A:46:VAL:CG1   | 1:A:83:GLU:HB3   | 0.44     | 2.32        | 9      | 2     |
| 1:A:24:VAL:HB    | 1:A:38:LEU:HD13  | 0.44     | 1.89        | 2      | 1     |
| 1:A:138:THR:HG21 | 1:A:153:VAL:HG11 | 0.44     | 1.89        | 14     | 2     |
| 1:A:137:ILE:CD1  | 1:A:195:VAL:HB   | 0.44     | 2.41        | 14     | 1     |
| 1:A:33:GLN:NE2   | 1:A:179:SER:O    | 0.44     | 2.51        | 19     | 1     |
| 1:A:71:GLN:OE1   | 1:A:71:GLN:O     | 0.44     | 2.36        | 4      | 1     |
| 1:A:92:LEU:O     | 1:A:93:THR:CB    | 0.44     | 2.66        | 11     | 1     |
| 1:A:25:LEU:O     | 1:A:26:VAL:CG1   | 0.44     | 2.66        | 10     | 1     |
| 1:A:6:ASN:HB3    | 1:A:9:LEU:CB     | 0.43     | 2.43        | 10     | 6     |
| 1:A:99:HIS:N     | 1:A:129:PRO:CB   | 0.43     | 2.81        | 15     | 2     |
| 1:A:74:PHE:CB    | 1:A:88:ASP:OD1   | 0.43     | 2.66        | 6      | 1     |
| 1:A:125:GLU:HB3  | 1:A:166:TRP:CE2  | 0.43     | 2.48        | 4      | 1     |
| 1:A:66:PRO:HB2   | 1:A:78:ALA:O     | 0.43     | 2.13        | 10     | 2     |
| 1:A:104:TYR:CE2  | 1:A:135:LEU:HB3  | 0.43     | 2.48        | 10     | 1     |
| 1:A:125:GLU:OE1  | 1:A:200:ARG:CG   | 0.43     | 2.65        | 12     | 1     |
| 1:A:23:ARG:HG3   | 1:A:97:ILE:O     | 0.43     | 2.14        | 19     | 5     |
| 1:A:94:ALA:O     | 1:A:98:GLY:CA    | 0.43     | 2.65        | 16     | 2     |
| 1:A:148:GLY:O    | 1:A:150:PRO:HD3  | 0.43     | 2.13        | 18     | 3     |
| 1:A:140:GLU:CG   | 1:A:192:ASP:HB2  | 0.43     | 2.43        | 5      | 1     |
| 1:A:89:PHE:O     | 1:A:90:PHE:HB2   | 0.43     | 2.12        | 8      | 1     |
| 1:A:146:LEU:HG   | 1:A:188:LEU:HD11 | 0.43     | 1.90        | 18     | 1     |
| 1:A:74:PHE:CD1   | 1:A:87:GLY:C     | 0.43     | 2.91        | 20     | 1     |
| 1:A:168:VAL:CG1  | 1:A:196:TYR:OH   | 0.43     | 2.60        | 20     | 1     |
| 1:A:142:ASP:O    | 1:A:150:PRO:HG2  | 0.43     | 2.14        | 13     | 1     |
| 1:A:146:LEU:CD2  | 1:A:191:MET:CE   | 0.43     | 2.96        | 11     | 1     |
| 1:A:59:PHE:N     | 1:A:59:PHE:HD1   | 0.43     | 2.11        | 12     | 2     |
| 1:A:28:LEU:CD1   | 1:A:50:LEU:HD23  | 0.43     | 2.40        | 12     | 1     |
| 1:A:109:MET:HB2  | 1:A:117:ARG:CD   | 0.43     | 2.43        | 16     | 2     |
| 1:A:131:ALA:C    | 1:A:132:CYS:SG   | 0.43     | 2.96        | 3      | 3     |
| 1:A:181:ALA:C    | 1:A:183:GLY:N    | 0.43     | 2.71        | 19     | 7     |
| 1:A:73:ASP:C     | 1:A:74:PHE:CG    | 0.43     | 2.92        | 14     | 1     |
| 1:A:142:ASP:OD2  | 1:A:150:PRO:HG3  | 0.43     | 2.12        | 18     | 1     |
| 1:A:177:LEU:HD22 | 1:A:189:GLU:CA   | 0.43     | 2.43        | 4      | 2     |
| 1:A:82:ILE:HD13  | 1:A:84:ILE:N     | 0.43     | 2.28        | 17     | 1     |
| 1:A:190:ARG:C    | 1:A:191:MET:HG2  | 0.43     | 2.34        | 20     | 1     |
| 1:A:189:GLU:O    | 1:A:189:GLU:CD   | 0.43     | 2.57        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:49:GLU:OE1   | 1:A:51:SER:N     | 0.43     | 2.51        | 2      | 1     |
| 1:A:139:LEU:HD22 | 1:A:146:LEU:CD2  | 0.43     | 2.43        | 16     | 1     |
| 1:A:92:LEU:C     | 1:A:92:LEU:CD2   | 0.43     | 2.86        | 13     | 2     |
| 1:A:34:ASP:OD2   | 1:A:38:LEU:HD11  | 0.43     | 2.14        | 14     | 1     |
| 1:A:79:ALA:HB1   | 1:A:80:PRO:HD2   | 0.43     | 1.90        | 6      | 1     |
| 1:A:6:ASN:HD21   | 1:A:137:ILE:HD12 | 0.43     | 1.74        | 9      | 1     |
| 1:A:119:ARG:HD3  | 1:A:123:HIS:CE1  | 0.43     | 2.48        | 7      | 1     |
| 1:A:29:CYS:SG    | 1:A:105:ASP:CA   | 0.43     | 3.06        | 20     | 1     |
| 1:A:13:TRP:HZ3   | 1:A:104:TYR:CE1  | 0.43     | 2.31        | 10     | 1     |
| 1:A:139:LEU:HD22 | 1:A:146:LEU:HD23 | 0.43     | 1.89        | 16     | 1     |
| 1:A:26:VAL:CG2   | 1:A:29:CYS:HB3   | 0.43     | 2.42        | 17     | 4     |
| 1:A:73:ASP:O     | 1:A:74:PHE:CG    | 0.43     | 2.71        | 14     | 1     |
| 1:A:140:GLU:CG   | 1:A:194:HIS:HB2  | 0.43     | 2.44        | 14     | 1     |
| 1:A:17:ASN:CG    | 1:A:17:ASN:O     | 0.43     | 2.57        | 9      | 2     |
| 1:A:102:ALA:N    | 1:A:132:CYS:HB3  | 0.43     | 2.27        | 4      | 3     |
| 1:A:121:VAL:O    | 1:A:166:TRP:CH2  | 0.43     | 2.71        | 8      | 1     |
| 1:A:98:GLY:C     | 1:A:99:HIS:CD2   | 0.43     | 2.91        | 18     | 1     |
| 1:A:151:PHE:O    | 1:A:153:VAL:N    | 0.43     | 2.51        | 18     | 1     |
| 1:A:28:LEU:O     | 1:A:106:ARG:CZ   | 0.43     | 2.67        | 10     | 1     |
| 1:A:46:VAL:HG11  | 1:A:97:ILE:HD11  | 0.43     | 1.89        | 16     | 1     |
| 1:A:28:LEU:CG    | 1:A:50:LEU:HG    | 0.43     | 2.44        | 8      | 2     |
| 1:A:90:PHE:O     | 1:A:91:ALA:HB2   | 0.43     | 2.12        | 8      | 2     |
| 1:A:139:LEU:N    | 1:A:139:LEU:HD13 | 0.43     | 2.28        | 3      | 1     |
| 1:A:117:ARG:HH22 | 1:A:158:LEU:HD11 | 0.43     | 1.72        | 19     | 1     |
| 1:A:18:VAL:HG13  | 1:A:43:TYR:HE2   | 0.43     | 1.73        | 19     | 1     |
| 1:A:94:ALA:N     | 1:A:127:LEU:HD13 | 0.43     | 2.27        | 4      | 1     |
| 1:A:112:LEU:HB2  | 1:A:117:ARG:CZ   | 0.43     | 2.42        | 13     | 1     |
| 1:A:32:SER:HB3   | 1:A:181:ALA:CB   | 0.43     | 2.44        | 15     | 1     |
| 1:A:9:LEU:HD22   | 1:A:104:TYR:CE2  | 0.43     | 2.47        | 10     | 1     |
| 1:A:59:PHE:CE1   | 1:A:68:ILE:HD12  | 0.43     | 2.49        | 1      | 1     |
| 1:A:88:ASP:CG    | 1:A:89:PHE:N     | 0.43     | 2.72        | 1      | 3     |
| 1:A:34:ASP:OD1   | 1:A:104:TYR:CD2  | 0.43     | 2.71        | 14     | 1     |
| 1:A:136:LEU:HD12 | 1:A:198:LEU:HD21 | 0.43     | 1.90        | 17     | 2     |
| 1:A:25:LEU:HD23  | 1:A:128:MET:CE   | 0.43     | 2.44        | 10     | 1     |
| 1:A:109:MET:HB2  | 1:A:117:ARG:NE   | 0.43     | 2.28        | 16     | 1     |
| 1:A:25:LEU:HD23  | 1:A:97:ILE:CD1   | 0.43     | 2.44        | 5      | 1     |
| 1:A:6:ASN:CB     | 1:A:9:LEU:HB3    | 0.43     | 2.43        | 10     | 3     |
| 1:A:109:MET:HA   | 1:A:112:LEU:CG   | 0.43     | 2.44        | 14     | 1     |
| 1:A:189:GLU:O    | 1:A:190:ARG:HB2  | 0.43     | 2.12        | 6      | 3     |
| 1:A:34:ASP:OD1   | 1:A:34:ASP:N     | 0.43     | 2.52        | 6      | 1     |
| 1:A:6:ASN:O      | 1:A:7:LYS:C      | 0.43     | 2.57        | 6      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:142:ASP:HB3  | 1:A:188:LEU:HD21 | 0.43     | 1.90        | 18     | 1     |
| 1:A:92:LEU:O     | 1:A:93:THR:C     | 0.43     | 2.56        | 19     | 1     |
| 1:A:82:ILE:HD12  | 1:A:84:ILE:CB    | 0.43     | 2.34        | 9      | 1     |
| 1:A:177:LEU:HD11 | 1:A:184:LEU:HD13 | 0.43     | 1.90        | 9      | 1     |
| 1:A:136:LEU:HD22 | 1:A:136:LEU:C    | 0.43     | 2.30        | 20     | 1     |
| 1:A:92:LEU:HD21  | 1:A:97:ILE:CD1   | 0.43     | 2.44        | 20     | 1     |
| 1:A:189:GLU:O    | 1:A:189:GLU:CG   | 0.43     | 2.66        | 2      | 1     |
| 1:A:74:PHE:CE2   | 1:A:88:ASP:CG    | 0.43     | 2.92        | 2      | 1     |
| 1:A:55:VAL:CG2   | 1:A:59:PHE:CZ    | 0.43     | 3.00        | 13     | 1     |
| 1:A:99:HIS:N     | 1:A:129:PRO:CG   | 0.43     | 2.82        | 15     | 1     |
| 1:A:104:TYR:CD1  | 1:A:135:LEU:HB3  | 0.43     | 2.48        | 10     | 1     |
| 1:A:158:LEU:CD2  | 1:A:162:MET:HE1  | 0.43     | 2.44        | 10     | 1     |
| 1:A:120:TYR:CD1  | 1:A:120:TYR:C    | 0.43     | 2.92        | 3      | 1     |
| 1:A:28:LEU:O     | 1:A:106:ARG:NE   | 0.43     | 2.51        | 8      | 1     |
| 1:A:141:TYR:O    | 1:A:143:GLN:CD   | 0.43     | 2.56        | 8      | 1     |
| 1:A:137:ILE:HG23 | 1:A:193:GLU:OE2  | 0.43     | 2.13        | 6      | 1     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:HG13  | 0.43     | 1.91        | 6      | 1     |
| 1:A:88:ASP:OD1   | 1:A:89:PHE:N     | 0.43     | 2.51        | 18     | 1     |
| 1:A:33:GLN:HE22  | 1:A:181:ALA:HB2  | 0.43     | 1.74        | 16     | 1     |
| 1:A:49:GLU:CB    | 1:A:86:CYS:HA    | 0.43     | 2.44        | 14     | 1     |
| 1:A:18:VAL:CG1   | 1:A:22:ALA:HB3   | 0.43     | 2.44        | 18     | 2     |
| 1:A:34:ASP:OD2   | 1:A:35:MET:SD    | 0.43     | 2.77        | 19     | 1     |
| 1:A:28:LEU:CD2   | 1:A:50:LEU:HB2   | 0.43     | 2.44        | 20     | 1     |
| 1:A:6:ASN:OD1    | 1:A:179:SER:O    | 0.43     | 2.37        | 15     | 1     |
| 1:A:172:GLY:CA   | 1:A:195:VAL:HG13 | 0.43     | 2.44        | 12     | 1     |
| 1:A:121:VAL:HB   | 1:A:162:MET:CG   | 0.42     | 2.44        | 20     | 5     |
| 1:A:31:LYS:O     | 1:A:32:SER:CB    | 0.42     | 2.66        | 1      | 1     |
| 1:A:68:ILE:CG2   | 1:A:75:LYS:HE2   | 0.42     | 2.44        | 16     | 1     |
| 1:A:155:GLN:CB   | 1:A:196:TYR:CE2  | 0.42     | 3.02        | 3      | 1     |
| 1:A:28:LEU:O     | 1:A:28:LEU:CD2   | 0.42     | 2.67        | 14     | 1     |
| 1:A:146:LEU:CG   | 1:A:188:LEU:HD21 | 0.42     | 2.38        | 6      | 4     |
| 1:A:103:PHE:HB3  | 1:A:200:ARG:NH2  | 0.42     | 2.29        | 6      | 1     |
| 1:A:112:LEU:H    | 1:A:112:LEU:HD12 | 0.42     | 1.74        | 19     | 1     |
| 1:A:59:PHE:HD1   | 1:A:59:PHE:N     | 0.42     | 2.12        | 4      | 2     |
| 1:A:125:GLU:HB3  | 1:A:166:TRP:CH2  | 0.42     | 2.49        | 4      | 1     |
| 1:A:109:MET:CB   | 1:A:117:ARG:HD3  | 0.42     | 2.44        | 13     | 1     |
| 1:A:25:LEU:O     | 1:A:103:PHE:CB   | 0.42     | 2.67        | 12     | 1     |
| 1:A:94:ALA:HA    | 1:A:97:ILE:CG1   | 0.42     | 2.44        | 6      | 1     |
| 1:A:113:PRO:HD2  | 1:A:116:MET:HB2  | 0.42     | 1.91        | 19     | 1     |
| 1:A:139:LEU:CD1  | 1:A:142:ASP:OD2  | 0.42     | 2.64        | 19     | 1     |
| 1:A:124:LEU:O    | 1:A:128:MET:SD   | 0.42     | 2.76        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:71:GLN:O     | 1:A:71:GLN:OE1   | 0.42     | 2.37        | 12     | 2     |
| 1:A:109:MET:HA   | 1:A:117:ARG:NH1  | 0.42     | 2.28        | 13     | 1     |
| 1:A:117:ARG:CB   | 1:A:157:TRP:CH2  | 0.42     | 3.02        | 15     | 1     |
| 1:A:124:LEU:HD13 | 1:A:128:MET:HG2  | 0.42     | 1.91        | 13     | 2     |
| 1:A:154:PRO:C    | 1:A:156:THR:N    | 0.42     | 2.73        | 16     | 2     |
| 1:A:34:ASP:OD1   | 1:A:35:MET:N     | 0.42     | 2.48        | 3      | 1     |
| 1:A:170:LYS:C    | 1:A:171:VAL:HG23 | 0.42     | 2.35        | 6      | 1     |
| 1:A:124:LEU:CD2  | 1:A:128:MET:CE   | 0.42     | 2.97        | 19     | 1     |
| 1:A:68:ILE:HD13  | 1:A:77:TYR:HA    | 0.42     | 1.89        | 17     | 1     |
| 1:A:117:ARG:NE   | 1:A:117:ARG:CA   | 0.42     | 2.81        | 13     | 1     |
| 1:A:107:ALA:HB2  | 1:A:137:ILE:O    | 0.42     | 2.14        | 1      | 1     |
| 1:A:21:GLY:O     | 1:A:22:ALA:O     | 0.42     | 2.35        | 16     | 2     |
| 1:A:177:LEU:C    | 1:A:177:LEU:CD1  | 0.42     | 2.88        | 14     | 1     |
| 1:A:139:LEU:CD2  | 1:A:191:MET:SD   | 0.42     | 3.08        | 18     | 1     |
| 1:A:97:ILE:HG13  | 1:A:98:GLY:N     | 0.42     | 2.29        | 15     | 2     |
| 1:A:141:TYR:CG   | 1:A:191:MET:HA   | 0.42     | 2.49        | 9      | 2     |
| 1:A:92:LEU:CD2   | 1:A:97:ILE:HG12  | 0.42     | 2.44        | 7      | 1     |
| 1:A:110:ILE:CG1  | 1:A:150:PRO:HB3  | 0.42     | 2.44        | 7      | 2     |
| 1:A:5:VAL:HG23   | 1:A:34:ASP:HA    | 0.42     | 1.90        | 4      | 1     |
| 1:A:75:LYS:O     | 1:A:88:ASP:OD1   | 0.42     | 2.38        | 13     | 1     |
| 1:A:8:ASP:OD1    | 1:A:171:VAL:CG2  | 0.42     | 2.67        | 10     | 1     |
| 1:A:160:ARG:HG3  | 1:A:161:VAL:HG12 | 0.42     | 1.92        | 1      | 2     |
| 1:A:114:ALA:O    | 1:A:115:ASP:C    | 0.42     | 2.58        | 14     | 17    |
| 1:A:112:LEU:N    | 1:A:112:LEU:HD23 | 0.42     | 2.30        | 1      | 1     |
| 1:A:109:MET:HB3  | 1:A:117:ARG:CD   | 0.42     | 2.44        | 5      | 1     |
| 1:A:28:LEU:CA    | 1:A:48:ALA:O     | 0.42     | 2.68        | 19     | 1     |
| 1:A:77:TYR:HB3   | 1:A:86:CYS:HB3   | 0.42     | 1.91        | 9      | 1     |
| 1:A:58:TYR:CE2   | 1:A:77:TYR:CE1   | 0.42     | 3.08        | 7      | 1     |
| 1:A:6:ASN:C      | 1:A:8:ASP:N      | 0.42     | 2.72        | 15     | 1     |
| 1:A:166:TRP:HA   | 1:A:199:GLU:O    | 0.42     | 2.15        | 16     | 3     |
| 1:A:155:GLN:HG3  | 1:A:196:TYR:CD2  | 0.42     | 2.50        | 3      | 1     |
| 1:A:106:ARG:CZ   | 1:A:182:ARG:HG3  | 0.42     | 2.45        | 3      | 1     |
| 1:A:141:TYR:O    | 1:A:143:GLN:HG2  | 0.42     | 2.15        | 7      | 2     |
| 1:A:28:LEU:HD12  | 1:A:89:PHE:CD2   | 0.42     | 2.50        | 6      | 1     |
| 1:A:23:ARG:HB3   | 1:A:97:ILE:O     | 0.42     | 2.12        | 7      | 3     |
| 1:A:142:ASP:O    | 1:A:150:PRO:HD2  | 0.42     | 2.15        | 4      | 1     |
| 1:A:105:ASP:OD1  | 1:A:135:LEU:C    | 0.42     | 2.57        | 2      | 1     |
| 1:A:184:LEU:N    | 1:A:184:LEU:CD2  | 0.42     | 2.82        | 2      | 1     |
| 1:A:158:LEU:HD21 | 1:A:162:MET:SD   | 0.42     | 2.54        | 1      | 1     |
| 1:A:157:TRP:C    | 1:A:157:TRP:CE3  | 0.42     | 2.93        | 16     | 1     |
| 1:A:32:SER:O     | 1:A:36:SER:OG    | 0.42     | 2.37        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:189:GLU:O    | 1:A:189:GLU:OE2  | 0.42     | 2.38        | 4      | 1     |
| 1:A:125:GLU:OE1  | 1:A:125:GLU:C    | 0.42     | 2.58        | 15     | 2     |
| 1:A:162:MET:HG2  | 1:A:166:TRP:CE2  | 0.42     | 2.50        | 12     | 1     |
| 1:A:24:VAL:HA    | 1:A:102:ALA:O    | 0.42     | 2.14        | 8      | 4     |
| 1:A:142:ASP:CB   | 1:A:146:LEU:CD1  | 0.42     | 2.98        | 1      | 1     |
| 1:A:158:LEU:HB3  | 1:A:196:TYR:CE2  | 0.42     | 2.49        | 16     | 1     |
| 1:A:95:ARG:CA    | 1:A:127:LEU:O    | 0.42     | 2.68        | 3      | 1     |
| 1:A:195:VAL:HG12 | 1:A:196:TYR:N    | 0.42     | 2.30        | 5      | 1     |
| 1:A:110:ILE:HD13 | 1:A:110:ILE:N    | 0.42     | 2.30        | 10     | 2     |
| 1:A:6:ASN:OD1    | 1:A:104:TYR:OH   | 0.42     | 2.38        | 14     | 1     |
| 1:A:102:ALA:CA   | 1:A:132:CYS:HB3  | 0.42     | 2.44        | 8      | 2     |
| 1:A:112:LEU:HB2  | 1:A:117:ARG:CD   | 0.42     | 2.44        | 9      | 1     |
| 1:A:155:GLN:CB   | 1:A:196:TYR:CZ   | 0.42     | 3.02        | 4      | 1     |
| 1:A:188:LEU:H    | 1:A:188:LEU:HD12 | 0.42     | 1.75        | 20     | 1     |
| 1:A:6:ASN:CB     | 1:A:9:LEU:CB     | 0.42     | 2.98        | 10     | 1     |
| 1:A:7:LYS:CE     | 1:A:173:GLY:HA3  | 0.42     | 2.45        | 14     | 1     |
| 1:A:196:TYR:HH   | 1:A:198:LEU:HD13 | 0.42     | 1.67        | 18     | 1     |
| 1:A:30:GLY:HA2   | 1:A:84:ILE:CD1   | 0.42     | 2.45        | 7      | 1     |
| 1:A:37:TRP:CE3   | 1:A:37:TRP:C     | 0.42     | 2.93        | 17     | 1     |
| 1:A:90:PHE:CD1   | 1:A:91:ALA:N     | 0.42     | 2.88        | 17     | 1     |
| 1:A:69:THR:HG23  | 1:A:71:GLN:OE1   | 0.42     | 2.13        | 17     | 1     |
| 1:A:136:LEU:CD1  | 1:A:162:MET:CE   | 0.42     | 2.98        | 11     | 1     |
| 1:A:169:THR:N    | 1:A:196:TYR:CE1  | 0.42     | 2.88        | 15     | 1     |
| 1:A:6:ASN:HB2    | 1:A:9:LEU:CB     | 0.42     | 2.44        | 20     | 2     |
| 1:A:95:ARG:HB2   | 1:A:127:LEU:O    | 0.42     | 2.15        | 3      | 2     |
| 1:A:169:THR:C    | 1:A:196:TYR:CE1  | 0.42     | 2.93        | 3      | 1     |
| 1:A:26:VAL:O     | 1:A:47:GLY:HA3   | 0.42     | 2.15        | 14     | 1     |
| 1:A:140:GLU:OE2  | 1:A:194:HIS:CG   | 0.42     | 2.73        | 14     | 1     |
| 1:A:200:ARG:O    | 1:A:200:ARG:HG3  | 0.42     | 2.14        | 8      | 1     |
| 1:A:124:LEU:CD2  | 1:A:128:MET:HG2  | 0.42     | 2.44        | 19     | 1     |
| 1:A:64:GLU:O     | 1:A:66:PRO:CD    | 0.42     | 2.68        | 17     | 1     |
| 1:A:16:LEU:O     | 1:A:17:ASN:HB3   | 0.41     | 2.15        | 13     | 3     |
| 1:A:22:ALA:HB1   | 1:A:101:ALA:HB1  | 0.41     | 1.86        | 5      | 1     |
| 1:A:84:ILE:CG2   | 1:A:84:ILE:O     | 0.41     | 2.68        | 6      | 2     |
| 1:A:12:TYR:CZ    | 1:A:197:VAL:HB   | 0.41     | 2.49        | 14     | 1     |
| 1:A:66:PRO:HB2   | 1:A:77:TYR:CD1   | 0.41     | 2.50        | 14     | 1     |
| 1:A:101:ALA:C    | 1:A:132:CYS:HB3  | 0.41     | 2.34        | 6      | 1     |
| 1:A:177:LEU:HD21 | 1:A:190:ARG:N    | 0.41     | 2.28        | 19     | 1     |
| 1:A:27:PRO:HD3   | 1:A:103:PHE:CD1  | 0.41     | 2.50        | 9      | 1     |
| 1:A:177:LEU:HD23 | 1:A:177:LEU:C    | 0.41     | 2.35        | 7      | 1     |
| 1:A:63:GLY:C     | 1:A:64:GLU:CG    | 0.41     | 2.87        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:128:MET:HG3  | 1:A:129:PRO:HD2  | 0.41     | 1.90        | 4      | 1     |
| 1:A:94:ALA:CA    | 1:A:97:ILE:HG23  | 0.41     | 2.43        | 4      | 1     |
| 1:A:99:HIS:HA    | 1:A:129:PRO:CB   | 0.41     | 2.45        | 15     | 1     |
| 1:A:16:LEU:O     | 1:A:17:ASN:C     | 0.41     | 2.58        | 15     | 1     |
| 1:A:155:GLN:HB2  | 1:A:196:TYR:CD1  | 0.41     | 2.50        | 12     | 1     |
| 1:A:109:MET:HB3  | 1:A:117:ARG:NH1  | 0.41     | 2.30        | 16     | 1     |
| 1:A:131:ALA:O    | 1:A:132:CYS:SG   | 0.41     | 2.78        | 8      | 4     |
| 1:A:110:ILE:HD12 | 1:A:110:ILE:C    | 0.41     | 2.35        | 14     | 1     |
| 1:A:116:MET:HE2  | 1:A:119:ARG:HG2  | 0.41     | 1.92        | 19     | 1     |
| 1:A:125:GLU:HG3  | 1:A:166:TRP:CZ3  | 0.41     | 2.50        | 19     | 1     |
| 1:A:50:LEU:CD2   | 1:A:89:PHE:N     | 0.41     | 2.83        | 7      | 1     |
| 1:A:57:ARG:O     | 1:A:57:ARG:HG2   | 0.41     | 2.15        | 17     | 1     |
| 1:A:196:TYR:CD1  | 1:A:196:TYR:O    | 0.41     | 2.73        | 20     | 1     |
| 1:A:26:VAL:HG21  | 1:A:29:CYS:SG    | 0.41     | 2.55        | 11     | 1     |
| 1:A:140:GLU:OE1  | 1:A:140:GLU:C    | 0.41     | 2.58        | 12     | 1     |
| 1:A:135:LEU:HG   | 1:A:137:ILE:HD11 | 0.41     | 1.91        | 14     | 1     |
| 1:A:26:VAL:CG2   | 1:A:35:MET:CE    | 0.41     | 2.98        | 14     | 1     |
| 1:A:46:VAL:HA    | 1:A:83:GLU:CB    | 0.41     | 2.46        | 8      | 1     |
| 1:A:110:ILE:CG2  | 1:A:138:THR:HG22 | 0.41     | 2.45        | 19     | 1     |
| 1:A:138:THR:O    | 1:A:194:HIS:O    | 0.41     | 2.38        | 19     | 2     |
| 1:A:177:LEU:HD12 | 1:A:177:LEU:C    | 0.41     | 2.36        | 19     | 1     |
| 1:A:189:GLU:HG2  | 1:A:189:GLU:O    | 0.41     | 2.14        | 19     | 1     |
| 1:A:51:SER:HB2   | 1:A:54:ALA:CB    | 0.41     | 2.45        | 19     | 1     |
| 1:A:125:GLU:CD   | 1:A:165:ASN:ND2  | 0.41     | 2.73        | 4      | 1     |
| 1:A:93:THR:C     | 1:A:95:ARG:H     | 0.41     | 2.18        | 4      | 1     |
| 1:A:110:ILE:CD1  | 1:A:150:PRO:HB3  | 0.41     | 2.46        | 17     | 1     |
| 1:A:103:PHE:CE1  | 1:A:200:ARG:HB2  | 0.41     | 2.50        | 12     | 1     |
| 1:A:158:LEU:HG   | 1:A:162:MET:SD   | 0.41     | 2.55        | 1      | 3     |
| 1:A:110:ILE:CD1  | 1:A:110:ILE:N    | 0.41     | 2.84        | 5      | 1     |
| 1:A:12:TYR:HB3   | 1:A:16:LEU:HD12  | 0.41     | 1.92        | 14     | 1     |
| 1:A:109:MET:O    | 1:A:112:LEU:O    | 0.41     | 2.38        | 18     | 1     |
| 1:A:48:ALA:HB2   | 1:A:85:TRP:CH2   | 0.41     | 2.50        | 9      | 1     |
| 1:A:188:LEU:O    | 1:A:189:GLU:CB   | 0.41     | 2.67        | 13     | 1     |
| 1:A:104:TYR:HH   | 1:A:137:ILE:HG13 | 0.41     | 1.75        | 15     | 1     |
| 1:A:169:THR:HB   | 1:A:197:VAL:HG12 | 0.41     | 1.92        | 1      | 1     |
| 1:A:164:GLY:C    | 1:A:165:ASN:ND2  | 0.41     | 2.74        | 3      | 1     |
| 1:A:169:THR:N    | 1:A:196:TYR:CD1  | 0.41     | 2.89        | 3      | 1     |
| 1:A:52:GLU:O     | 1:A:56:GLU:OE2   | 0.41     | 2.38        | 14     | 1     |
| 1:A:28:LEU:CD1   | 1:A:89:PHE:CD2   | 0.41     | 3.03        | 6      | 1     |
| 1:A:106:ARG:HG2  | 1:A:106:ARG:NH1  | 0.41     | 2.30        | 4      | 1     |
| 1:A:6:ASN:CG     | 1:A:179:SER:OG   | 0.41     | 2.59        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:121:VAL:CB   | 1:A:162:MET:HG2  | 0.41     | 2.45        | 20     | 1     |
| 1:A:190:ARG:O    | 1:A:191:MET:HE2  | 0.41     | 2.15        | 20     | 1     |
| 1:A:117:ARG:NH2  | 1:A:151:PHE:CD2  | 0.41     | 2.88        | 2      | 1     |
| 1:A:157:TRP:CD2  | 1:A:161:VAL:CG1  | 0.41     | 3.03        | 13     | 1     |
| 1:A:125:GLU:OE1  | 1:A:200:ARG:NH1  | 0.41     | 2.53        | 12     | 2     |
| 1:A:103:PHE:O    | 1:A:134:GLY:CA   | 0.41     | 2.66        | 10     | 1     |
| 1:A:23:ARG:NH1   | 1:A:44:HIS:CD2   | 0.41     | 2.89        | 12     | 1     |
| 1:A:13:TRP:CH2   | 1:A:38:LEU:HD11  | 0.41     | 2.51        | 1      | 1     |
| 1:A:177:LEU:HD22 | 1:A:191:MET:SD   | 0.41     | 2.55        | 14     | 1     |
| 1:A:144:ALA:C    | 1:A:145:LEU:HD12 | 0.41     | 2.36        | 19     | 2     |
| 1:A:138:THR:C    | 1:A:139:LEU:CD2  | 0.41     | 2.81        | 19     | 1     |
| 1:A:12:TYR:O     | 1:A:15:SER:N     | 0.41     | 2.54        | 20     | 1     |
| 1:A:71:GLN:O     | 1:A:74:PHE:HB2   | 0.41     | 2.16        | 20     | 1     |
| 1:A:23:ARG:HB2   | 1:A:98:GLY:O     | 0.41     | 2.16        | 2      | 1     |
| 1:A:99:HIS:CA    | 1:A:129:PRO:HB3  | 0.41     | 2.46        | 15     | 1     |
| 1:A:28:LEU:HD12  | 1:A:89:PHE:HB3   | 0.41     | 1.91        | 12     | 1     |
| 1:A:68:ILE:CG2   | 1:A:75:LYS:HD3   | 0.41     | 2.46        | 14     | 1     |
| 1:A:50:LEU:HD23  | 1:A:89:PHE:HB3   | 0.41     | 1.93        | 6      | 2     |
| 1:A:139:LEU:HB2  | 1:A:142:ASP:OD2  | 0.41     | 2.15        | 2      | 1     |
| 1:A:167:GLU:O    | 1:A:197:VAL:O    | 0.41     | 2.39        | 11     | 1     |
| 1:A:93:THR:HG22  | 1:A:95:ARG:CD    | 0.41     | 2.45        | 1      | 1     |
| 1:A:174:GLN:HA   | 1:A:192:ASP:HA   | 0.41     | 1.93        | 16     | 1     |
| 1:A:92:LEU:HD23  | 1:A:97:ILE:HD13  | 0.41     | 1.92        | 3      | 1     |
| 1:A:135:LEU:O    | 1:A:137:ILE:HD12 | 0.41     | 2.14        | 6      | 1     |
| 1:A:177:LEU:HD23 | 1:A:191:MET:HE2  | 0.41     | 1.91        | 18     | 1     |
| 1:A:25:LEU:HD23  | 1:A:94:ALA:HA    | 0.41     | 1.93        | 9      | 1     |
| 1:A:71:GLN:O     | 1:A:71:GLN:NE2   | 0.41     | 2.54        | 7      | 1     |
| 1:A:139:LEU:HB3  | 1:A:142:ASP:OD2  | 0.41     | 2.15        | 20     | 1     |
| 1:A:37:TRP:C     | 1:A:37:TRP:CE3   | 0.41     | 2.94        | 15     | 1     |
| 1:A:157:TRP:CE3  | 1:A:158:LEU:HG   | 0.41     | 2.51        | 10     | 1     |
| 1:A:113:PRO:O    | 1:A:117:ARG:HG2  | 0.41     | 2.16        | 16     | 1     |
| 1:A:29:CYS:HG    | 1:A:104:TYR:HD1  | 0.41     | 1.50        | 16     | 1     |
| 1:A:124:LEU:HD22 | 1:A:127:LEU:CD1  | 0.41     | 2.45        | 3      | 1     |
| 1:A:28:LEU:H     | 1:A:28:LEU:HD13  | 0.41     | 1.68        | 3      | 1     |
| 1:A:139:LEU:HD21 | 1:A:150:PRO:HG2  | 0.41     | 1.86        | 3      | 1     |
| 1:A:125:GLU:HB3  | 1:A:200:ARG:NH2  | 0.41     | 2.31        | 5      | 1     |
| 1:A:92:LEU:CD1   | 1:A:92:LEU:O     | 0.41     | 2.59        | 5      | 1     |
| 1:A:103:PHE:CD2  | 1:A:103:PHE:O    | 0.41     | 2.74        | 5      | 1     |
| 1:A:181:ALA:O    | 1:A:182:ARG:C    | 0.41     | 2.59        | 5      | 1     |
| 1:A:23:ARG:HG2   | 1:A:97:ILE:O     | 0.41     | 2.15        | 14     | 1     |
| 1:A:103:PHE:N    | 1:A:200:ARG:NH2  | 0.41     | 2.69        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:10:GLN:HG3   | 1:A:37:TRP:NE1   | 0.41     | 2.30        | 6      | 1     |
| 1:A:107:ALA:C    | 1:A:110:ILE:HD11 | 0.41     | 2.36        | 18     | 1     |
| 1:A:145:LEU:HD22 | 1:A:188:LEU:HG   | 0.41     | 1.93        | 19     | 1     |
| 1:A:140:GLU:CG   | 1:A:141:TYR:N    | 0.41     | 2.84        | 7      | 1     |
| 1:A:177:LEU:HD13 | 1:A:189:GLU:N    | 0.41     | 2.31        | 7      | 1     |
| 1:A:121:VAL:CG2  | 1:A:162:MET:HG2  | 0.41     | 2.45        | 20     | 2     |
| 1:A:105:ASP:HB3  | 1:A:136:LEU:HD23 | 0.41     | 1.93        | 20     | 1     |
| 1:A:85:TRP:CE3   | 1:A:88:ASP:O     | 0.41     | 2.74        | 20     | 1     |
| 1:A:49:GLU:OE1   | 1:A:51:SER:CB    | 0.41     | 2.69        | 2      | 1     |
| 1:A:94:ALA:CB    | 1:A:128:MET:HE1  | 0.41     | 2.38        | 15     | 1     |
| 1:A:27:PRO:HG2   | 1:A:105:ASP:OD2  | 0.41     | 2.16        | 10     | 1     |
| 1:A:171:VAL:HG13 | 1:A:196:TYR:HA   | 0.41     | 1.93        | 10     | 1     |
| 1:A:117:ARG:NH1  | 1:A:158:LEU:HD21 | 0.41     | 2.31        | 12     | 1     |
| 1:A:177:LEU:HD13 | 1:A:184:LEU:CD1  | 0.41     | 2.46        | 12     | 1     |
| 1:A:7:LYS:HD3    | 1:A:8:ASP:N      | 0.41     | 2.31        | 16     | 1     |
| 1:A:95:ARG:HG3   | 1:A:96:ASP:N     | 0.41     | 2.30        | 9      | 2     |
| 1:A:171:VAL:HG13 | 1:A:196:TYR:CA   | 0.41     | 2.46        | 5      | 1     |
| 1:A:158:LEU:CD2  | 1:A:168:VAL:HG11 | 0.41     | 2.43        | 19     | 1     |
| 1:A:110:ILE:O    | 1:A:150:PRO:HA   | 0.41     | 2.16        | 9      | 1     |
| 1:A:183:GLY:HA2  | 1:A:188:LEU:CD1  | 0.41     | 2.46        | 7      | 1     |
| 1:A:154:PRO:HB2  | 1:A:156:THR:CG2  | 0.41     | 2.45        | 7      | 1     |
| 1:A:173:GLY:C    | 1:A:193:GLU:O    | 0.41     | 2.59        | 4      | 1     |
| 1:A:124:LEU:C    | 1:A:128:MET:HG3  | 0.40     | 2.37        | 5      | 1     |
| 1:A:109:MET:HE2  | 1:A:158:LEU:HD11 | 0.40     | 1.91        | 5      | 1     |
| 1:A:153:VAL:CG1  | 1:A:153:VAL:O    | 0.40     | 2.68        | 14     | 1     |
| 1:A:55:VAL:CG2   | 1:A:86:CYS:SG    | 0.40     | 3.08        | 14     | 1     |
| 1:A:144:ALA:O    | 1:A:145:LEU:CB   | 0.40     | 2.69        | 19     | 1     |
| 1:A:26:VAL:HB    | 1:A:47:GLY:HA3   | 0.40     | 1.93        | 9      | 1     |
| 1:A:66:PRO:O     | 1:A:68:ILE:N     | 0.40     | 2.54        | 17     | 1     |
| 1:A:175:ASP:N    | 1:A:191:MET:O    | 0.40     | 2.55        | 20     | 1     |
| 1:A:175:ASP:HA   | 1:A:192:ASP:HA   | 0.40     | 1.93        | 13     | 1     |
| 1:A:101:ALA:C    | 1:A:132:CYS:HA   | 0.40     | 2.36        | 15     | 1     |
| 1:A:162:MET:CB   | 1:A:168:VAL:HG11 | 0.40     | 2.46        | 10     | 1     |
| 1:A:71:GLN:O     | 1:A:71:GLN:CD    | 0.40     | 2.59        | 12     | 1     |
| 1:A:120:TYR:C    | 1:A:120:TYR:CD1  | 0.40     | 2.95        | 1      | 1     |
| 1:A:157:TRP:CZ3  | 1:A:158:LEU:HD12 | 0.40     | 2.51        | 1      | 1     |
| 1:A:78:ALA:HA    | 1:A:84:ILE:O     | 0.40     | 2.15        | 3      | 1     |
| 1:A:109:MET:HA   | 1:A:112:LEU:HG   | 0.40     | 1.93        | 14     | 1     |
| 1:A:82:ILE:CD1   | 1:A:83:GLU:N     | 0.40     | 2.82        | 8      | 1     |
| 1:A:196:TYR:O    | 1:A:196:TYR:CD2  | 0.40     | 2.73        | 18     | 1     |
| 1:A:119:ARG:HG3  | 1:A:120:TYR:N    | 0.40     | 2.31        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:141:TYR:O    | 1:A:143:GLN:OE1  | 0.40     | 2.39        | 11     | 1     |
| 1:A:188:LEU:O    | 1:A:190:ARG:HG3  | 0.40     | 2.16        | 11     | 1     |
| 1:A:109:MET:HA   | 1:A:112:LEU:HD21 | 0.40     | 1.92        | 12     | 1     |
| 1:A:30:GLY:C     | 1:A:49:GLU:OE2   | 0.40     | 2.59        | 1      | 1     |
| 1:A:35:MET:HG3   | 1:A:36:SER:N     | 0.40     | 2.31        | 6      | 2     |
| 1:A:5:VAL:HG11   | 1:A:37:TRP:CD1   | 0.40     | 2.51        | 19     | 2     |
| 1:A:27:PRO:HG3   | 1:A:103:PHE:CE1  | 0.40     | 2.51        | 9      | 1     |
| 1:A:128:MET:HG3  | 1:A:129:PRO:CD   | 0.40     | 2.46        | 4      | 1     |
| 1:A:98:GLY:HA3   | 1:A:129:PRO:HG3  | 0.40     | 1.92        | 15     | 1     |
| 1:A:66:PRO:CB    | 1:A:78:ALA:O     | 0.40     | 2.69        | 10     | 1     |
| 1:A:45:VAL:O     | 1:A:83:GLU:HB2   | 0.40     | 2.16        | 10     | 1     |
| 1:A:64:GLU:O     | 1:A:65:GLN:HB2   | 0.40     | 2.16        | 12     | 1     |
| 1:A:112:LEU:CB   | 1:A:113:PRO:CD   | 0.40     | 3.00        | 1      | 1     |
| 1:A:130:GLN:HG3  | 1:A:131:ALA:N    | 0.40     | 2.30        | 5      | 1     |
| 1:A:27:PRO:O     | 1:A:48:ALA:HB3   | 0.40     | 2.15        | 5      | 1     |
| 1:A:110:ILE:O    | 1:A:151:PHE:HB2  | 0.40     | 2.16        | 14     | 1     |
| 1:A:16:LEU:CD2   | 1:A:133:SER:CB   | 0.40     | 3.00        | 6      | 1     |
| 1:A:125:GLU:CD   | 1:A:166:TRP:NE1  | 0.40     | 2.74        | 19     | 1     |
| 1:A:4:GLU:O      | 1:A:33:GLN:CG    | 0.40     | 2.69        | 19     | 1     |
| 1:A:16:LEU:HD13  | 1:A:133:SER:OG   | 0.40     | 2.16        | 20     | 1     |
| 1:A:112:LEU:HB2  | 1:A:117:ARG:NH2  | 0.40     | 2.31        | 13     | 1     |
| 1:A:108:ALA:O    | 1:A:112:LEU:HD23 | 0.40     | 2.16        | 15     | 1     |
| 1:A:171:VAL:CG1  | 1:A:196:TYR:CA   | 0.40     | 2.98        | 15     | 1     |
| 1:A:7:LYS:CE     | 1:A:8:ASP:OD1    | 0.40     | 2.69        | 10     | 1     |
| 1:A:95:ARG:HB3   | 1:A:127:LEU:O    | 0.40     | 2.17        | 1      | 1     |
| 1:A:157:TRP:O    | 1:A:161:VAL:HG13 | 0.40     | 2.16        | 16     | 1     |
| 1:A:189:GLU:C    | 1:A:190:ARG:HG2  | 0.40     | 2.37        | 3      | 1     |
| 1:A:110:ILE:HG12 | 1:A:150:PRO:HA   | 0.40     | 1.93        | 18     | 1     |
| 1:A:197:VAL:CA   | 1:A:198:LEU:HD23 | 0.40     | 2.47        | 18     | 1     |
| 1:A:182:ARG:NH2  | 1:A:185:LYS:NZ   | 0.40     | 2.70        | 17     | 1     |
| 1:A:171:VAL:HG23 | 1:A:172:GLY:H    | 0.40     | 1.76        | 20     | 1     |
| 1:A:161:VAL:O    | 1:A:162:MET:C    | 0.40     | 2.60        | 13     | 1     |
| 1:A:30:GLY:HA2   | 1:A:49:GLU:CD    | 0.40     | 2.36        | 13     | 1     |
| 1:A:74:PHE:HB3   | 1:A:88:ASP:HB3   | 0.40     | 1.92        | 13     | 1     |
| 1:A:169:THR:O    | 1:A:169:THR:HG22 | 0.40     | 2.16        | 15     | 1     |
| 1:A:188:LEU:O    | 1:A:191:MET:HG2  | 0.40     | 2.16        | 15     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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     | 198/203 (98%)   | 140±4 (70±2%) | 39±4 (19±2%) | 20±2 (10±1%) | 1           | 10 |
| All | All   | 3960/4060 (98%) | 2791 (70%)    | 771 (19%)    | 398 (10%)    | 1           | 10 |

All 48 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 90  | PHE  | 20             |
| 1   | A     | 145 | LEU  | 20             |
| 1   | A     | 101 | ALA  | 20             |
| 1   | A     | 143 | GLN  | 20             |
| 1   | A     | 99  | HIS  | 19             |
| 1   | A     | 142 | ASP  | 19             |
| 1   | A     | 190 | ARG  | 19             |
| 1   | A     | 65  | GLN  | 18             |
| 1   | A     | 162 | MET  | 18             |
| 1   | A     | 6   | ASN  | 18             |
| 1   | A     | 141 | TYR  | 17             |
| 1   | A     | 165 | ASN  | 17             |
| 1   | A     | 164 | GLY  | 17             |
| 1   | A     | 28  | LEU  | 16             |
| 1   | A     | 22  | ALA  | 14             |
| 1   | A     | 107 | ALA  | 10             |
| 1   | A     | 91  | ALA  | 10             |
| 1   | A     | 129 | PRO  | 10             |
| 1   | A     | 3   | SER  | 9              |
| 1   | A     | 11  | GLN  | 8              |
| 1   | A     | 32  | SER  | 6              |
| 1   | A     | 152 | SER  | 6              |
| 1   | A     | 147 | GLU  | 6              |
| 1   | A     | 72  | GLY  | 6              |
| 1   | A     | 30  | GLY  | 5              |
| 1   | A     | 113 | PRO  | 5              |
| 1   | A     | 31  | LYS  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 93  | THR  | 4              |
| 1   | A     | 189 | GLU  | 4              |
| 1   | A     | 163 | SER  | 3              |
| 1   | A     | 50  | LEU  | 3              |
| 1   | A     | 66  | PRO  | 3              |
| 1   | A     | 130 | GLN  | 3              |
| 1   | A     | 148 | GLY  | 2              |
| 1   | A     | 18  | VAL  | 2              |
| 1   | A     | 179 | SER  | 2              |
| 1   | A     | 171 | VAL  | 2              |
| 1   | A     | 182 | ARG  | 2              |
| 1   | A     | 200 | ARG  | 2              |
| 1   | A     | 21  | GLY  | 1              |
| 1   | A     | 128 | MET  | 1              |
| 1   | A     | 94  | ALA  | 1              |
| 1   | A     | 174 | GLN  | 1              |
| 1   | A     | 155 | GLN  | 1              |
| 1   | A     | 67  | HIS  | 1              |
| 1   | A     | 27  | PRO  | 1              |
| 1   | A     | 73  | ASP  | 1              |
| 1   | A     | 98  | GLY  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 163/166 (98%)   | 97±4 (59±2%) | 66±4 (41±2%) | 0           | 4 |
| All | All   | 3260/3320 (98%) | 1933 (59%)   | 1327 (41%)   | 0           | 4 |

All 131 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 60  | THR  | 20             |
| 1   | A     | 124 | LEU  | 20             |
| 1   | A     | 28  | LEU  | 20             |
| 1   | A     | 198 | LEU  | 20             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 142 | ASP  | 20             |
| 1   | A     | 127 | LEU  | 20             |
| 1   | A     | 169 | THR  | 20             |
| 1   | A     | 82  | ILE  | 20             |
| 1   | A     | 69  | THR  | 20             |
| 1   | A     | 139 | LEU  | 20             |
| 1   | A     | 90  | PHE  | 20             |
| 1   | A     | 145 | LEU  | 20             |
| 1   | A     | 161 | VAL  | 20             |
| 1   | A     | 166 | TRP  | 20             |
| 1   | A     | 84  | ILE  | 20             |
| 1   | A     | 92  | LEU  | 20             |
| 1   | A     | 162 | MET  | 19             |
| 1   | A     | 7   | LYS  | 19             |
| 1   | A     | 83  | GLU  | 19             |
| 1   | A     | 97  | ILE  | 19             |
| 1   | A     | 85  | TRP  | 19             |
| 1   | A     | 49  | GLU  | 19             |
| 1   | A     | 200 | ARG  | 18             |
| 1   | A     | 133 | SER  | 18             |
| 1   | A     | 146 | LEU  | 18             |
| 1   | A     | 160 | ARG  | 18             |
| 1   | A     | 185 | LYS  | 17             |
| 1   | A     | 110 | ILE  | 17             |
| 1   | A     | 171 | VAL  | 16             |
| 1   | A     | 109 | MET  | 16             |
| 1   | A     | 136 | LEU  | 16             |
| 1   | A     | 106 | ARG  | 15             |
| 1   | A     | 32  | SER  | 15             |
| 1   | A     | 65  | GLN  | 15             |
| 1   | A     | 55  | VAL  | 15             |
| 1   | A     | 125 | GLU  | 15             |
| 1   | A     | 50  | LEU  | 14             |
| 1   | A     | 199 | GLU  | 14             |
| 1   | A     | 77  | TYR  | 14             |
| 1   | A     | 67  | HIS  | 14             |
| 1   | A     | 151 | PHE  | 13             |
| 1   | A     | 4   | GLU  | 13             |
| 1   | A     | 170 | LYS  | 13             |
| 1   | A     | 119 | ARG  | 13             |
| 1   | A     | 35  | MET  | 13             |
| 1   | A     | 135 | LEU  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 15  | SER  | 12             |
| 1   | A     | 190 | ARG  | 12             |
| 1   | A     | 44  | HIS  | 12             |
| 1   | A     | 177 | LEU  | 12             |
| 1   | A     | 103 | PHE  | 12             |
| 1   | A     | 112 | LEU  | 12             |
| 1   | A     | 39  | SER  | 11             |
| 1   | A     | 34  | ASP  | 11             |
| 1   | A     | 191 | MET  | 11             |
| 1   | A     | 132 | CYS  | 11             |
| 1   | A     | 71  | GLN  | 11             |
| 1   | A     | 99  | HIS  | 11             |
| 1   | A     | 16  | LEU  | 10             |
| 1   | A     | 184 | LEU  | 10             |
| 1   | A     | 158 | LEU  | 10             |
| 1   | A     | 156 | THR  | 9              |
| 1   | A     | 89  | PHE  | 9              |
| 1   | A     | 19  | VAL  | 9              |
| 1   | A     | 29  | CYS  | 9              |
| 1   | A     | 31  | LYS  | 9              |
| 1   | A     | 95  | ARG  | 9              |
| 1   | A     | 88  | ASP  | 9              |
| 1   | A     | 57  | ARG  | 9              |
| 1   | A     | 3   | SER  | 9              |
| 1   | A     | 38  | LEU  | 9              |
| 1   | A     | 182 | ARG  | 9              |
| 1   | A     | 117 | ARG  | 9              |
| 1   | A     | 93  | THR  | 9              |
| 1   | A     | 51  | SER  | 8              |
| 1   | A     | 75  | LYS  | 8              |
| 1   | A     | 141 | TYR  | 8              |
| 1   | A     | 175 | ASP  | 8              |
| 1   | A     | 189 | GLU  | 8              |
| 1   | A     | 8   | ASP  | 7              |
| 1   | A     | 192 | ASP  | 7              |
| 1   | A     | 196 | TYR  | 7              |
| 1   | A     | 194 | HIS  | 7              |
| 1   | A     | 10  | GLN  | 7              |
| 1   | A     | 130 | GLN  | 7              |
| 1   | A     | 25  | LEU  | 7              |
| 1   | A     | 6   | ASN  | 7              |
| 1   | A     | 73  | ASP  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 58  | TYR  | 6              |
| 1   | A     | 26  | VAL  | 6              |
| 1   | A     | 105 | ASP  | 6              |
| 1   | A     | 76  | VAL  | 6              |
| 1   | A     | 52  | GLU  | 6              |
| 1   | A     | 86  | CYS  | 5              |
| 1   | A     | 179 | SER  | 5              |
| 1   | A     | 159 | HIS  | 5              |
| 1   | A     | 193 | GLU  | 5              |
| 1   | A     | 178 | HIS  | 5              |
| 1   | A     | 62  | ARG  | 4              |
| 1   | A     | 155 | GLN  | 4              |
| 1   | A     | 140 | GLU  | 4              |
| 1   | A     | 96  | ASP  | 4              |
| 1   | A     | 41  | GLN  | 4              |
| 1   | A     | 174 | GLN  | 4              |
| 1   | A     | 115 | ASP  | 4              |
| 1   | A     | 152 | SER  | 4              |
| 1   | A     | 36  | SER  | 4              |
| 1   | A     | 180 | SER  | 4              |
| 1   | A     | 143 | GLN  | 4              |
| 1   | A     | 167 | GLU  | 4              |
| 1   | A     | 128 | MET  | 3              |
| 1   | A     | 46  | VAL  | 3              |
| 1   | A     | 168 | VAL  | 3              |
| 1   | A     | 188 | LEU  | 3              |
| 1   | A     | 197 | VAL  | 3              |
| 1   | A     | 120 | TYR  | 3              |
| 1   | A     | 5   | VAL  | 2              |
| 1   | A     | 163 | SER  | 2              |
| 1   | A     | 118 | GLU  | 2              |
| 1   | A     | 147 | GLU  | 2              |
| 1   | A     | 33  | GLN  | 2              |
| 1   | A     | 23  | ARG  | 2              |
| 1   | A     | 195 | VAL  | 2              |
| 1   | A     | 13  | TRP  | 1              |
| 1   | A     | 59  | PHE  | 1              |
| 1   | A     | 74  | PHE  | 1              |
| 1   | A     | 100 | CYS  | 1              |
| 1   | A     | 121 | VAL  | 1              |
| 1   | A     | 165 | ASN  | 1              |
| 1   | A     | 123 | HIS  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 9   | LEU  | 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 carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5820

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|   |      |
|---|------|
| Total number of shifts                  | 2157 |
| Number of shifts mapped to atoms        | 2157 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 7    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 199      | $-0.89 \pm 0.16$                | Should be applied          |
| $^{13}\text{C}_\beta$  | 183      | $-0.55 \pm 0.14$                | Should be applied          |
| $^{13}\text{C}'$       | 190      | $-0.05 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 190      | $-0.46 \pm 0.31$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1894 atoms were assigned a chemical shift out of a possible 2403. 31 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 957/977 (98%)  | 382/389 (98%) | 386/398 (97%)   | 189/190 (99%)   |
| Sidechain | 863/1199 (72%) | 504/703 (72%) | 359/444 (81%)   | 0/52 (0%)       |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 74/227 (33%)    | 38/120 (32%)         | 32/95 (34%)           | 4/12 (33%)            |
| Overall  | 1894/2403 (79%) | 924/1212 (76%)       | 777/937 (83%)         | 193/254 (76%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1906 atoms were assigned a chemical shift out of a possible 2433. 31 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 963/987 (98%)   | 384/393 (98%)        | 389/402 (97%)         | 190/192 (99%)         |
| Sidechain | 869/1212 (72%)  | 507/711 (71%)        | 362/448 (81%)         | 0/53 (0%)             |
| Aromatic  | 74/234 (32%)    | 38/124 (31%)         | 32/97 (33%)           | 4/13 (31%)            |
| Overall   | 1906/2433 (78%) | 929/1228 (76%)       | 783/947 (83%)         | 194/258 (75%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | A     | 27  | PRO  | CD   | 40.05      | 55.31 – 45.41       | -10.4   |
| 1   | A     | 152 | SER  | HB2  | 2.07       | 5.18 – 2.58         | -7.0    |
| 1   | A     | 41  | GLN  | HG2  | 0.66       | 3.67 – 0.97         | -6.2    |
| 1   | A     | 76  | VAL  | HG13 | -0.65      | 2.13 – -0.47        | -5.7    |
| 1   | A     | 76  | VAL  | HG12 | -0.65      | 2.13 – -0.47        | -5.7    |
| 1   | A     | 76  | VAL  | HG11 | -0.65      | 2.13 – -0.47        | -5.7    |
| 1   | A     | 96  | ASP  | HB2  | 1.20       | 4.07 – 1.37         | -5.6    |

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

