# Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:52 pm BST

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|---|---|---|
| PDB ID | : | 2KX9 |
| Title | : | Solution Structure of the Enzyme I dimer Using Residual Dipolar Couplings and Small Angle X-Ray Scattering |
| Authors | : | Schwieters, C.D.; Suh, J.; Grishaev, A.; Takayama, Y.; Guirlando, R.; Clore, G. |
| Deposited on | : | 2010-04-29 |

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

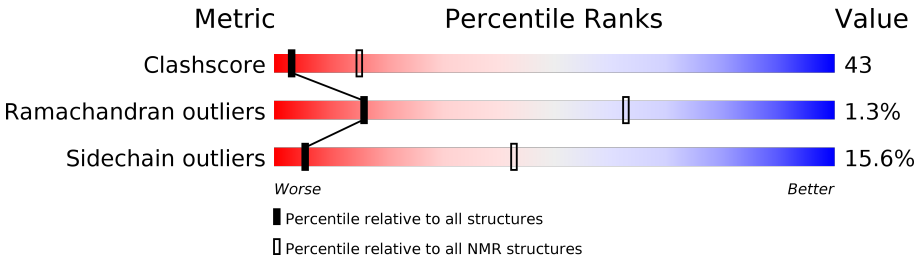
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 573 | 53% 35% 12% |
| 1 | B | 573 | 53% 35% 11% |

## 2 Ensemble composition and analysis

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

# 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17912 atoms, of which 9028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phosphoenolpyruvate-protein phosphotransferase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 573 | Total | C | H | N | O | S | 0 |
| | | | 8956 | 2790 | 4514 | 757 | 874 | 21 | |
| 1 | B | 573 | Total | C | H | N | O | S | 0 |
| | | | 8956 | 2790 | 4514 | 757 | 874 | 21 | |

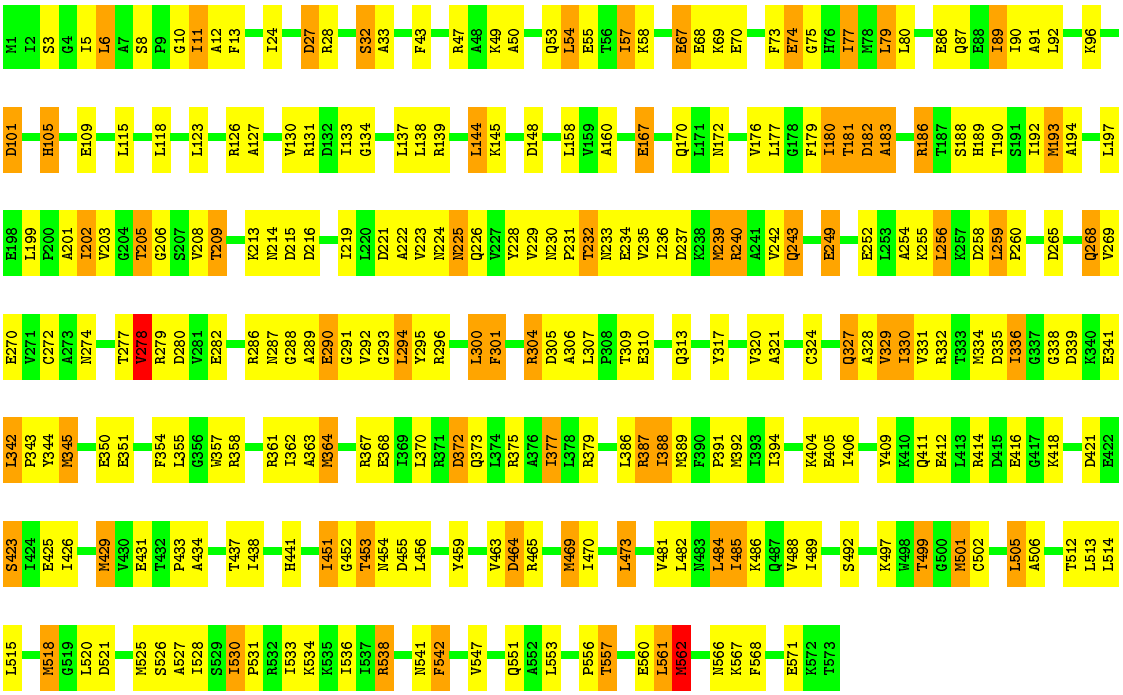
# 4 Residue-property plots

## 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.

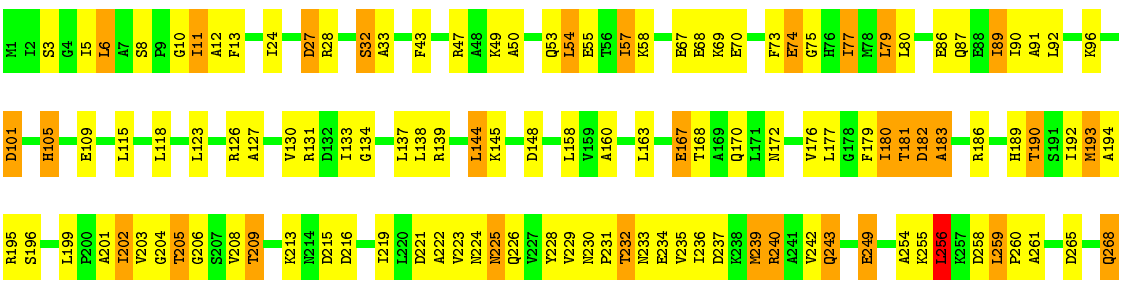
- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

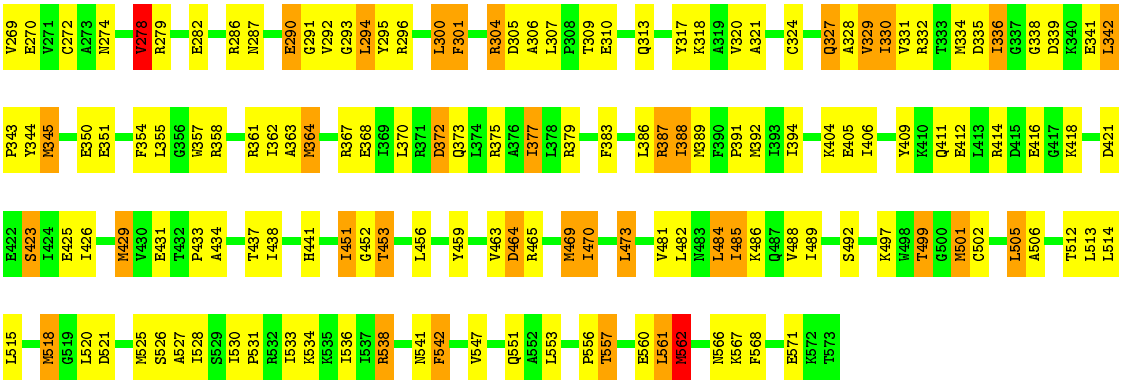
Chain A:


- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain B:



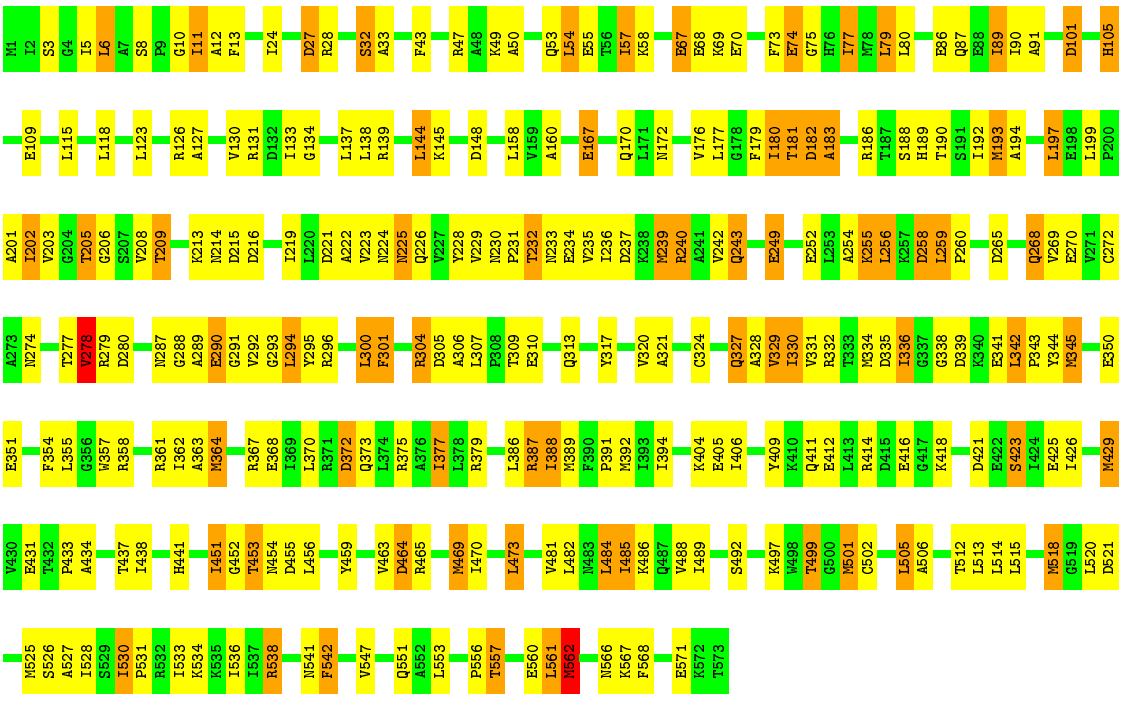
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1 (medoid)

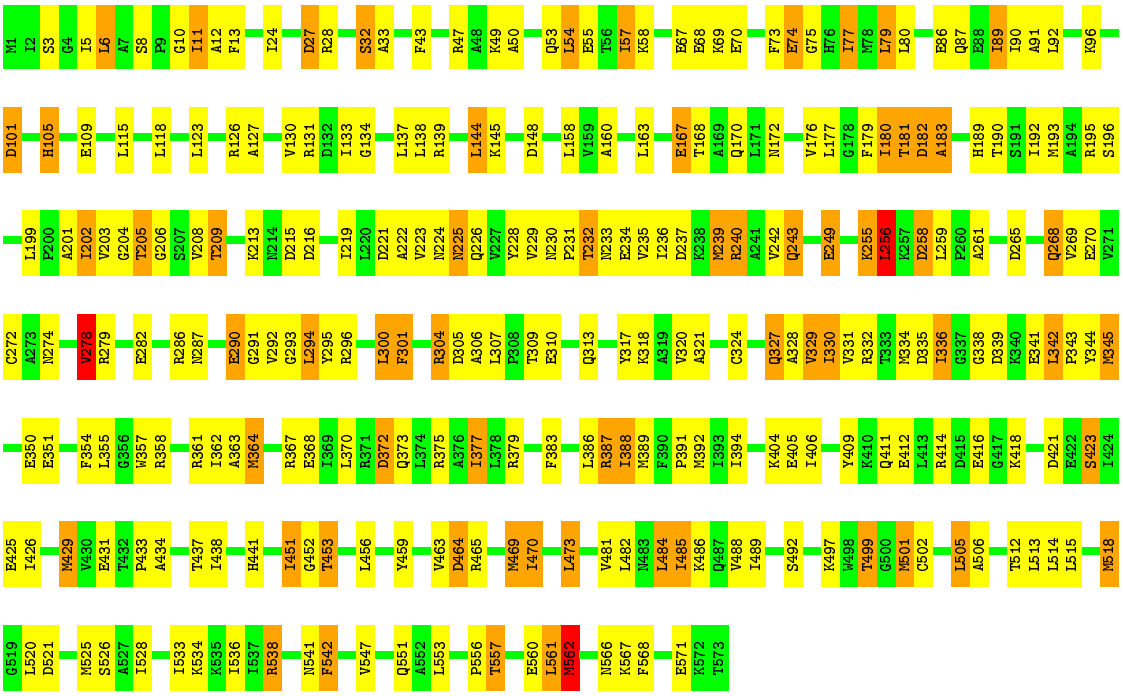
- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain A:

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

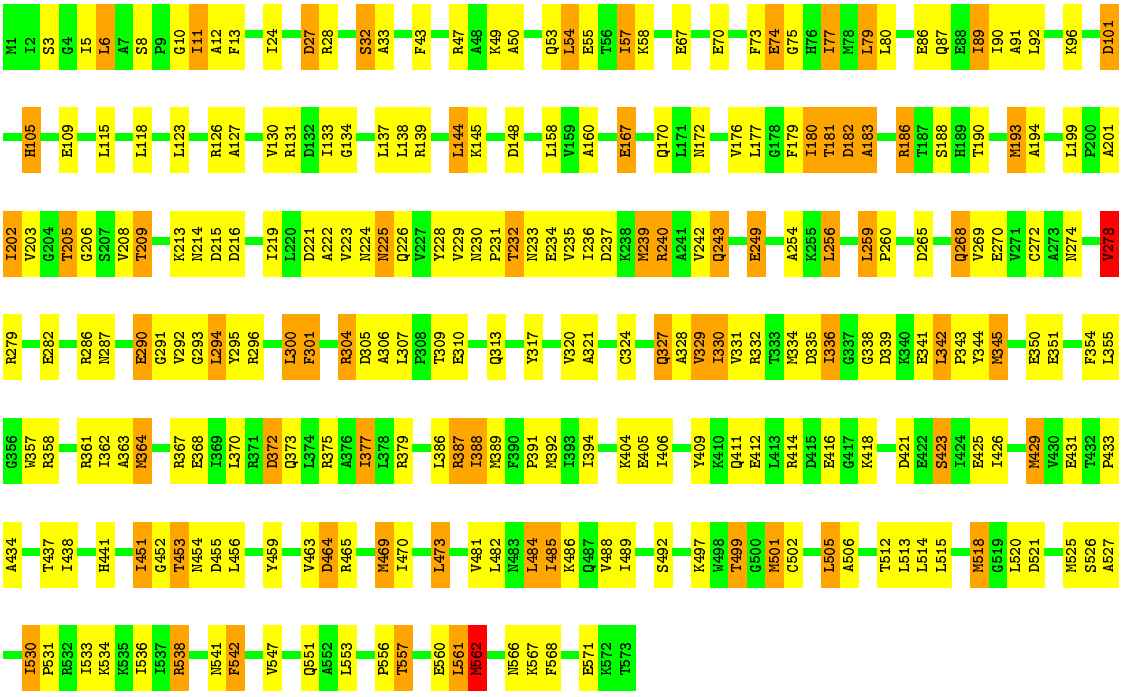
Chain B:



### 4.2.2 Score per residue for model 2

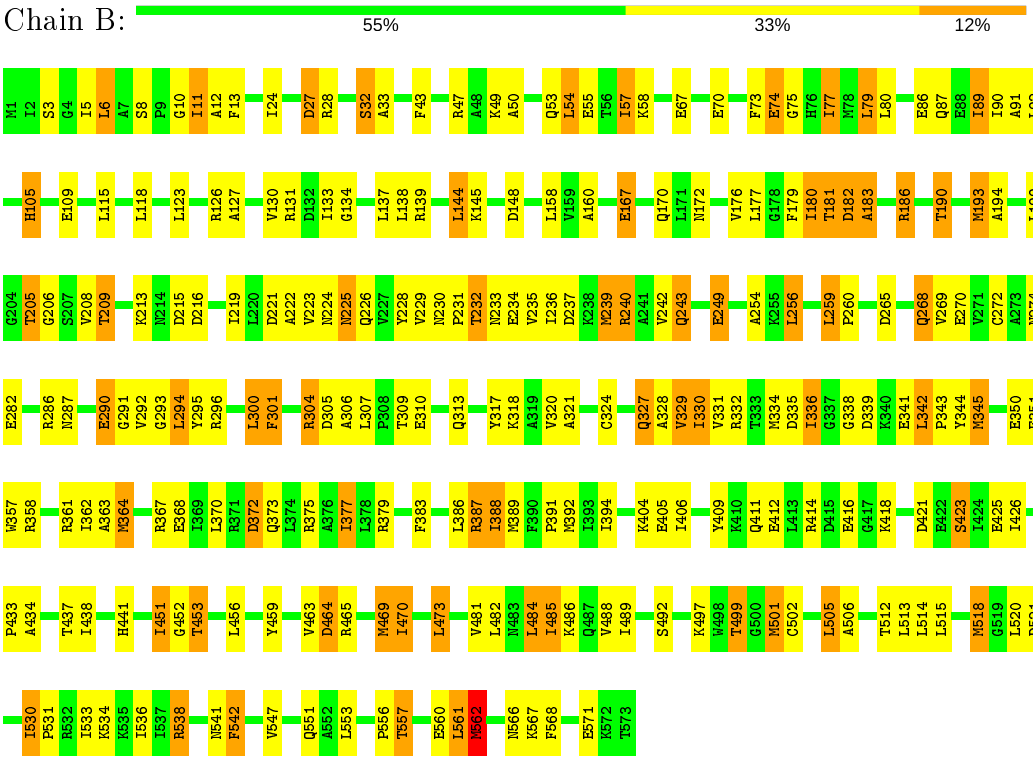
• Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain A:

• Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain B:


55%
33%
12%
M1 I2 S3 G4 I5 L6 A7 S8 P9 G10 I11 A12 F13 I24 D27 R28 S32 A33 F43 R47 A48 K49 A50 Q53 L54 E55 T56 I57 K58 E67 E70 F73 E74 G75 H76 I77 N78 L79 L80 E86 Q87 E88 I89 I90 A91 L92 K96 D101
H105 E109 L115 L118 L123 R126 A127 V130 R131 D132 I133 G134 L137 L138 R139 L144 K145 D148 L158 V159 A160 E167 Q170 L171 N172 V176 L177 G178 F179 I180 T181 D182 A183 R186 T190 M193 A194 L199 P200 A201 I202 V203
G204 T205 G206 S207 V208 T209 K213 N214 D215 D216 I219 L220 D221 A222 Y223 N224 N225 Q226 Y227 Y228 V229 N230 P231 T232 N233 E234 V235 I236 D237 K238 M239 R240 A241 V242 Q243 E249 A254 K255 I256 L259 P260 D265 Q268 V269 E270 V271 C272 A273 N274 V278 R279
E282 R286 N287 E290 G291 V292 G293 L294 Y295 R296 L300 F301 R304 D305 A306 L307 P308 T309 E310 Q313 Y317 K318 A319 V320 A321 C324 Q327 A328 V329 I330 V331 R332 T333 M334 D335 I336 G337 G338 D339 K340 E341 L342 P343 Y344 M345 E350 E351 F354 L355 G356
W357 R358 R361 I362 A363 M364 R367 E368 I369 L370 R371 D372 Q373 L374 R375 A376 I377 L378 R379 F383 L386 R387 I388 M389 F390 P391 M392 I393 I394 K404 E405 I406 Y409 K410 Q411 E412 L413 R414 D415 E416 G417 K418 D421 E422 S423 I424 E425 I426 M429 V430 E431 T432
P433 A434 T437 I438 H441 I451 G452 T453 L456 Y459 V463 D464 R465 M469 I470 L473 V481 L482 N483 L484 I485 K486 Q487 V488 I489 S492 K497 W498 T499 G500 M501 C502 L505 A506 T512 L513 L514 L515 M518 G519 L520 D521 M525 S526 A527
I530 P531 R532 I533 K534 K535 I536 I537 R538 N541 F542 V547 Q551 A552 L553 P556 T557 E560 L561 M562 N566 K567 F568 E571 K572 T573

# 5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 2 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 |
|---|---|---|
| Xplor-NIH | structure solution | 2.25 |
| Xplor-NIH | refinement | 2.25 |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

## 5.1 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 | 4442 | 4514 | 4506 | 394±0 |
| 1 | B | 4442 | 4514 | 4506 | 386±4 |
| All | All | 17768 | 18056 | 18024 | 1524 |

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 43.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:562:MET:CE | 1:B:562:MET:SD | 1.48 | 2.01 | 1 | 1 |
| 1:B:562:MET:SD | 1:B:562:MET:CE | 1.48 | 2.01 | 2 | 1 |
| 1:B:364:MET:SD | 1:B:364:MET:CE | 1.43 | 2.06 | 1 | 2 |
| 1:A:364:MET:CE | 1:A:364:MET:SD | 1.42 | 2.06 | 1 | 2 |
| 1:A:469:MET:CE | 1:A:469:MET:SD | 1.36 | 2.14 | 1 | 1 |
| 1:B:469:MET:SD | 1:B:469:MET:CE | 1.36 | 2.14 | 1 | 1 |
| 1:A:469:MET:SD | 1:A:469:MET:CE | 1.36 | 2.14 | 2 | 1 |
| 1:B:469:MET:CE | 1:B:469:MET:SD | 1.36 | 2.14 | 2 | 1 |
| 1:B:345:MET:SD | 1:B:345:MET:CE | 1.35 | 2.14 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:345:MET:CE | 1:B:345:MET:SD | 1.35 | 2.14 | 2 | 1 |
| 1:A:345:MET:SD | 1:A:345:MET:CE | 1.35 | 2.14 | 1 | 2 |
| 1:B:54:LEU:HD22 | 1:B:54:LEU:O | 1.25 | 1.27 | 2 | 2 |
| 1:A:54:LEU:O | 1:A:54:LEU:HD22 | 1.24 | 1.28 | 1 | 1 |
| 1:A:54:LEU:HD22 | 1:A:54:LEU:O | 1.22 | 1.28 | 2 | 1 |
| 1:B:54:LEU:HD13 | 1:B:55:GLU:N | 1.20 | 1.52 | 1 | 2 |
| 1:A:54:LEU:HD13 | 1:A:55:GLU:N | 1.19 | 1.52 | 1 | 2 |
| 1:B:527:ALA:O | 1:B:530:ILE:CG2 | 1.18 | 1.92 | 2 | 1 |
| 1:A:527:ALA:O | 1:A:530:ILE:CG2 | 1.17 | 1.92 | 2 | 2 |
| 1:A:54:LEU:C | 1:A:54:LEU:HD22 | 1.16 | 1.60 | 1 | 1 |
| 1:A:54:LEU:HD22 | 1:A:54:LEU:C | 1.15 | 1.60 | 2 | 1 |
| 1:A:301:PHE:O | 1:A:304:ARG:NE | 1.14 | 1.79 | 1 | 2 |
| 1:B:301:PHE:O | 1:B:304:ARG:NE | 1.14 | 1.80 | 1 | 2 |
| 1:B:54:LEU:C | 1:B:54:LEU:HD22 | 1.12 | 1.61 | 1 | 1 |
| 1:B:54:LEU:HD22 | 1:B:54:LEU:C | 1.12 | 1.61 | 2 | 1 |
| 1:B:144:LEU:O | 1:B:144:LEU:HD13 | 1.11 | 1.46 | 2 | 2 |
| 1:A:144:LEU:O | 1:A:144:LEU:HD13 | 1.07 | 1.46 | 1 | 1 |
| 1:B:291:GLY:HA2 | 1:B:327:GLN:CG | 1.07 | 1.79 | 1 | 2 |
| 1:A:144:LEU:HD13 | 1:A:144:LEU:O | 1.06 | 1.46 | 2 | 1 |
| 1:A:291:GLY:HA2 | 1:A:327:GLN:CG | 1.06 | 1.79 | 1 | 2 |
| 1:B:11:ILE:HD12 | 1:B:12:ALA:N | 1.04 | 1.67 | 2 | 2 |
| 1:A:527:ALA:O | 1:A:530:ILE:HG22 | 1.04 | 1.52 | 1 | 2 |
| 1:A:11:ILE:HD12 | 1:A:12:ALA:N | 1.02 | 1.67 | 1 | 2 |
| 1:A:77:ILE:HD13 | 1:A:77:ILE:N | 1.02 | 1.68 | 1 | 1 |
| 1:B:77:ILE:N | 1:B:77:ILE:HD13 | 1.02 | 1.68 | 2 | 1 |
| 1:B:77:ILE:HD13 | 1:B:77:ILE:N | 1.01 | 1.68 | 1 | 1 |
| 1:A:77:ILE:N | 1:A:77:ILE:HD13 | 1.01 | 1.68 | 2 | 1 |
| 1:A:291:GLY:HA2 | 1:A:327:GLN:HG3 | 1.00 | 1.03 | 1 | 2 |
| 1:B:232:THR:CG2 | 1:B:233:ASN:H | 1.00 | 1.69 | 2 | 2 |
| 1:A:221:ASP:HA | 1:A:239:MET:CE | 0.99 | 1.87 | 2 | 2 |
| 1:A:232:THR:CG2 | 1:A:233:ASN:H | 0.99 | 1.69 | 2 | 2 |
| 1:B:291:GLY:HA2 | 1:B:327:GLN:HG3 | 0.99 | 1.02 | 1 | 2 |
| 1:B:221:ASP:HA | 1:B:239:MET:CE | 0.98 | 1.87 | 1 | 2 |
| 1:A:232:THR:CG2 | 1:A:233:ASN:N | 0.98 | 2.26 | 2 | 2 |
| 1:A:232:THR:HG22 | 1:A:233:ASN:N | 0.98 | 1.71 | 2 | 2 |
| 1:B:232:THR:HG22 | 1:B:233:ASN:N | 0.98 | 1.71 | 2 | 2 |
| 1:B:232:THR:CG2 | 1:B:233:ASN:N | 0.97 | 2.26 | 2 | 2 |
| 1:B:304:ARG:NE | 1:B:304:ARG:O | 0.96 | 1.97 | 1 | 2 |
| 1:A:304:ARG:NE | 1:A:304:ARG:O | 0.96 | 1.98 | 1 | 1 |
| 1:A:304:ARG:O | 1:A:304:ARG:NE | 0.96 | 1.98 | 2 | 1 |
| 1:B:527:ALA:O | 1:B:530:ILE:HG22 | 0.94 | 1.58 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:527:ALA:O | 1:B:530:ILE:HG23 | 0.94 | 1.61 | 2 | 1 |
| 1:A:527:ALA:O | 1:A:530:ILE:HG23 | 0.93 | 1.61 | 2 | 1 |
| 1:A:11:ILE:HG21 | 1:A:243:GLN:CA | 0.92 | 1.95 | 1 | 2 |
| 1:A:484:LEU:HD23 | 1:A:485:ILE:N | 0.92 | 1.80 | 1 | 2 |
| 1:A:54:LEU:C | 1:A:54:LEU:CD2 | 0.92 | 2.37 | 1 | 1 |
| 1:B:11:ILE:HG21 | 1:B:243:GLN:HA | 0.91 | 1.42 | 2 | 2 |
| 1:A:160:ALA:O | 1:A:181:THR:HG22 | 0.91 | 1.65 | 1 | 2 |
| 1:A:54:LEU:CD2 | 1:A:54:LEU:C | 0.91 | 2.37 | 2 | 1 |
| 1:B:484:LEU:HD23 | 1:B:485:ILE:N | 0.91 | 1.80 | 1 | 2 |
| 1:B:11:ILE:HG21 | 1:B:243:GLN:CA | 0.91 | 1.95 | 2 | 2 |
| 1:B:160:ALA:O | 1:B:181:THR:HG22 | 0.91 | 1.65 | 1 | 2 |
| 1:A:481:VAL:O | 1:A:485:ILE:HG23 | 0.90 | 1.66 | 1 | 2 |
| 1:A:11:ILE:HG21 | 1:A:243:GLN:HA | 0.89 | 1.42 | 1 | 2 |
| 1:A:456:LEU:HD13 | 1:A:484:LEU:HD21 | 0.89 | 1.45 | 1 | 2 |
| 1:B:228:TYR:HB3 | 1:B:231:PRO:HG3 | 0.88 | 1.45 | 2 | 2 |
| 1:A:228:TYR:HB3 | 1:A:231:PRO:HG3 | 0.88 | 1.46 | 1 | 2 |
| 1:B:481:VAL:O | 1:B:485:ILE:HG23 | 0.87 | 1.66 | 1 | 2 |
| 1:A:11:ILE:HD12 | 1:A:12:ALA:H | 0.87 | 1.27 | 2 | 2 |
| 1:A:388:ILE:HD12 | 1:A:389:MET:N | 0.87 | 1.83 | 1 | 2 |
| 1:B:54:LEU:CD2 | 1:B:54:LEU:C | 0.87 | 2.37 | 2 | 2 |
| 1:B:456:LEU:HD13 | 1:B:484:LEU:HD21 | 0.87 | 1.45 | 1 | 2 |
| 1:B:144:LEU:C | 1:B:144:LEU:HD22 | 0.86 | 1.91 | 1 | 1 |
| 1:A:180:ILE:HD11 | 1:A:208:VAL:HG11 | 0.86 | 1.47 | 2 | 2 |
| 1:B:144:LEU:HD22 | 1:B:144:LEU:C | 0.86 | 1.90 | 2 | 1 |
| 1:B:388:ILE:HD12 | 1:B:389:MET:N | 0.86 | 1.86 | 1 | 2 |
| 1:B:221:ASP:HA | 1:B:239:MET:HE2 | 0.85 | 1.48 | 2 | 2 |
| 1:A:144:LEU:C | 1:A:144:LEU:HD22 | 0.85 | 1.91 | 1 | 1 |
| 1:A:221:ASP:HA | 1:A:239:MET:HE2 | 0.85 | 1.46 | 1 | 2 |
| 1:A:144:LEU:HD22 | 1:A:144:LEU:C | 0.85 | 1.91 | 2 | 1 |
| 1:B:518:MET:SD | 1:B:553:LEU:HD11 | 0.84 | 2.13 | 1 | 2 |
| 1:A:518:MET:SD | 1:A:553:LEU:HD11 | 0.83 | 2.13 | 1 | 2 |
| 1:B:11:ILE:HD12 | 1:B:12:ALA:H | 0.83 | 1.27 | 1 | 2 |
| 1:A:473:LEU:HD12 | 1:B:394:ILE:HD11 | 0.82 | 1.51 | 1 | 2 |
| 1:B:225:ASN:O | 1:B:225:ASN:CG | 0.81 | 2.19 | 2 | 1 |
| 1:A:54:LEU:O | 1:A:54:LEU:CD2 | 0.81 | 2.23 | 1 | 1 |
| 1:B:225:ASN:CG | 1:B:225:ASN:O | 0.81 | 2.19 | 1 | 1 |
| 1:B:291:GLY:CA | 1:B:327:GLN:HG3 | 0.81 | 1.98 | 1 | 2 |
| 1:A:556:PRO:HB3 | 1:B:441:HIS:ND1 | 0.81 | 1.89 | 1 | 2 |
| 1:B:429:MET:SD | 1:B:431:GLU:HG3 | 0.81 | 2.16 | 1 | 2 |
| 1:B:77:ILE:N | 1:B:77:ILE:CD1 | 0.81 | 2.44 | 2 | 2 |
| 1:B:180:ILE:HD11 | 1:B:208:VAL:HG11 | 0.81 | 1.51 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:77:ILE:CD1 | 1:A:77:ILE:N | 0.80 | 2.43 | 2 | 2 |
| 1:A:225:ASN:CG | 1:A:225:ASN:O | 0.80 | 2.19 | 1 | 1 |
| 1:A:429:MET:SD | 1:A:431:GLU:HG3 | 0.80 | 2.16 | 1 | 2 |
| 1:A:225:ASN:O | 1:A:225:ASN:CG | 0.80 | 2.19 | 2 | 1 |
| 1:A:291:GLY:CA | 1:A:327:GLN:HG3 | 0.79 | 1.99 | 1 | 2 |
| 1:A:189:HIS:O | 1:A:192:ILE:HG22 | 0.79 | 1.77 | 1 | 1 |
| 1:A:54:LEU:CD2 | 1:A:54:LEU:O | 0.79 | 2.23 | 2 | 1 |
| 1:A:11:ILE:HD11 | 1:A:13:PHE:CZ | 0.79 | 2.13 | 2 | 2 |
| 1:B:54:LEU:CD2 | 1:B:54:LEU:O | 0.79 | 2.23 | 1 | 2 |
| 1:B:163:LEU:HB3 | 1:B:190:THR:HG21 | 0.79 | 1.53 | 1 | 1 |
| 1:B:11:ILE:HD11 | 1:B:13:PHE:CZ | 0.78 | 2.13 | 1 | 2 |
| 1:B:482:LEU:O | 1:B:485:ILE:HG12 | 0.78 | 1.79 | 1 | 2 |
| 1:B:139:ARG:HB3 | 1:B:144:LEU:HG | 0.78 | 1.55 | 1 | 2 |
| 1:A:139:ARG:HB3 | 1:A:144:LEU:HG | 0.77 | 1.56 | 2 | 2 |
| 1:B:13:PHE:CZ | 1:B:240:ARG:HD2 | 0.77 | 2.15 | 1 | 2 |
| 1:A:13:PHE:CZ | 1:A:240:ARG:HD2 | 0.77 | 2.15 | 2 | 2 |
| 1:B:54:LEU:CD1 | 1:B:55:GLU:N | 0.76 | 2.44 | 2 | 2 |
| 1:A:144:LEU:O | 1:A:144:LEU:CD1 | 0.76 | 2.32 | 1 | 2 |
| 1:A:372:ASP:OD1 | 1:A:372:ASP:C | 0.76 | 2.24 | 1 | 1 |
| 1:A:372:ASP:C | 1:A:372:ASP:OD1 | 0.76 | 2.24 | 2 | 1 |
| 1:A:482:LEU:O | 1:A:485:ILE:HG12 | 0.76 | 1.79 | 1 | 2 |
| 1:A:505:LEU:HD13 | 1:A:506:ALA:H | 0.76 | 1.41 | 1 | 2 |
| 1:A:394:ILE:HD11 | 1:B:473:LEU:HD12 | 0.76 | 1.58 | 1 | 2 |
| 1:B:530:ILE:O | 1:B:530:ILE:HD12 | 0.76 | 1.81 | 2 | 1 |
| 1:A:330:ILE:HD12 | 1:A:330:ILE:C | 0.75 | 2.02 | 1 | 1 |
| 1:A:330:ILE:C | 1:A:330:ILE:HD12 | 0.75 | 2.02 | 2 | 1 |
| 1:B:372:ASP:OD1 | 1:B:372:ASP:C | 0.75 | 2.24 | 1 | 2 |
| 1:B:330:ILE:HD12 | 1:B:330:ILE:C | 0.74 | 2.02 | 1 | 1 |
| 1:A:530:ILE:HD12 | 1:A:530:ILE:O | 0.74 | 1.80 | 2 | 1 |
| 1:B:330:ILE:C | 1:B:330:ILE:HD12 | 0.74 | 2.02 | 2 | 1 |
| 1:B:505:LEU:CD1 | 1:B:505:LEU:N | 0.74 | 2.50 | 1 | 1 |
| 1:B:505:LEU:N | 1:B:505:LEU:CD1 | 0.74 | 2.50 | 2 | 1 |
| 1:A:54:LEU:CD1 | 1:A:55:GLU:N | 0.74 | 2.44 | 1 | 2 |
| 1:B:144:LEU:CD2 | 1:B:145:LYS:O | 0.74 | 2.35 | 2 | 2 |
| 1:A:11:ILE:CG2 | 1:A:243:GLN:HA | 0.74 | 2.13 | 1 | 2 |
| 1:A:144:LEU:CD2 | 1:A:145:LYS:O | 0.74 | 2.35 | 1 | 2 |
| 1:B:144:LEU:O | 1:B:144:LEU:CD1 | 0.74 | 2.32 | 2 | 1 |
| 1:A:54:LEU:HD21 | 1:A:77:ILE:HG13 | 0.74 | 1.60 | 2 | 2 |
| 1:B:144:LEU:CD1 | 1:B:144:LEU:O | 0.74 | 2.32 | 1 | 1 |
| 1:B:11:ILE:CG2 | 1:B:243:GLN:HA | 0.74 | 2.13 | 1 | 2 |
| 1:B:429:MET:SD | 1:B:431:GLU:CG | 0.74 | 2.76 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:429:MET:SD | 1:A:431:GLU:CG | 0.73 | 2.76 | 1 | 2 |
| 1:A:505:LEU:N | 1:A:505:LEU:CD1 | 0.73 | 2.50 | 1 | 2 |
| 1:A:193:MET:SD | 1:A:197:LEU:HD22 | 0.73 | 2.24 | 1 | 1 |
| 1:B:294:LEU:HD12 | 1:B:502:CYS:SG | 0.73 | 2.23 | 1 | 2 |
| 1:A:228:TYR:CD1 | 1:A:235:VAL:HG11 | 0.73 | 2.19 | 2 | 2 |
| 1:B:456:LEU:HD22 | 1:B:484:LEU:HD11 | 0.73 | 1.60 | 1 | 2 |
| 1:B:228:TYR:CB | 1:B:231:PRO:HG3 | 0.73 | 2.14 | 2 | 2 |
| 1:B:168:THR:CG2 | 1:B:193:MET:SD | 0.73 | 2.76 | 1 | 1 |
| 1:A:228:TYR:CB | 1:A:231:PRO:HG3 | 0.73 | 2.14 | 1 | 2 |
| 1:A:73:PHE:O | 1:A:77:ILE:HG12 | 0.73 | 1.84 | 1 | 2 |
| 1:A:294:LEU:HD12 | 1:A:502:CYS:SG | 0.72 | 2.24 | 1 | 2 |
| 1:B:202:ILE:HD13 | 1:B:202:ILE:O | 0.72 | 1.84 | 2 | 1 |
| 1:A:291:GLY:CA | 1:A:327:GLN:CG | 0.72 | 2.65 | 1 | 2 |
| 1:B:505:LEU:HD13 | 1:B:506:ALA:H | 0.72 | 1.42 | 1 | 2 |
| 1:A:232:THR:O | 1:A:236:ILE:HG13 | 0.72 | 1.84 | 1 | 2 |
| 1:A:441:HIS:ND1 | 1:B:556:PRO:HB3 | 0.72 | 1.99 | 1 | 2 |
| 1:B:11:ILE:CD1 | 1:B:12:ALA:N | 0.72 | 2.51 | 1 | 2 |
| 1:B:202:ILE:O | 1:B:202:ILE:HD13 | 0.72 | 1.84 | 1 | 1 |
| 1:B:232:THR:O | 1:B:236:ILE:HG13 | 0.72 | 1.84 | 1 | 2 |
| 1:B:73:PHE:O | 1:B:77:ILE:HG12 | 0.72 | 1.84 | 2 | 2 |
| 1:A:202:ILE:O | 1:A:202:ILE:HD13 | 0.72 | 1.85 | 2 | 1 |
| 1:A:202:ILE:HD13 | 1:A:202:ILE:O | 0.72 | 1.85 | 1 | 1 |
| 1:B:228:TYR:CD1 | 1:B:235:VAL:HG11 | 0.71 | 2.19 | 1 | 2 |
| 1:B:54:LEU:HD21 | 1:B:77:ILE:HG13 | 0.71 | 1.61 | 1 | 2 |
| 1:A:130:VAL:O | 1:A:133:ILE:HG22 | 0.71 | 1.85 | 2 | 2 |
| 1:A:530:ILE:HG23 | 1:A:531:PRO:HD3 | 0.71 | 1.61 | 1 | 2 |
| 1:A:464:ASP:CG | 1:B:355:LEU:O | 0.71 | 2.29 | 1 | 2 |
| 1:B:221:ASP:HA | 1:B:239:MET:HE1 | 0.71 | 1.59 | 2 | 2 |
| 1:A:221:ASP:HA | 1:A:239:MET:HE1 | 0.71 | 1.60 | 2 | 2 |
| 1:B:130:VAL:O | 1:B:133:ILE:HG22 | 0.71 | 1.85 | 1 | 2 |
| 1:A:11:ILE:CD1 | 1:A:12:ALA:N | 0.71 | 2.51 | 1 | 2 |
| 1:A:219:ILE:HD11 | 1:A:236:ILE:HG12 | 0.70 | 1.62 | 1 | 2 |
| 1:A:301:PHE:CD1 | 1:A:342:LEU:HD13 | 0.70 | 2.21 | 1 | 2 |
| 1:B:287:ASN:O | 1:B:530:ILE:HG12 | 0.70 | 1.86 | 2 | 1 |
| 1:A:567:LYS:O | 1:A:571:GLU:HG3 | 0.70 | 1.87 | 1 | 2 |
| 1:B:321:ALA:O | 1:B:324:CYS:SG | 0.70 | 2.49 | 1 | 2 |
| 1:A:433:PRO:O | 1:A:437:THR:HG23 | 0.70 | 1.85 | 1 | 2 |
| 1:A:287:ASN:O | 1:A:530:ILE:HG12 | 0.70 | 1.86 | 2 | 1 |
| 1:A:321:ALA:O | 1:A:324:CYS:SG | 0.70 | 2.49 | 1 | 2 |
| 1:A:530:ILE:HD12 | 1:A:530:ILE:C | 0.70 | 2.07 | 2 | 1 |
| 1:B:224:ASN:O | 1:B:225:ASN:OD1 | 0.70 | 2.09 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:11:ILE:HD11 | 1:A:13:PHE:CE1 | 0.70 | 2.22 | 1 | 2 |
| 1:B:287:ASN:O | 1:B:530:ILE:CG1 | 0.70 | 2.40 | 2 | 1 |
| 1:A:180:ILE:HD11 | 1:A:208:VAL:CG1 | 0.70 | 2.16 | 1 | 2 |
| 1:A:392:MET:N | 1:A:429:MET:SD | 0.70 | 2.64 | 1 | 2 |
| 1:B:219:ILE:HD11 | 1:B:236:ILE:HG12 | 0.70 | 1.62 | 2 | 2 |
| 1:B:11:ILE:HD11 | 1:B:13:PHE:CE1 | 0.70 | 2.22 | 2 | 2 |
| 1:B:179:PHE:CZ | 1:B:181:THR:OG1 | 0.69 | 2.45 | 1 | 2 |
| 1:B:567:LYS:O | 1:B:571:GLU:HG3 | 0.69 | 1.87 | 1 | 2 |
| 1:B:13:PHE:CE2 | 1:B:240:ARG:HD2 | 0.69 | 2.23 | 1 | 2 |
| 1:B:392:MET:N | 1:B:429:MET:SD | 0.69 | 2.64 | 1 | 2 |
| 1:A:456:LEU:HD22 | 1:A:484:LEU:HD11 | 0.69 | 1.62 | 1 | 2 |
| 1:B:291:GLY:CA | 1:B:327:GLN:CG | 0.69 | 2.65 | 1 | 2 |
| 1:B:301:PHE:CD1 | 1:B:342:LEU:HD13 | 0.69 | 2.22 | 1 | 2 |
| 1:A:224:ASN:O | 1:A:225:ASN:OD1 | 0.69 | 2.10 | 1 | 2 |
| 1:A:287:ASN:O | 1:A:530:ILE:CG1 | 0.69 | 2.40 | 2 | 1 |
| 1:A:317:TYR:CE2 | 1:A:377:ILE:HD13 | 0.69 | 2.23 | 1 | 2 |
| 1:A:13:PHE:CE2 | 1:A:240:ARG:HD2 | 0.69 | 2.23 | 1 | 2 |
| 1:B:228:TYR:CG | 1:B:235:VAL:HG11 | 0.69 | 2.23 | 1 | 2 |
| 1:B:144:LEU:HD22 | 1:B:145:LYS:O | 0.69 | 1.88 | 2 | 2 |
| 1:A:556:PRO:HB3 | 1:B:441:HIS:CG | 0.69 | 2.23 | 1 | 2 |
| 1:A:144:LEU:HD22 | 1:A:145:LYS:O | 0.68 | 1.88 | 1 | 2 |
| 1:B:274:ASN:ND2 | 1:B:526:SER:N | 0.68 | 2.42 | 1 | 2 |
| 1:B:429:MET:O | 1:B:429:MET:HG3 | 0.68 | 1.88 | 1 | 1 |
| 1:B:429:MET:HG3 | 1:B:429:MET:O | 0.68 | 1.88 | 2 | 1 |
| 1:B:530:ILE:HD12 | 1:B:530:ILE:C | 0.68 | 2.08 | 2 | 1 |
| 1:A:429:MET:HG3 | 1:A:429:MET:O | 0.68 | 1.88 | 1 | 2 |
| 1:B:317:TYR:CE2 | 1:B:377:ILE:HD13 | 0.68 | 2.22 | 1 | 2 |
| 1:A:54:LEU:HD13 | 1:A:55:GLU:H | 0.68 | 1.46 | 2 | 2 |
| 1:A:228:TYR:CG | 1:A:235:VAL:HG11 | 0.68 | 2.22 | 2 | 2 |
| 1:A:431:GLU:HA | 1:A:456:LEU:HG | 0.68 | 1.65 | 1 | 2 |
| 1:B:304:ARG:CD | 1:B:306:ALA:O | 0.68 | 2.42 | 1 | 2 |
| 1:B:431:GLU:HA | 1:B:456:LEU:HG | 0.68 | 1.66 | 1 | 2 |
| 1:B:139:ARG:HB3 | 1:B:144:LEU:CG | 0.68 | 2.18 | 2 | 2 |
| 1:B:434:ALA:O | 1:B:437:THR:OG1 | 0.68 | 2.11 | 1 | 2 |
| 1:A:464:ASP:N | 1:A:464:ASP:OD1 | 0.68 | 2.27 | 1 | 2 |
| 1:B:433:PRO:O | 1:B:437:THR:HG23 | 0.68 | 1.89 | 1 | 2 |
| 1:A:139:ARG:HB3 | 1:A:144:LEU:CG | 0.67 | 2.18 | 1 | 2 |
| 1:B:464:ASP:N | 1:B:464:ASP:OD1 | 0.67 | 2.27 | 1 | 1 |
| 1:B:464:ASP:OD1 | 1:B:464:ASP:N | 0.67 | 2.27 | 2 | 1 |
| 1:A:232:THR:HG23 | 1:A:233:ASN:H | 0.67 | 1.47 | 1 | 2 |
| 1:A:274:ASN:ND2 | 1:A:526:SER:N | 0.67 | 2.41 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:13:PHE:CG | 1:B:240:ARG:NH1 | 0.67 | 2.63 | 2 | 2 |
| 1:A:304:ARG:CD | 1:A:306:ALA:O | 0.67 | 2.43 | 1 | 2 |
| 1:A:179:PHE:CZ | 1:A:181:THR:OG1 | 0.67 | 2.46 | 1 | 2 |
| 1:A:13:PHE:CG | 1:A:240:ARG:NH1 | 0.67 | 2.63 | 2 | 2 |
| 1:B:232:THR:HG23 | 1:B:233:ASN:H | 0.67 | 1.48 | 1 | 2 |
| 1:B:505:LEU:HD13 | 1:B:505:LEU:N | 0.67 | 2.04 | 1 | 1 |
| 1:B:505:LEU:N | 1:B:505:LEU:HD13 | 0.67 | 2.04 | 2 | 1 |
| 1:A:232:THR:HG22 | 1:A:234:GLU:H | 0.66 | 1.51 | 1 | 2 |
| 1:B:54:LEU:HD13 | 1:B:55:GLU:H | 0.66 | 1.47 | 2 | 2 |
| 1:A:434:ALA:O | 1:A:437:THR:OG1 | 0.66 | 2.12 | 1 | 2 |
| 1:B:304:ARG:CZ | 1:B:304:ARG:O | 0.66 | 2.43 | 1 | 1 |
| 1:B:304:ARG:O | 1:B:304:ARG:CZ | 0.66 | 2.43 | 2 | 1 |
| 1:A:505:LEU:N | 1:A:505:LEU:HD13 | 0.66 | 2.05 | 1 | 2 |
| 1:B:180:ILE:HD11 | 1:B:208:VAL:CG1 | 0.66 | 2.21 | 1 | 2 |
| 1:A:230:ASN:N | 1:A:231:PRO:CD | 0.66 | 2.59 | 1 | 2 |
| 1:A:127:ALA:O | 1:A:130:VAL:HG22 | 0.66 | 1.90 | 2 | 2 |
| 1:A:230:ASN:N | 1:A:231:PRO:HD3 | 0.65 | 2.07 | 1 | 2 |
| 1:A:375:ARG:HH11 | 1:A:379:ARG:HH21 | 0.65 | 1.33 | 1 | 2 |
| 1:A:160:ALA:O | 1:A:181:THR:CG2 | 0.65 | 2.44 | 2 | 2 |
| 1:A:301:PHE:O | 1:A:304:ARG:CD | 0.65 | 2.44 | 1 | 2 |
| 1:A:304:ARG:CZ | 1:A:304:ARG:O | 0.65 | 2.44 | 1 | 1 |
| 1:B:438:ILE:O | 1:B:438:ILE:HG23 | 0.65 | 1.91 | 1 | 1 |
| 1:B:160:ALA:O | 1:B:181:THR:CG2 | 0.65 | 2.43 | 2 | 2 |
| 1:A:304:ARG:O | 1:A:304:ARG:CZ | 0.65 | 2.44 | 2 | 1 |
| 1:B:438:ILE:HG23 | 1:B:438:ILE:O | 0.65 | 1.91 | 2 | 1 |
| 1:A:10:GLY:O | 1:A:222:ALA:HB3 | 0.65 | 1.92 | 1 | 2 |
| 1:A:406:ILE:HD13 | 1:A:426:ILE:HD13 | 0.65 | 1.68 | 1 | 2 |
| 1:B:232:THR:HG22 | 1:B:234:GLU:H | 0.65 | 1.51 | 1 | 2 |
| 1:B:406:ILE:HD13 | 1:B:426:ILE:HD13 | 0.65 | 1.68 | 1 | 2 |
| 1:A:180:ILE:CD1 | 1:A:208:VAL:HG11 | 0.65 | 2.21 | 1 | 2 |
| 1:A:258:ASP:N | 1:A:258:ASP:OD1 | 0.65 | 2.30 | 1 | 1 |
| 1:B:230:ASN:N | 1:B:231:PRO:CD | 0.65 | 2.59 | 1 | 2 |
| 1:B:232:THR:HG22 | 1:B:233:ASN:H | 0.65 | 1.34 | 1 | 2 |
| 1:B:456:LEU:CD2 | 1:B:484:LEU:HD11 | 0.65 | 2.22 | 1 | 2 |
| 1:B:230:ASN:N | 1:B:231:PRO:HD3 | 0.64 | 2.07 | 1 | 2 |
| 1:B:505:LEU:HD22 | 1:B:506:ALA:N | 0.64 | 2.07 | 1 | 2 |
| 1:A:355:LEU:O | 1:B:464:ASP:CG | 0.64 | 2.36 | 1 | 2 |
| 1:A:373:GLN:O | 1:A:377:ILE:HG12 | 0.64 | 1.92 | 1 | 2 |
| 1:B:301:PHE:O | 1:B:304:ARG:CD | 0.64 | 2.45 | 1 | 2 |
| 1:B:375:ARG:HH11 | 1:B:379:ARG:HH21 | 0.64 | 1.34 | 1 | 2 |
| 1:A:438:ILE:O | 1:A:438:ILE:HG23 | 0.64 | 1.91 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:259:LEU:CB | 1:A:260:PRO:CD | 0.64 | 2.75 | 1 | 1 |
| 1:B:10:GLY:O | 1:B:222:ALA:HB3 | 0.64 | 1.92 | 1 | 2 |
| 1:B:127:ALA:O | 1:B:130:VAL:HG22 | 0.63 | 1.93 | 2 | 2 |
| 1:B:373:GLN:O | 1:B:377:ILE:HG12 | 0.63 | 1.93 | 1 | 2 |
| 1:A:431:GLU:CD | 1:A:452:GLY:HA3 | 0.63 | 2.13 | 1 | 2 |
| 1:A:505:LEU:HD22 | 1:A:506:ALA:N | 0.63 | 2.08 | 1 | 2 |
| 1:B:431:GLU:CD | 1:B:452:GLY:HA3 | 0.63 | 2.14 | 1 | 2 |
| 1:B:54:LEU:C | 1:B:54:LEU:HD13 | 0.63 | 2.14 | 2 | 2 |
| 1:B:304:ARG:HD2 | 1:B:306:ALA:O | 0.63 | 1.94 | 1 | 2 |
| 1:A:456:LEU:CD2 | 1:A:484:LEU:HD11 | 0.63 | 2.24 | 1 | 2 |
| 1:B:54:LEU:CD2 | 1:B:77:ILE:HG13 | 0.63 | 2.24 | 2 | 2 |
| 1:A:441:HIS:CG | 1:B:556:PRO:HB3 | 0.62 | 2.28 | 1 | 2 |
| 1:B:180:ILE:CD1 | 1:B:208:VAL:HG11 | 0.62 | 2.25 | 1 | 2 |
| 1:B:505:LEU:H | 1:B:505:LEU:CD1 | 0.62 | 2.07 | 1 | 1 |
| 1:B:505:LEU:CD1 | 1:B:505:LEU:H | 0.62 | 2.07 | 2 | 1 |
| 1:A:505:LEU:H | 1:A:505:LEU:CD1 | 0.62 | 2.07 | 1 | 2 |
| 1:A:228:TYR:HB3 | 1:A:231:PRO:CG | 0.62 | 2.25 | 1 | 2 |
| 1:A:501:MET:SD | 1:A:520:LEU:HD22 | 0.62 | 2.35 | 1 | 2 |
| 1:A:301:PHE:O | 1:A:304:ARG:CZ | 0.62 | 2.47 | 1 | 2 |
| 1:B:205:THR:CG2 | 1:B:208:VAL:H | 0.62 | 2.08 | 1 | 2 |
| 1:A:304:ARG:HD2 | 1:A:306:ALA:O | 0.61 | 1.94 | 1 | 2 |
| 1:A:54:LEU:CD2 | 1:A:77:ILE:HG13 | 0.61 | 2.24 | 1 | 2 |
| 1:B:533:ILE:O | 1:B:536:ILE:HG22 | 0.61 | 1.95 | 2 | 2 |
| 1:A:489:ILE:O | 1:A:492:SER:HB2 | 0.61 | 1.95 | 1 | 2 |
| 1:A:205:THR:CG2 | 1:A:208:VAL:H | 0.61 | 2.08 | 2 | 2 |
| 1:A:391:PRO:HA | 1:A:429:MET:HG2 | 0.61 | 1.73 | 1 | 2 |
| 1:A:431:GLU:HG2 | 1:A:452:GLY:H | 0.61 | 1.54 | 1 | 2 |
| 1:B:139:ARG:HB3 | 1:B:144:LEU:CD1 | 0.61 | 2.25 | 1 | 2 |
| 1:A:533:ILE:O | 1:A:536:ILE:HG22 | 0.61 | 1.96 | 2 | 2 |
| 1:A:144:LEU:C | 1:A:144:LEU:HD13 | 0.61 | 2.10 | 2 | 2 |
| 1:A:139:ARG:HB3 | 1:A:144:LEU:CD1 | 0.61 | 2.26 | 2 | 2 |
| 1:B:501:MET:SD | 1:B:520:LEU:HD22 | 0.61 | 2.36 | 1 | 2 |
| 1:B:296:ARG:NE | 1:B:332:ARG:NH2 | 0.61 | 2.49 | 1 | 2 |
| 1:B:391:PRO:HA | 1:B:429:MET:HG2 | 0.61 | 1.72 | 1 | 2 |
| 1:A:90:ILE:HD12 | 1:A:91:ALA:N | 0.60 | 2.11 | 1 | 2 |
| 1:B:228:TYR:HB3 | 1:B:231:PRO:CG | 0.60 | 2.25 | 2 | 2 |
| 1:A:193:MET:HG3 | 1:A:194:ALA:N | 0.60 | 2.11 | 2 | 2 |
| 1:A:287:ASN:HB3 | 1:A:530:ILE:HG23 | 0.60 | 1.72 | 1 | 2 |
| 1:B:90:ILE:HD12 | 1:B:91:ALA:N | 0.60 | 2.10 | 1 | 2 |
| 1:B:489:ILE:O | 1:B:492:SER:HB2 | 0.60 | 1.95 | 1 | 2 |
| 1:A:375:ARG:NH2 | 1:A:416:GLU:OE1 | 0.60 | 2.35 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:193:MET:HG3 | 1:B:194:ALA:N | 0.60 | 2.10 | 2 | 1 |
| 1:A:296:ARG:NE | 1:A:332:ARG:NH2 | 0.60 | 2.49 | 1 | 2 |
| 1:B:387:ARG:HH21 | 1:B:425:GLU:H | 0.60 | 1.40 | 1 | 2 |
| 1:B:301:PHE:O | 1:B:304:ARG:CZ | 0.60 | 2.48 | 1 | 2 |
| 1:B:193:MET:C | 1:B:193:MET:SD | 0.60 | 2.80 | 2 | 1 |
| 1:A:321:ALA:C | 1:A:324:CYS:SG | 0.60 | 2.80 | 1 | 2 |
| 1:A:193:MET:SD | 1:A:197:LEU:CD2 | 0.59 | 2.90 | 1 | 1 |
| 1:B:79:LEU:O | 1:B:79:LEU:HD13 | 0.59 | 1.98 | 2 | 2 |
| 1:A:310:GLU:N | 1:A:372:ASP:OD2 | 0.59 | 2.34 | 1 | 2 |
| 1:B:431:GLU:HG2 | 1:B:452:GLY:H | 0.59 | 1.54 | 1 | 2 |
| 1:A:79:LEU:O | 1:A:79:LEU:HD13 | 0.59 | 1.98 | 1 | 1 |
| 1:B:321:ALA:C | 1:B:324:CYS:SG | 0.59 | 2.81 | 1 | 2 |
| 1:B:320:VAL:O | 1:B:324:CYS:SG | 0.59 | 2.61 | 1 | 2 |
| 1:A:505:LEU:HD13 | 1:A:506:ALA:N | 0.59 | 2.12 | 1 | 2 |
| 1:A:54:LEU:O | 1:A:57:ILE:HG12 | 0.59 | 1.98 | 1 | 2 |
| 1:B:375:ARG:NH2 | 1:B:416:GLU:OE1 | 0.58 | 2.36 | 1 | 2 |
| 1:A:79:LEU:HD13 | 1:A:79:LEU:O | 0.58 | 1.98 | 2 | 1 |
| 1:A:387:ARG:HH21 | 1:A:425:GLU:H | 0.58 | 1.40 | 1 | 2 |
| 1:B:225:ASN:ND2 | 1:B:225:ASN:O | 0.58 | 2.37 | 2 | 2 |
| 1:A:193:MET:C | 1:A:193:MET:SD | 0.58 | 2.81 | 2 | 1 |
| 1:A:320:VAL:O | 1:A:324:CYS:SG | 0.58 | 2.61 | 1 | 2 |
| 1:A:562:MET:SD | 1:A:566:ASN:ND2 | 0.58 | 2.77 | 1 | 2 |
| 1:B:310:GLU:N | 1:B:372:ASP:OD2 | 0.58 | 2.36 | 1 | 2 |
| 1:B:484:LEU:C | 1:B:484:LEU:HD23 | 0.58 | 2.18 | 1 | 1 |
| 1:B:484:LEU:HD23 | 1:B:484:LEU:C | 0.58 | 2.18 | 2 | 1 |
| 1:A:421:ASP:OD1 | 1:A:423:SER:HB2 | 0.58 | 1.99 | 1 | 2 |
| 1:B:514:LEU:O | 1:B:518:MET:CG | 0.58 | 2.52 | 1 | 2 |
| 1:B:421:ASP:OD1 | 1:B:423:SER:HB2 | 0.58 | 1.99 | 1 | 2 |
| 1:A:89:ILE:O | 1:A:89:ILE:HD13 | 0.58 | 1.99 | 1 | 1 |
| 1:A:89:ILE:HD13 | 1:A:89:ILE:O | 0.58 | 1.99 | 2 | 1 |
| 1:A:481:VAL:O | 1:A:485:ILE:CG2 | 0.57 | 2.48 | 1 | 2 |
| 1:B:481:VAL:O | 1:B:485:ILE:CG2 | 0.57 | 2.48 | 1 | 2 |
| 1:B:562:MET:SD | 1:B:566:ASN:ND2 | 0.57 | 2.78 | 1 | 2 |
| 1:B:54:LEU:HG | 1:B:77:ILE:HD12 | 0.57 | 1.76 | 1 | 2 |
| 1:B:182:ASP:OD1 | 1:B:182:ASP:N | 0.57 | 2.38 | 2 | 2 |
| 1:A:484:LEU:HD23 | 1:A:484:LEU:C | 0.57 | 2.19 | 1 | 1 |
| 1:A:464:ASP:OD1 | 1:B:355:LEU:O | 0.57 | 2.23 | 1 | 2 |
| 1:A:484:LEU:C | 1:A:484:LEU:HD23 | 0.57 | 2.19 | 2 | 1 |
| 1:B:451:ILE:N | 1:B:451:ILE:CD1 | 0.57 | 2.68 | 1 | 1 |
| 1:B:505:LEU:HD13 | 1:B:506:ALA:N | 0.57 | 2.13 | 1 | 2 |
| 1:B:54:LEU:HG | 1:B:77:ILE:CD1 | 0.57 | 2.29 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:451:ILE:CD1 | 1:B:451:ILE:N | 0.57 | 2.68 | 2 | 1 |
| 1:A:514:LEU:O | 1:A:518:MET:CG | 0.57 | 2.52 | 1 | 2 |
| 1:A:225:ASN:ND2 | 1:A:225:ASN:O | 0.57 | 2.37 | 1 | 2 |
| 1:B:54:LEU:O | 1:B:57:ILE:HG12 | 0.57 | 1.99 | 1 | 2 |
| 1:B:176:VAL:HG13 | 1:B:176:VAL:O | 0.57 | 1.99 | 2 | 2 |
| 1:A:11:ILE:HG21 | 1:A:243:GLN:CB | 0.57 | 2.30 | 1 | 2 |
| 1:A:287:ASN:HB3 | 1:A:530:ILE:CG2 | 0.57 | 2.30 | 1 | 1 |
| 1:A:89:ILE:CG2 | 1:A:90:ILE:N | 0.57 | 2.68 | 2 | 2 |
| 1:A:13:PHE:CD2 | 1:A:240:ARG:NH1 | 0.57 | 2.73 | 1 | 2 |
| 1:A:451:ILE:CD1 | 1:A:451:ILE:N | 0.57 | 2.68 | 1 | 2 |
| 1:A:133:ILE:CG2 | 1:A:134:GLY:N | 0.57 | 2.67 | 2 | 2 |
| 1:A:176:VAL:HG13 | 1:A:176:VAL:O | 0.57 | 2.00 | 2 | 1 |
| 1:A:179:PHE:CE2 | 1:A:190:THR:OG1 | 0.56 | 2.51 | 2 | 1 |
| 1:B:179:PHE:CE2 | 1:B:190:THR:OG1 | 0.56 | 2.51 | 2 | 1 |
| 1:A:292:VAL:HG12 | 1:A:327:GLN:NE2 | 0.56 | 2.15 | 1 | 2 |
| 1:A:486:LYS:HD2 | 1:A:553:LEU:HD13 | 0.56 | 1.76 | 1 | 2 |
| 1:A:54:LEU:HG | 1:A:77:ILE:HD12 | 0.56 | 1.76 | 2 | 2 |
| 1:A:54:LEU:C | 1:A:54:LEU:HD13 | 0.56 | 2.15 | 2 | 1 |
| 1:B:486:LYS:HD2 | 1:B:553:LEU:HD13 | 0.56 | 1.75 | 1 | 2 |
| 1:B:223:VAL:HG23 | 1:B:224:ASN:N | 0.56 | 2.16 | 1 | 2 |
| 1:B:294:LEU:CB | 1:B:502:CYS:SG | 0.56 | 2.94 | 1 | 2 |
| 1:B:321:ALA:HA | 1:B:324:CYS:SG | 0.56 | 2.40 | 1 | 2 |
| 1:B:13:PHE:CD2 | 1:B:240:ARG:NH1 | 0.56 | 2.73 | 2 | 2 |
| 1:B:89:ILE:CG2 | 1:B:90:ILE:N | 0.56 | 2.68 | 2 | 2 |
| 1:A:182:ASP:N | 1:A:182:ASP:OD1 | 0.56 | 2.37 | 2 | 2 |
| 1:B:133:ILE:CG2 | 1:B:134:GLY:N | 0.56 | 2.67 | 2 | 2 |
| 1:B:485:ILE:CG1 | 1:B:486:LYS:N | 0.56 | 2.68 | 1 | 2 |
| 1:A:176:VAL:O | 1:A:176:VAL:HG13 | 0.56 | 2.00 | 1 | 1 |
| 1:A:74:GLU:HG3 | 1:A:75:GLY:N | 0.56 | 2.16 | 2 | 2 |
| 1:A:54:LEU:HG | 1:A:77:ILE:CD1 | 0.56 | 2.31 | 1 | 2 |
| 1:B:278:VAL:HG23 | 1:B:279:ARG:N | 0.56 | 2.16 | 1 | 2 |
| 1:B:89:ILE:O | 1:B:89:ILE:HD13 | 0.56 | 1.99 | 2 | 1 |
| 1:A:485:ILE:CG1 | 1:A:486:LYS:N | 0.56 | 2.68 | 1 | 2 |
| 1:B:330:ILE:CD1 | 1:B:330:ILE:C | 0.56 | 2.72 | 1 | 1 |
| 1:B:412:GLU:O | 1:B:416:GLU:HG3 | 0.56 | 2.01 | 1 | 2 |
| 1:B:330:ILE:C | 1:B:330:ILE:CD1 | 0.56 | 2.72 | 2 | 1 |
| 1:A:294:LEU:CB | 1:A:502:CYS:SG | 0.56 | 2.93 | 1 | 2 |
| 1:A:77:ILE:H | 1:A:77:ILE:HD13 | 0.56 | 1.57 | 2 | 1 |
| 1:A:321:ALA:HA | 1:A:324:CYS:SG | 0.56 | 2.41 | 1 | 2 |
| 1:B:11:ILE:HG21 | 1:B:243:GLN:CB | 0.56 | 2.30 | 1 | 2 |
| 1:B:292:VAL:HG12 | 1:B:327:GLN:NE2 | 0.56 | 2.15 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:505:LEU:HD12 | 1:B:505:LEU:H | 0.56 | 1.61 | 1 | 2 |
| 1:A:223:VAL:HG23 | 1:A:224:ASN:N | 0.55 | 2.16 | 2 | 2 |
| 1:A:412:GLU:O | 1:A:416:GLU:HG3 | 0.55 | 2.01 | 1 | 2 |
| 1:B:89:ILE:HD13 | 1:B:89:ILE:O | 0.55 | 1.99 | 1 | 1 |
| 1:B:74:GLU:HG3 | 1:B:75:GLY:N | 0.55 | 2.17 | 2 | 2 |
| 1:A:324:CYS:CB | 1:A:327:GLN:NE2 | 0.55 | 2.70 | 1 | 2 |
| 1:A:54:LEU:HD13 | 1:A:54:LEU:C | 0.55 | 2.15 | 1 | 1 |
| 1:B:221:ASP:OD2 | 1:B:226:GLN:HB2 | 0.55 | 2.02 | 1 | 2 |
| 1:A:105:HIS:CE1 | 1:A:109:GLU:OE1 | 0.55 | 2.60 | 1 | 2 |
| 1:A:278:VAL:HG23 | 1:A:279:ARG:N | 0.55 | 2.16 | 1 | 2 |
| 1:B:74:GLU:C | 1:B:74:GLU:CD | 0.55 | 2.64 | 1 | 1 |
| 1:A:67:GLU:CD | 1:A:67:GLU:H | 0.55 | 2.05 | 2 | 1 |
| 1:B:530:ILE:CD1 | 1:B:530:ILE:C | 0.55 | 2.72 | 2 | 1 |
| 1:A:221:ASP:OD2 | 1:A:226:GLN:HB2 | 0.55 | 2.02 | 1 | 2 |
| 1:B:13:PHE:CD1 | 1:B:13:PHE:N | 0.55 | 2.74 | 2 | 2 |
| 1:B:105:HIS:CE1 | 1:B:109:GLU:OE1 | 0.55 | 2.60 | 1 | 2 |
| 1:B:67:GLU:CD | 1:B:67:GLU:H | 0.55 | 2.04 | 2 | 1 |
| 1:B:74:GLU:CD | 1:B:74:GLU:C | 0.55 | 2.64 | 2 | 1 |
| 1:A:505:LEU:HD12 | 1:A:505:LEU:H | 0.55 | 1.61 | 1 | 2 |
| 1:A:74:GLU:C | 1:A:74:GLU:CD | 0.55 | 2.65 | 1 | 2 |
| 1:B:179:PHE:CE2 | 1:B:181:THR:OG1 | 0.55 | 2.60 | 1 | 2 |
| 1:A:252:GLU:O | 1:A:255:LYS:HG2 | 0.54 | 2.02 | 1 | 1 |
| 1:A:13:PHE:CD1 | 1:A:13:PHE:N | 0.54 | 2.74 | 1 | 1 |
| 1:A:144:LEU:HD22 | 1:A:145:LYS:C | 0.54 | 2.22 | 1 | 2 |
| 1:A:221:ASP:CA | 1:A:239:MET:CE | 0.54 | 2.78 | 1 | 2 |
| 1:A:259:LEU:HB3 | 1:A:260:PRO:CD | 0.54 | 2.31 | 1 | 1 |
| 1:B:330:ILE:O | 1:B:330:ILE:CG1 | 0.54 | 2.55 | 1 | 2 |
| 1:A:330:ILE:O | 1:A:330:ILE:CG1 | 0.54 | 2.55 | 1 | 1 |
| 1:A:330:ILE:CG1 | 1:A:330:ILE:O | 0.54 | 2.55 | 2 | 1 |
| 1:A:179:PHE:CE2 | 1:A:181:THR:OG1 | 0.54 | 2.61 | 1 | 2 |
| 1:A:294:LEU:CD1 | 1:A:502:CYS:SG | 0.54 | 2.95 | 1 | 2 |
| 1:A:405:GLU:HG3 | 1:A:409:TYR:CE2 | 0.54 | 2.38 | 1 | 2 |
| 1:B:324:CYS:CB | 1:B:327:GLN:NE2 | 0.54 | 2.71 | 1 | 2 |
| 1:B:144:LEU:CD2 | 1:B:144:LEU:C | 0.54 | 2.63 | 2 | 1 |
| 1:B:268:GLN:CD | 1:B:268:GLN:H | 0.54 | 2.06 | 1 | 2 |
| 1:A:13:PHE:N | 1:A:13:PHE:CD1 | 0.54 | 2.74 | 2 | 1 |
| 1:B:54:LEU:CD1 | 1:B:54:LEU:C | 0.54 | 2.76 | 2 | 1 |
| 1:A:77:ILE:HD13 | 1:A:77:ILE:H | 0.54 | 1.57 | 1 | 1 |
| 1:A:388:ILE:HD12 | 1:A:388:ILE:C | 0.54 | 2.23 | 1 | 1 |
| 1:B:513:LEU:CD2 | 1:B:568:PHE:CE1 | 0.54 | 2.91 | 1 | 2 |
| 1:A:388:ILE:C | 1:A:388:ILE:HD12 | 0.54 | 2.23 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:193:MET:CG | 1:B:194:ALA:N | 0.54 | 2.71 | 2 | 1 |
| 1:A:513:LEU:CD2 | 1:A:568:PHE:CE1 | 0.53 | 2.92 | 1 | 2 |
| 1:B:331:VAL:HG11 | 1:B:377:ILE:HD12 | 0.53 | 1.80 | 1 | 2 |
| 1:B:294:LEU:CD1 | 1:B:502:CYS:SG | 0.53 | 2.94 | 1 | 2 |
| 1:B:221:ASP:OD2 | 1:B:224:ASN:ND2 | 0.53 | 2.41 | 2 | 2 |
| 1:A:221:ASP:OD2 | 1:A:224:ASN:ND2 | 0.53 | 2.41 | 1 | 2 |
| 1:A:473:LEU:N | 1:A:473:LEU:CD2 | 0.53 | 2.71 | 1 | 1 |
| 1:B:350:GLU:N | 1:B:350:GLU:OE1 | 0.53 | 2.41 | 1 | 2 |
| 1:B:144:LEU:HD22 | 1:B:145:LYS:C | 0.53 | 2.22 | 2 | 2 |
| 1:A:202:ILE:HD11 | 1:A:205:THR:HB | 0.53 | 1.79 | 2 | 2 |
| 1:A:473:LEU:CD2 | 1:A:473:LEU:N | 0.53 | 2.71 | 2 | 1 |
| 1:A:355:LEU:O | 1:B:464:ASP:OD1 | 0.53 | 2.25 | 1 | 2 |
| 1:B:54:LEU:CG | 1:B:77:ILE:HG13 | 0.53 | 2.33 | 1 | 2 |
| 1:B:144:LEU:HD22 | 1:B:145:LYS:N | 0.53 | 2.19 | 2 | 2 |
| 1:B:405:GLU:HG3 | 1:B:409:TYR:CE2 | 0.53 | 2.38 | 1 | 2 |
| 1:A:73:PHE:O | 1:A:77:ILE:CG1 | 0.53 | 2.57 | 1 | 2 |
| 1:B:202:ILE:HD11 | 1:B:205:THR:HB | 0.53 | 1.80 | 2 | 2 |
| 1:B:265:ASP:OD2 | 1:B:541:ASN:ND2 | 0.53 | 2.42 | 1 | 2 |
| 1:B:473:LEU:N | 1:B:473:LEU:CD2 | 0.53 | 2.72 | 1 | 1 |
| 1:A:54:LEU:CD1 | 1:A:54:LEU:C | 0.53 | 2.77 | 2 | 1 |
| 1:B:473:LEU:CD2 | 1:B:473:LEU:N | 0.53 | 2.72 | 2 | 1 |
| 1:A:268:GLN:H | 1:A:268:GLN:CD | 0.53 | 2.06 | 1 | 2 |
| 1:A:278:VAL:CG2 | 1:A:279:ARG:N | 0.53 | 2.72 | 1 | 2 |
| 1:A:309:THR:C | 1:A:372:ASP:OD2 | 0.53 | 2.48 | 1 | 2 |
| 1:A:375:ARG:NH1 | 1:A:379:ARG:NH2 | 0.53 | 2.57 | 1 | 2 |
| 1:B:294:LEU:HA | 1:B:330:ILE:HG13 | 0.53 | 1.81 | 1 | 2 |
| 1:B:73:PHE:O | 1:B:77:ILE:CG1 | 0.53 | 2.57 | 1 | 2 |
| 1:B:453:THR:OG1 | 1:B:505:LEU:CD1 | 0.52 | 2.58 | 1 | 2 |
| 1:A:265:ASP:OD2 | 1:A:541:ASN:ND2 | 0.52 | 2.42 | 1 | 2 |
| 1:A:350:GLU:N | 1:A:350:GLU:OE1 | 0.52 | 2.42 | 1 | 1 |
| 1:A:54:LEU:HD21 | 1:A:77:ILE:CG1 | 0.52 | 2.33 | 1 | 2 |
| 1:B:451:ILE:HD13 | 1:B:499:THR:HG23 | 0.52 | 1.81 | 1 | 2 |
| 1:A:193:MET:CG | 1:A:194:ALA:N | 0.52 | 2.71 | 2 | 1 |
| 1:A:350:GLU:OE1 | 1:A:350:GLU:N | 0.52 | 2.42 | 2 | 1 |
| 1:B:438:ILE:CG2 | 1:B:438:ILE:O | 0.52 | 2.57 | 1 | 1 |
| 1:B:438:ILE:O | 1:B:438:ILE:CG2 | 0.52 | 2.57 | 2 | 1 |
| 1:B:54:LEU:HD13 | 1:B:55:GLU:CA | 0.52 | 2.32 | 1 | 2 |
| 1:A:438:ILE:O | 1:A:438:ILE:CG2 | 0.52 | 2.58 | 1 | 2 |
| 1:A:514:LEU:O | 1:A:518:MET:HG3 | 0.52 | 2.05 | 1 | 2 |
| 1:A:453:THR:OG1 | 1:A:505:LEU:CD1 | 0.52 | 2.57 | 1 | 2 |
| 1:A:463:VAL:CG1 | 1:B:361:ARG:NH1 | 0.52 | 2.73 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:451:ILE:HD13 | 1:A:499:THR:HG23 | 0.52 | 1.81 | 1 | 2 |
| 1:B:309:THR:C | 1:B:372:ASP:OD2 | 0.52 | 2.48 | 1 | 2 |
| 1:A:205:THR:HG21 | 1:A:208:VAL:HG12 | 0.52 | 1.81 | 2 | 2 |
| 1:A:274:ASN:ND2 | 1:A:525:MET:C | 0.52 | 2.63 | 1 | 2 |
| 1:A:331:VAL:HG11 | 1:A:377:ILE:HD12 | 0.52 | 1.80 | 1 | 2 |
| 1:B:229:VAL:C | 1:B:231:PRO:HD3 | 0.52 | 2.25 | 1 | 2 |
| 1:B:278:VAL:CG2 | 1:B:279:ARG:N | 0.52 | 2.72 | 1 | 2 |
| 1:B:375:ARG:NH1 | 1:B:379:ARG:NH2 | 0.52 | 2.58 | 1 | 2 |
| 1:B:68:GLU:CB | 1:B:279:ARG:HH21 | 0.52 | 2.18 | 1 | 1 |
| 1:B:292:VAL:HG22 | 1:B:329:VAL:HA | 0.52 | 1.82 | 1 | 2 |
| 1:B:54:LEU:HD21 | 1:B:77:ILE:CG1 | 0.52 | 2.33 | 1 | 2 |
| 1:B:86:GLU:O | 1:B:90:ILE:CG1 | 0.52 | 2.58 | 2 | 2 |
| 1:A:205:THR:CG2 | 1:A:206:GLY:N | 0.52 | 2.73 | 1 | 2 |
| 1:A:321:ALA:CA | 1:A:324:CYS:SG | 0.52 | 2.98 | 1 | 2 |
| 1:A:54:LEU:CG | 1:A:77:ILE:HG13 | 0.52 | 2.34 | 1 | 2 |
| 1:B:321:ALA:CA | 1:B:324:CYS:SG | 0.52 | 2.98 | 1 | 2 |
| 1:B:514:LEU:O | 1:B:518:MET:HG3 | 0.52 | 2.05 | 1 | 2 |
| 1:A:515:LEU:N | 1:A:515:LEU:CD1 | 0.51 | 2.74 | 1 | 2 |
| 1:A:86:GLU:O | 1:A:90:ILE:CG1 | 0.51 | 2.58 | 1 | 2 |
| 1:B:274:ASN:ND2 | 1:B:525:MET:C | 0.51 | 2.64 | 1 | 2 |
| 1:B:292:VAL:O | 1:B:330:ILE:HG23 | 0.51 | 2.05 | 1 | 2 |
| 1:A:229:VAL:C | 1:A:231:PRO:HD3 | 0.51 | 2.25 | 1 | 2 |
| 1:A:221:ASP:OD1 | 1:A:239:MET:SD | 0.51 | 2.68 | 1 | 2 |
| 1:A:144:LEU:HD22 | 1:A:145:LYS:N | 0.51 | 2.19 | 1 | 2 |
| 1:A:3:SER:OG | 1:A:225:ASN:ND2 | 0.51 | 2.43 | 1 | 2 |
| 1:B:205:THR:CG2 | 1:B:206:GLY:N | 0.51 | 2.73 | 2 | 2 |
| 1:B:221:ASP:OD1 | 1:B:239:MET:SD | 0.51 | 2.69 | 1 | 2 |
| 1:B:255:LYS:NZ | 1:B:258:ASP:OD2 | 0.51 | 2.40 | 1 | 1 |
| 1:B:557:THR:HB | 1:B:560:GLU:OE1 | 0.51 | 2.05 | 1 | 2 |
| 1:A:294:LEU:HA | 1:A:330:ILE:HG13 | 0.51 | 1.81 | 1 | 2 |
| 1:B:202:ILE:C | 1:B:202:ILE:HD13 | 0.51 | 2.26 | 1 | 1 |
| 1:B:77:ILE:HD13 | 1:B:77:ILE:H | 0.51 | 1.58 | 1 | 1 |
| 1:B:168:THR:HG21 | 1:B:193:MET:SD | 0.51 | 2.45 | 1 | 1 |
| 1:A:292:VAL:HG22 | 1:A:329:VAL:HA | 0.51 | 1.81 | 1 | 2 |
| 1:B:3:SER:OG | 1:B:225:ASN:ND2 | 0.51 | 2.43 | 2 | 2 |
| 1:A:292:VAL:O | 1:A:330:ILE:HG23 | 0.51 | 2.04 | 1 | 2 |
| 1:A:324:CYS:HB2 | 1:A:327:GLN:NE2 | 0.51 | 2.21 | 1 | 2 |
| 1:B:431:GLU:HG2 | 1:B:452:GLY:N | 0.51 | 2.21 | 1 | 2 |
| 1:A:219:ILE:CD1 | 1:A:236:ILE:HG12 | 0.51 | 2.36 | 2 | 2 |
| 1:B:202:ILE:HD13 | 1:B:202:ILE:C | 0.51 | 2.26 | 2 | 1 |
| 1:A:451:ILE:HD12 | 1:A:451:ILE:N | 0.50 | 2.20 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:221:ASP:CA | 1:B:239:MET:CE | 0.50 | 2.78 | 1 | 2 |
| 1:B:388:ILE:C | 1:B:388:ILE:HD12 | 0.50 | 2.26 | 1 | 1 |
| 1:B:388:ILE:HD12 | 1:B:388:ILE:C | 0.50 | 2.26 | 2 | 1 |
| 1:B:219:ILE:CD1 | 1:B:236:ILE:HG12 | 0.50 | 2.36 | 1 | 2 |
| 1:B:451:ILE:HD12 | 1:B:451:ILE:N | 0.50 | 2.20 | 1 | 1 |
| 1:B:451:ILE:N | 1:B:451:ILE:HD12 | 0.50 | 2.20 | 2 | 1 |
| 1:B:205:THR:HG22 | 1:B:206:GLY:N | 0.50 | 2.21 | 1 | 2 |
| 1:B:375:ARG:HH11 | 1:B:379:ARG:NH2 | 0.50 | 2.04 | 1 | 2 |
| 1:B:144:LEU:O | 1:B:144:LEU:HD22 | 0.50 | 2.07 | 1 | 2 |
| 1:A:172:ASN:O | 1:A:176:VAL:HG12 | 0.50 | 2.06 | 2 | 2 |
| 1:B:324:CYS:HB2 | 1:B:327:GLN:NE2 | 0.50 | 2.22 | 1 | 2 |
| 1:A:375:ARG:HH11 | 1:A:379:ARG:NH2 | 0.50 | 2.03 | 1 | 2 |
| 1:A:294:LEU:HB2 | 1:A:502:CYS:SG | 0.50 | 2.46 | 1 | 2 |
| 1:A:556:PRO:HB3 | 1:B:441:HIS:CE1 | 0.50 | 2.41 | 1 | 2 |
| 1:B:256:LEU:CD1 | 1:B:256:LEU:C | 0.50 | 2.80 | 1 | 1 |
| 1:B:386:LEU:O | 1:B:387:ARG:CZ | 0.50 | 2.59 | 1 | 2 |
| 1:B:456:LEU:HD22 | 1:B:484:LEU:CD1 | 0.50 | 2.36 | 1 | 2 |
| 1:B:205:THR:HG21 | 1:B:208:VAL:HG12 | 0.50 | 1.83 | 2 | 2 |
| 1:B:294:LEU:HB2 | 1:B:502:CYS:SG | 0.50 | 2.47 | 1 | 2 |
| 1:B:53:GLN:O | 1:B:57:ILE:HG23 | 0.50 | 2.06 | 1 | 2 |
| 1:B:221:ASP:O | 1:B:223:VAL:HG13 | 0.50 | 2.06 | 2 | 2 |
| 1:A:144:LEU:O | 1:A:144:LEU:HD22 | 0.50 | 2.07 | 1 | 1 |
| 1:A:431:GLU:HG2 | 1:A:452:GLY:N | 0.50 | 2.21 | 1 | 2 |
| 1:A:557:THR:HB | 1:A:560:GLU:OE1 | 0.50 | 2.05 | 1 | 2 |
| 1:A:205:THR:HG22 | 1:A:206:GLY:N | 0.49 | 2.22 | 1 | 2 |
| 1:A:330:ILE:O | 1:A:330:ILE:HD12 | 0.49 | 2.06 | 1 | 1 |
| 1:A:293:GLY:O | 1:A:330:ILE:HG12 | 0.49 | 2.07 | 1 | 2 |
| 1:A:54:LEU:C | 1:A:54:LEU:CD1 | 0.49 | 2.77 | 1 | 1 |
| 1:B:515:LEU:CD1 | 1:B:515:LEU:N | 0.49 | 2.74 | 1 | 1 |
| 1:A:330:ILE:HD12 | 1:A:330:ILE:O | 0.49 | 2.06 | 2 | 1 |
| 1:B:515:LEU:N | 1:B:515:LEU:CD1 | 0.49 | 2.74 | 2 | 1 |
| 1:A:53:GLN:O | 1:A:57:ILE:HG23 | 0.49 | 2.06 | 1 | 2 |
| 1:A:459:TYR:HB3 | 1:B:459:TYR:O | 0.49 | 2.07 | 1 | 2 |
| 1:A:386:LEU:O | 1:A:387:ARG:CZ | 0.49 | 2.59 | 1 | 2 |
| 1:A:80:LEU:HD13 | 1:A:137:LEU:HD11 | 0.49 | 1.84 | 2 | 2 |
| 1:B:144:LEU:CD1 | 1:B:144:LEU:C | 0.49 | 2.78 | 2 | 2 |
| 1:A:105:HIS:NE2 | 1:A:109:GLU:CD | 0.49 | 2.66 | 1 | 2 |
| 1:A:293:GLY:O | 1:A:330:ILE:CG1 | 0.49 | 2.61 | 1 | 2 |
| 1:B:68:GLU:OE2 | 1:B:69:LYS:NZ | 0.49 | 2.36 | 1 | 1 |
| 1:A:202:ILE:C | 1:A:202:ILE:HD13 | 0.49 | 2.27 | 2 | 2 |
| 1:B:158:LEU:O | 1:B:180:ILE:HG23 | 0.49 | 2.07 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:54:LEU:C | 1:B:54:LEU:CD1 | 0.49 | 2.76 | 1 | 1 |
| 1:A:144:LEU:HD22 | 1:A:144:LEU:O | 0.49 | 2.07 | 2 | 1 |
| 1:A:182:ASP:OD2 | 1:A:209:THR:CG2 | 0.49 | 2.61 | 1 | 2 |
| 1:A:252:GLU:O | 1:A:255:LYS:CG | 0.49 | 2.61 | 1 | 1 |
| 1:B:105:HIS:NE2 | 1:B:109:GLU:CD | 0.49 | 2.66 | 1 | 2 |
| 1:A:57:ILE:CG1 | 1:A:58:LYS:N | 0.49 | 2.76 | 1 | 2 |
| 1:B:182:ASP:OD2 | 1:B:209:THR:CG2 | 0.49 | 2.60 | 1 | 2 |
| 1:B:233:ASN:O | 1:B:237:ASP:OD2 | 0.49 | 2.31 | 1 | 2 |
| 1:B:363:ALA:HB1 | 1:B:370:LEU:HB2 | 0.49 | 1.85 | 1 | 2 |
| 1:B:57:ILE:CG1 | 1:B:58:LYS:N | 0.49 | 2.76 | 1 | 2 |
| 1:B:80:LEU:HD13 | 1:B:137:LEU:HD11 | 0.49 | 1.84 | 1 | 2 |
| 1:A:233:ASN:O | 1:A:237:ASP:OD2 | 0.49 | 2.31 | 2 | 2 |
| 1:A:221:ASP:O | 1:A:223:VAL:HG13 | 0.49 | 2.08 | 1 | 2 |
| 1:B:330:ILE:O | 1:B:330:ILE:HD12 | 0.49 | 2.06 | 1 | 2 |
| 1:B:330:ILE:O | 1:B:330:ILE:HG13 | 0.49 | 2.08 | 1 | 2 |
| 1:A:330:ILE:CD1 | 1:A:330:ILE:C | 0.49 | 2.72 | 1 | 1 |
| 1:B:341:GLU:OE1 | 1:B:343:PRO:N | 0.49 | 2.46 | 1 | 2 |
| 1:A:330:ILE:C | 1:A:330:ILE:CD1 | 0.49 | 2.72 | 2 | 1 |
| 1:B:77:ILE:H | 1:B:77:ILE:HD13 | 0.49 | 1.58 | 2 | 1 |
| 1:A:431:GLU:CA | 1:A:456:LEU:HG | 0.48 | 2.37 | 1 | 2 |
| 1:B:293:GLY:O | 1:B:330:ILE:CG1 | 0.48 | 2.61 | 1 | 2 |
| 1:A:74:GLU:CG | 1:A:75:GLY:N | 0.48 | 2.76 | 1 | 2 |
| 1:A:101:ASP:N | 1:A:101:ASP:OD1 | 0.48 | 2.45 | 2 | 1 |
| 1:A:557:THR:HG22 | 1:A:560:GLU:H | 0.48 | 1.69 | 1 | 2 |
| 1:A:101:ASP:OD1 | 1:A:101:ASP:N | 0.48 | 2.45 | 1 | 1 |
| 1:A:341:GLU:OE1 | 1:A:343:PRO:N | 0.48 | 2.47 | 1 | 2 |
| 1:B:172:ASN:O | 1:B:176:VAL:HG12 | 0.48 | 2.08 | 1 | 2 |
| 1:B:293:GLY:O | 1:B:330:ILE:HG12 | 0.48 | 2.08 | 1 | 2 |
| 1:B:429:MET:CE | 1:B:431:GLU:CD | 0.48 | 2.82 | 1 | 2 |
| 1:B:74:GLU:CG | 1:B:75:GLY:N | 0.48 | 2.76 | 1 | 2 |
| 1:B:144:LEU:CD1 | 1:B:144:LEU:N | 0.48 | 2.77 | 2 | 2 |
| 1:A:8:SER:OG | 1:A:199:LEU:O | 0.48 | 2.28 | 2 | 2 |
| 1:A:144:LEU:C | 1:A:144:LEU:CD2 | 0.48 | 2.63 | 2 | 2 |
| 1:A:270:GLU:N | 1:A:270:GLU:OE1 | 0.48 | 2.47 | 1 | 1 |
| 1:A:388:ILE:CD1 | 1:A:388:ILE:C | 0.48 | 2.81 | 1 | 1 |
| 1:A:139:ARG:CB | 1:A:144:LEU:CD1 | 0.48 | 2.92 | 2 | 2 |
| 1:B:139:ARG:CB | 1:B:144:LEU:CD1 | 0.48 | 2.92 | 2 | 2 |
| 1:A:270:GLU:OE1 | 1:A:270:GLU:N | 0.48 | 2.47 | 2 | 1 |
| 1:A:388:ILE:C | 1:A:388:ILE:CD1 | 0.48 | 2.81 | 2 | 1 |
| 1:B:10:GLY:O | 1:B:221:ASP:O | 0.48 | 2.32 | 1 | 2 |
| 1:B:301:PHE:HD1 | 1:B:301:PHE:O | 0.48 | 1.92 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:10:GLY:O | 1:A:221:ASP:O | 0.48 | 2.32 | 2 | 2 |
| 1:B:282:GLU:O | 1:B:286:ARG:HG2 | 0.48 | 2.09 | 2 | 1 |
| 1:A:330:ILE:O | 1:A:330:ILE:HG13 | 0.47 | 2.08 | 1 | 1 |
| 1:A:363:ALA:HB1 | 1:A:370:LEU:HB2 | 0.47 | 1.85 | 1 | 2 |
| 1:A:54:LEU:HD13 | 1:A:55:GLU:CA | 0.47 | 2.33 | 1 | 2 |
| 1:B:557:THR:HG22 | 1:B:560:GLU:H | 0.47 | 1.69 | 1 | 2 |
| 1:A:330:ILE:HG13 | 1:A:330:ILE:O | 0.47 | 2.08 | 2 | 1 |
| 1:A:324:CYS:HB2 | 1:A:327:GLN:CD | 0.47 | 2.30 | 1 | 2 |
| 1:A:327:GLN:C | 1:A:327:GLN:OE1 | 0.47 | 2.52 | 1 | 2 |
| 1:B:221:ASP:C | 1:B:223:VAL:N | 0.47 | 2.66 | 1 | 2 |
| 1:B:221:ASP:O | 1:B:223:VAL:N | 0.47 | 2.48 | 1 | 2 |
| 1:B:530:ILE:HG23 | 1:B:531:PRO:HD3 | 0.47 | 1.85 | 2 | 1 |
| 1:B:388:ILE:C | 1:B:388:ILE:CD1 | 0.47 | 2.83 | 1 | 2 |
| 1:A:144:LEU:N | 1:A:144:LEU:CD1 | 0.47 | 2.77 | 2 | 2 |
| 1:A:335:ASP:O | 1:A:335:ASP:OD1 | 0.47 | 2.33 | 1 | 2 |
| 1:B:391:PRO:CA | 1:B:429:MET:HG2 | 0.47 | 2.38 | 1 | 2 |
| 1:B:202:ILE:C | 1:B:202:ILE:CD1 | 0.47 | 2.83 | 2 | 2 |
| 1:A:126:ARG:O | 1:A:130:VAL:HG13 | 0.47 | 2.10 | 1 | 2 |
| 1:A:330:ILE:O | 1:A:330:ILE:CD1 | 0.47 | 2.62 | 1 | 1 |
| 1:A:429:MET:CE | 1:A:431:GLU:CD | 0.47 | 2.83 | 1 | 2 |
| 1:B:274:ASN:HD22 | 1:B:525:MET:C | 0.47 | 2.13 | 1 | 2 |
| 1:A:330:ILE:CD1 | 1:A:330:ILE:O | 0.47 | 2.62 | 2 | 1 |
| 1:A:358:ARG:NH1 | 1:A:392:MET:SD | 0.47 | 2.87 | 1 | 2 |
| 1:A:538:ARG:NE | 1:A:538:ARG:O | 0.47 | 2.45 | 1 | 2 |
| 1:B:324:CYS:HB2 | 1:B:327:GLN:CD | 0.47 | 2.30 | 1 | 2 |
| 1:B:11:ILE:CD1 | 1:B:13:PHE:CZ | 0.47 | 2.94 | 2 | 2 |
| 1:B:330:ILE:O | 1:B:330:ILE:CD1 | 0.47 | 2.62 | 1 | 1 |
| 1:B:562:MET:CG | 1:B:562:MET:CE | 0.47 | 2.92 | 1 | 1 |
| 1:B:68:GLU:HB2 | 1:B:279:ARG:HH21 | 0.47 | 1.69 | 1 | 1 |
| 1:A:254:ALA:O | 1:A:255:LYS:C | 0.47 | 2.53 | 1 | 1 |
| 1:B:270:GLU:OE1 | 1:B:270:GLU:N | 0.47 | 2.48 | 1 | 1 |
| 1:B:335:ASP:OD1 | 1:B:335:ASP:O | 0.47 | 2.33 | 1 | 1 |
| 1:B:451:ILE:HG23 | 1:B:456:LEU:HD12 | 0.47 | 1.86 | 1 | 2 |
| 1:B:542:PHE:C | 1:B:542:PHE:CD1 | 0.47 | 2.88 | 1 | 1 |
| 1:B:123:LEU:HD12 | 1:B:123:LEU:N | 0.47 | 2.24 | 2 | 2 |
| 1:B:330:ILE:CD1 | 1:B:330:ILE:O | 0.47 | 2.62 | 2 | 1 |
| 1:B:562:MET:CE | 1:B:562:MET:CG | 0.47 | 2.92 | 2 | 1 |
| 1:B:270:GLU:N | 1:B:270:GLU:OE1 | 0.47 | 2.48 | 2 | 1 |
| 1:B:335:ASP:O | 1:B:335:ASP:OD1 | 0.47 | 2.33 | 2 | 1 |
| 1:B:542:PHE:CD1 | 1:B:542:PHE:C | 0.47 | 2.88 | 2 | 1 |
| 1:A:11:ILE:CG2 | 1:A:243:GLN:HB2 | 0.47 | 2.40 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:451:ILE:HG23 | 1:A:456:LEU:HD12 | 0.47 | 1.86 | 1 | 2 |
| 1:B:8:SER:OG | 1:B:199:LEU:O | 0.47 | 2.28 | 1 | 2 |
| 1:B:27:ASP:OD1 | 1:B:27:ASP:N | 0.47 | 2.48 | 2 | 2 |
| 1:A:221:ASP:O | 1:A:223:VAL:N | 0.47 | 2.48 | 1 | 2 |
| 1:B:43:PHE:CZ | 1:B:47:ARG:NE | 0.47 | 2.83 | 1 | 2 |
| 1:B:431:GLU:CA | 1:B:456:LEU:HG | 0.47 | 2.37 | 1 | 2 |
| 1:A:123:LEU:N | 1:A:123:LEU:HD12 | 0.47 | 2.24 | 1 | 2 |
| 1:A:300:LEU:HD12 | 1:A:313:GLN:HE22 | 0.47 | 1.70 | 1 | 2 |
| 1:A:339:ASP:OD1 | 1:B:351:GLU:OE1 | 0.47 | 2.33 | 1 | 2 |
| 1:A:391:PRO:CA | 1:A:429:MET:HG2 | 0.47 | 2.39 | 1 | 2 |
| 1:B:327:GLN:OE1 | 1:B:327:GLN:C | 0.47 | 2.53 | 1 | 2 |
| 1:B:429:MET:HE1 | 1:B:431:GLU:CD | 0.47 | 2.30 | 1 | 2 |
| 1:A:202:ILE:C | 1:A:202:ILE:CD1 | 0.47 | 2.84 | 2 | 2 |
| 1:A:11:ILE:CD1 | 1:A:13:PHE:CZ | 0.46 | 2.94 | 1 | 2 |
| 1:A:27:ASP:N | 1:A:27:ASP:OD1 | 0.46 | 2.48 | 1 | 2 |
| 1:A:377:ILE:HG22 | 1:A:386:LEU:CD2 | 0.46 | 2.40 | 1 | 2 |
| 1:A:130:VAL:CG2 | 1:A:131:ARG:N | 0.46 | 2.77 | 2 | 2 |
| 1:A:292:VAL:CG1 | 1:A:327:GLN:NE2 | 0.46 | 2.79 | 1 | 2 |
| 1:B:313:GLN:OE1 | 1:B:317:TYR:OH | 0.46 | 2.28 | 1 | 2 |
| 1:B:377:ILE:HG22 | 1:B:386:LEU:CD2 | 0.46 | 2.40 | 1 | 2 |
| 1:B:429:MET:SD | 1:B:431:GLU:HB2 | 0.46 | 2.49 | 1 | 2 |
| 1:B:11:ILE:CG2 | 1:B:243:GLN:HB2 | 0.46 | 2.40 | 2 | 2 |
| 1:A:282:GLU:O | 1:A:286:ARG:HG2 | 0.46 | 2.10 | 2 | 1 |
| 1:A:301:PHE:O | 1:A:301:PHE:HD1 | 0.46 | 1.92 | 1 | 1 |
| 1:A:542:PHE:C | 1:A:542:PHE:CD1 | 0.46 | 2.88 | 1 | 1 |
| 1:A:67:GLU:N | 1:A:67:GLU:OE1 | 0.46 | 2.48 | 1 | 1 |
| 1:B:223:VAL:CG2 | 1:B:224:ASN:N | 0.46 | 2.79 | 1 | 2 |
| 1:A:301:PHE:HD1 | 1:A:301:PHE:O | 0.46 | 1.92 | 2 | 1 |
| 1:A:542:PHE:CD1 | 1:A:542:PHE:C | 0.46 | 2.88 | 2 | 1 |
| 1:A:361:ARG:NH2 | 1:A:394:ILE:HG21 | 0.46 | 2.25 | 1 | 2 |
| 1:B:358:ARG:NH1 | 1:B:392:MET:SD | 0.46 | 2.87 | 1 | 2 |
| 1:A:221:ASP:C | 1:A:223:VAL:N | 0.46 | 2.66 | 2 | 2 |
| 1:B:123:LEU:N | 1:B:123:LEU:CD1 | 0.46 | 2.79 | 2 | 2 |
| 1:A:274:ASN:HD22 | 1:A:525:MET:C | 0.46 | 2.13 | 1 | 2 |
| 1:A:429:MET:SD | 1:A:431:GLU:HB2 | 0.46 | 2.49 | 1 | 2 |
| 1:A:459:TYR:O | 1:B:459:TYR:HB3 | 0.46 | 2.10 | 1 | 2 |
| 1:B:202:ILE:HG12 | 1:B:203:VAL:N | 0.46 | 2.26 | 1 | 2 |
| 1:A:43:PHE:CZ | 1:A:47:ARG:NE | 0.46 | 2.83 | 2 | 2 |
| 1:A:256:LEU:O | 1:A:259:LEU:HD21 | 0.46 | 2.11 | 1 | 1 |
| 1:B:300:LEU:HD12 | 1:B:313:GLN:HE22 | 0.46 | 1.69 | 1 | 2 |
| 1:A:249:GLU:C | 1:A:249:GLU:CD | 0.46 | 2.74 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:512:THR:CB | 1:B:536:ILE:HG21 | 0.46 | 2.41 | 1 | 2 |
| 1:A:256:LEU:HD23 | 1:A:256:LEU:H | 0.46 | 1.71 | 2 | 1 |
| 1:A:294:LEU:HD23 | 1:A:295:TYR:N | 0.46 | 2.26 | 1 | 2 |
| 1:A:512:THR:CB | 1:A:536:ILE:HG21 | 0.46 | 2.41 | 1 | 2 |
| 1:B:318:LYS:NZ | 1:B:383:PHE:CE2 | 0.46 | 2.81 | 1 | 2 |
| 1:B:11:ILE:CG2 | 1:B:243:GLN:CA | 0.46 | 2.82 | 2 | 2 |
| 1:A:463:VAL:CG1 | 1:B:361:ARG:HH12 | 0.46 | 2.24 | 1 | 2 |
| 1:B:361:ARG:NH2 | 1:B:394:ILE:HG21 | 0.46 | 2.26 | 1 | 2 |
| 1:B:5:ILE:O | 1:B:6:LEU:O | 0.46 | 2.34 | 2 | 2 |
| 1:B:521:ASP:O | 1:B:521:ASP:OD1 | 0.46 | 2.34 | 1 | 1 |
| 1:B:521:ASP:OD1 | 1:B:521:ASP:O | 0.46 | 2.34 | 2 | 1 |
| 1:A:429:MET:HE1 | 1:A:431:GLU:CD | 0.45 | 2.31 | 1 | 2 |
| 1:A:54:LEU:CD2 | 1:A:77:ILE:CG1 | 0.45 | 2.94 | 1 | 2 |
| 1:B:87:GLN:O | 1:B:90:ILE:HG13 | 0.45 | 2.11 | 1 | 2 |
| 1:B:54:LEU:CD2 | 1:B:77:ILE:CG1 | 0.45 | 2.94 | 2 | 2 |
| 1:A:158:LEU:O | 1:A:180:ILE:HG23 | 0.45 | 2.11 | 1 | 2 |
| 1:A:190:THR:O | 1:A:193:MET:HG3 | 0.45 | 2.11 | 1 | 2 |
| 1:A:255:LYS:O | 1:A:256:LEU:HG | 0.45 | 2.11 | 1 | 1 |
| 1:A:562:MET:CE | 1:A:566:ASN:HD21 | 0.45 | 2.24 | 1 | 2 |
| 1:B:249:GLU:C | 1:B:249:GLU:CD | 0.45 | 2.74 | 1 | 1 |
| 1:B:290:GLU:OE1 | 1:B:290:GLU:O | 0.45 | 2.34 | 1 | 2 |
| 1:A:223:VAL:CG2 | 1:A:224:ASN:N | 0.45 | 2.79 | 2 | 2 |
| 1:A:5:ILE:O | 1:A:6:LEU:O | 0.45 | 2.34 | 2 | 2 |
| 1:B:249:GLU:CD | 1:B:249:GLU:C | 0.45 | 2.74 | 2 | 1 |
| 1:B:292:VAL:CG1 | 1:B:327:GLN:NE2 | 0.45 | 2.79 | 1 | 2 |
| 1:A:133:ILE:HG23 | 1:A:134:GLY:N | 0.45 | 2.25 | 2 | 2 |
| 1:B:130:VAL:CG2 | 1:B:131:ARG:N | 0.45 | 2.79 | 2 | 2 |
| 1:A:202:ILE:HG12 | 1:A:203:VAL:N | 0.45 | 2.26 | 2 | 2 |
| 1:A:118:LEU:CD2 | 1:A:118:LEU:N | 0.45 | 2.80 | 2 | 1 |
| 1:B:144:LEU:HD13 | 1:B:144:LEU:C | 0.45 | 2.10 | 2 | 2 |
| 1:B:101:ASP:OD1 | 1:B:101:ASP:N | 0.45 | 2.47 | 2 | 1 |
| 1:B:256:LEU:HD23 | 1:B:256:LEU:H | 0.45 | 1.72 | 2 | 1 |
| 1:A:118:LEU:N | 1:A:118:LEU:CD2 | 0.45 | 2.80 | 1 | 1 |
| 1:A:123:LEU:N | 1:A:123:LEU:CD1 | 0.45 | 2.79 | 1 | 2 |
| 1:B:101:ASP:N | 1:B:101:ASP:OD1 | 0.45 | 2.47 | 1 | 1 |
| 1:B:294:LEU:HD23 | 1:B:295:TYR:N | 0.45 | 2.26 | 1 | 2 |
| 1:A:361:ARG:NH1 | 1:B:463:VAL:CG1 | 0.45 | 2.79 | 1 | 2 |
| 1:A:265:ASP:OD2 | 1:A:541:ASN:OD1 | 0.45 | 2.34 | 1 | 2 |
| 1:B:118:LEU:CD2 | 1:B:118:LEU:N | 0.45 | 2.79 | 1 | 2 |
| 1:B:133:ILE:HG23 | 1:B:134:GLY:N | 0.45 | 2.25 | 1 | 2 |
| 1:A:186:ARG:CG | 1:A:186:ARG:HH11 | 0.45 | 2.25 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:195:ARG:O | 1:B:195:ARG:NH1 | 0.45 | 2.50 | 1 | 1 |
| 1:A:290:GLU:O | 1:A:290:GLU:OE1 | 0.45 | 2.35 | 1 | 2 |
| 1:B:562:MET:CE | 1:B:566:ASN:HD21 | 0.45 | 2.25 | 1 | 2 |
| 1:A:205:THR:HG23 | 1:A:208:VAL:H | 0.45 | 1.71 | 2 | 2 |
| 1:B:186:ARG:CG | 1:B:186:ARG:HH11 | 0.45 | 2.25 | 2 | 1 |
| 1:B:126:ARG:O | 1:B:130:VAL:HG13 | 0.45 | 2.12 | 1 | 2 |
| 1:B:189:HIS:O | 1:B:192:ILE:HG22 | 0.45 | 2.12 | 1 | 1 |
| 1:B:224:ASN:C | 1:B:224:ASN:OD1 | 0.45 | 2.55 | 2 | 1 |
| 1:A:68:GLU:OE1 | 1:A:69:LYS:NZ | 0.45 | 2.35 | 1 | 1 |
| 1:B:375:ARG:HH22 | 1:B:418:LYS:HZ2 | 0.45 | 1.53 | 1 | 2 |
| 1:A:274:ASN:O | 1:A:274:ASN:OD1 | 0.44 | 2.35 | 1 | 2 |
| 1:A:521:ASP:O | 1:A:521:ASP:OD1 | 0.44 | 2.35 | 1 | 2 |
| 1:A:177:LEU:CD2 | 1:A:177:LEU:N | 0.44 | 2.80 | 1 | 1 |
| 1:A:289:ALA:N | 1:A:530:ILE:HD13 | 0.44 | 2.28 | 1 | 1 |
| 1:B:57:ILE:HD11 | 1:B:73:PHE:CD1 | 0.44 | 2.48 | 1 | 2 |
| 1:A:224:ASN:C | 1:A:224:ASN:OD1 | 0.44 | 2.56 | 2 | 2 |
| 1:A:86:GLU:OE1 | 1:A:87:GLN:NE2 | 0.44 | 2.50 | 2 | 2 |
| 1:A:530:ILE:C | 1:A:530:ILE:CD1 | 0.44 | 2.72 | 2 | 1 |
| 1:A:50:ALA:O | 1:A:54:LEU:HB3 | 0.44 | 2.11 | 1 | 2 |
| 1:A:87:GLN:O | 1:A:90:ILE:HG13 | 0.44 | 2.12 | 1 | 2 |
| 1:A:351:GLU:OE1 | 1:B:339:ASP:OD1 | 0.44 | 2.35 | 1 | 2 |
| 1:B:484:LEU:O | 1:B:488:VAL:HG23 | 0.44 | 2.12 | 1 | 2 |
| 1:A:473:LEU:N | 1:A:473:LEU:HD22 | 0.44 | 2.28 | 1 | 1 |
| 1:B:177:LEU:N | 1:B:177:LEU:CD2 | 0.44 | 2.80 | 1 | 1 |
| 1:B:163:LEU:CB | 1:B:190:THR:HG21 | 0.44 | 2.35 | 1 | 1 |
| 1:B:274:ASN:OD1 | 1:B:274:ASN:O | 0.44 | 2.35 | 1 | 2 |
| 1:B:327:GLN:HG2 | 1:B:328:ALA:N | 0.44 | 2.27 | 1 | 2 |
| 1:A:473:LEU:HD22 | 1:A:473:LEU:N | 0.44 | 2.28 | 2 | 1 |
| 1:A:484:LEU:O | 1:A:488:VAL:HG23 | 0.44 | 2.12 | 1 | 2 |
| 1:B:224:ASN:OD1 | 1:B:224:ASN:C | 0.44 | 2.55 | 1 | 1 |
| 1:B:50:ALA:O | 1:B:54:LEU:HB3 | 0.44 | 2.12 | 2 | 2 |
| 1:A:144:LEU:C | 1:A:144:LEU:CD1 | 0.44 | 2.78 | 2 | 2 |
| 1:A:138:LEU:N | 1:A:138:LEU:CD2 | 0.44 | 2.80 | 1 | 2 |
| 1:A:391:PRO:HA | 1:A:429:MET:CG | 0.44 | 2.42 | 1 | 2 |
| 1:A:538:ARG:HE | 1:A:538:ARG:C | 0.44 | 2.16 | 1 | 2 |
| 1:B:243:GLN:C | 1:B:243:GLN:CD | 0.44 | 2.76 | 1 | 2 |
| 1:B:388:ILE:O | 1:B:388:ILE:HG13 | 0.44 | 2.13 | 1 | 2 |
| 1:B:86:GLU:OE1 | 1:B:87:GLN:NE2 | 0.44 | 2.51 | 1 | 2 |
| 1:B:92:LEU:O | 1:B:96:LYS:N | 0.44 | 2.50 | 1 | 2 |
| 1:A:243:GLN:C | 1:A:243:GLN:CD | 0.44 | 2.76 | 2 | 2 |
| 1:A:177:LEU:N | 1:A:177:LEU:CD2 | 0.44 | 2.80 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:327:GLN:HG2 | 1:A:328:ALA:N | 0.44 | 2.27 | 1 | 2 |
| 1:A:429:MET:SD | 1:A:431:GLU:CB | 0.44 | 3.06 | 1 | 2 |
| 1:B:305:ASP:O | 1:B:344:TYR:CD1 | 0.44 | 2.71 | 1 | 2 |
| 1:A:224:ASN:OD1 | 1:A:226:GLN:N | 0.44 | 2.51 | 1 | 2 |
| 1:A:324:CYS:HB3 | 1:A:327:GLN:HE22 | 0.44 | 1.73 | 1 | 2 |
| 1:A:305:ASP:O | 1:A:344:TYR:CD1 | 0.44 | 2.70 | 1 | 2 |
| 1:B:324:CYS:HB3 | 1:B:327:GLN:HE22 | 0.44 | 1.73 | 1 | 2 |
| 1:B:265:ASP:OD2 | 1:B:541:ASN:OD1 | 0.44 | 2.35 | 1 | 2 |
| 1:A:11:ILE:CG2 | 1:A:243:GLN:CA | 0.44 | 2.82 | 2 | 2 |
| 1:B:301:PHE:CZ | 1:B:307:LEU:HA | 0.43 | 2.48 | 1 | 2 |
| 1:A:57:ILE:HD11 | 1:A:73:PHE:CD1 | 0.43 | 2.48 | 2 | 2 |
| 1:B:287:ASN:O | 1:B:530:ILE:HG13 | 0.43 | 2.11 | 2 | 1 |
| 1:B:538:ARG:NE | 1:B:538:ARG:O | 0.43 | 2.45 | 1 | 2 |
| 1:B:177:LEU:CD2 | 1:B:177:LEU:N | 0.43 | 2.80 | 2 | 1 |
| 1:A:221:ASP:CA | 1:A:239:MET:HE1 | 0.43 | 2.38 | 1 | 1 |
| 1:A:301:PHE:CZ | 1:A:307:LEU:HA | 0.43 | 2.49 | 1 | 2 |
| 1:A:105:HIS:HE2 | 1:A:109:GLU:CD | 0.43 | 2.17 | 2 | 2 |
| 1:B:224:ASN:OD1 | 1:B:226:GLN:N | 0.43 | 2.51 | 1 | 2 |
| 1:B:274:ASN:OD1 | 1:B:274:ASN:C | 0.43 | 2.57 | 1 | 2 |
| 1:A:182:ASP:O | 1:A:183:ALA:O | 0.43 | 2.37 | 1 | 2 |
| 1:A:336:ILE:HG23 | 1:A:362:ILE:HD12 | 0.43 | 1.89 | 1 | 2 |
| 1:B:429:MET:SD | 1:B:431:GLU:CB | 0.43 | 3.06 | 1 | 2 |
| 1:A:92:LEU:O | 1:A:96:LYS:N | 0.43 | 2.50 | 2 | 1 |
| 1:A:361:ARG:HH22 | 1:A:394:ILE:HG21 | 0.43 | 1.73 | 1 | 2 |
| 1:B:57:ILE:HG12 | 1:B:58:LYS:N | 0.43 | 2.28 | 1 | 2 |
| 1:A:49:LYS:O | 1:A:50:ALA:C | 0.43 | 2.57 | 2 | 2 |
| 1:B:49:LYS:O | 1:B:50:ALA:C | 0.43 | 2.57 | 2 | 2 |
| 1:B:336:ILE:HG23 | 1:B:362:ILE:HD12 | 0.43 | 1.89 | 1 | 2 |
| 1:A:268:GLN:CD | 1:A:268:GLN:N | 0.43 | 2.72 | 1 | 1 |
| 1:B:138:LEU:CD2 | 1:B:138:LEU:N | 0.43 | 2.81 | 1 | 1 |
| 1:A:24:ILE:CG1 | 1:A:139:ARG:HH11 | 0.43 | 2.27 | 2 | 2 |
| 1:A:268:GLN:N | 1:A:268:GLN:CD | 0.43 | 2.72 | 2 | 1 |
| 1:A:274:ASN:OD1 | 1:A:274:ASN:C | 0.43 | 2.57 | 1 | 1 |
| 1:B:208:VAL:CG1 | 1:B:209:THR:N | 0.43 | 2.82 | 1 | 2 |
| 1:A:274:ASN:C | 1:A:274:ASN:OD1 | 0.43 | 2.57 | 2 | 1 |
| 1:B:186:ARG:CG | 1:B:186:ARG:NH1 | 0.43 | 2.81 | 2 | 1 |
| 1:A:305:ASP:O | 1:A:344:TYR:CE1 | 0.43 | 2.72 | 1 | 2 |
| 1:B:547:VAL:O | 1:B:551:GLN:HG3 | 0.43 | 2.14 | 1 | 2 |
| 1:A:208:VAL:CG1 | 1:A:209:THR:N | 0.42 | 2.82 | 2 | 2 |
| 1:B:182:ASP:O | 1:B:183:ALA:O | 0.42 | 2.37 | 2 | 2 |
| 1:B:138:LEU:N | 1:B:138:LEU:CD2 | 0.42 | 2.81 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:341:GLU:OE2 | 1:A:342:LEU:O | 0.42 | 2.37 | 1 | 2 |
| 1:A:441:HIS:CE1 | 1:B:556:PRO:HB3 | 0.42 | 2.48 | 1 | 2 |
| 1:A:287:ASN:O | 1:A:530:ILE:HG13 | 0.42 | 2.10 | 2 | 1 |
| 1:B:287:ASN:HB3 | 1:B:530:ILE:HG23 | 0.42 | 1.90 | 2 | 1 |
| 1:B:205:THR:HG23 | 1:B:208:VAL:H | 0.42 | 1.72 | 1 | 2 |
| 1:B:287:ASN:HD21 | 1:B:528:ILE:HD13 | 0.42 | 1.73 | 1 | 1 |
| 1:A:221:ASP:CB | 1:A:224:ASN:OD1 | 0.42 | 2.68 | 2 | 2 |
| 1:A:282:GLU:OE2 | 1:A:286:ARG:NH2 | 0.42 | 2.52 | 2 | 1 |
| 1:A:304:ARG:C | 1:A:304:ARG:CD | 0.42 | 2.88 | 1 | 1 |
| 1:B:8:SER:CB | 1:B:199:LEU:O | 0.42 | 2.67 | 1 | 2 |
| 1:A:186:ARG:NH1 | 1:A:186:ARG:CG | 0.42 | 2.82 | 2 | 1 |
| 1:A:259:LEU:N | 1:A:260:PRO:HD2 | 0.42 | 2.29 | 2 | 1 |
| 1:A:304:ARG:CD | 1:A:304:ARG:C | 0.42 | 2.88 | 2 | 1 |
| 1:A:277:THR:N | 1:A:280:ASP:OD2 | 0.42 | 2.52 | 1 | 1 |
| 1:A:294:LEU:C | 1:A:294:LEU:CD2 | 0.42 | 2.88 | 1 | 2 |
| 1:A:375:ARG:HH22 | 1:A:418:LYS:NZ | 0.42 | 2.12 | 1 | 2 |
| 1:A:513:LEU:HD22 | 1:A:568:PHE:CD1 | 0.42 | 2.50 | 1 | 2 |
| 1:A:8:SER:CB | 1:A:199:LEU:O | 0.42 | 2.68 | 1 | 2 |
| 1:B:282:GLU:OE1 | 1:B:286:ARG:NH2 | 0.42 | 2.52 | 1 | 1 |
| 1:B:330:ILE:HD13 | 1:B:389:MET:HB2 | 0.42 | 1.91 | 1 | 2 |
| 1:B:361:ARG:HH22 | 1:B:394:ILE:HG21 | 0.42 | 1.74 | 1 | 2 |
| 1:A:301:PHE:O | 1:A:301:PHE:CD1 | 0.42 | 2.73 | 1 | 2 |
| 1:B:221:ASP:CB | 1:B:224:ASN:OD1 | 0.42 | 2.67 | 1 | 2 |
| 1:A:547:VAL:O | 1:A:551:GLN:HG3 | 0.42 | 2.14 | 1 | 2 |
| 1:B:105:HIS:HE2 | 1:B:109:GLU:CD | 0.42 | 2.17 | 1 | 2 |
| 1:B:304:ARG:C | 1:B:304:ARG:CD | 0.42 | 2.88 | 1 | 1 |
| 1:B:32:SER:OG | 1:B:33:ALA:N | 0.42 | 2.52 | 1 | 2 |
| 1:B:392:MET:H | 1:B:429:MET:CE | 0.42 | 2.27 | 1 | 2 |
| 1:B:89:ILE:HG23 | 1:B:90:ILE:N | 0.42 | 2.30 | 1 | 2 |
| 1:B:167:GLU:N | 1:B:167:GLU:OE1 | 0.42 | 2.52 | 2 | 1 |
| 1:B:304:ARG:CD | 1:B:304:ARG:C | 0.42 | 2.88 | 2 | 1 |
| 1:A:179:PHE:O | 1:A:201:ALA:HB1 | 0.42 | 2.15 | 1 | 2 |
| 1:A:57:ILE:HG12 | 1:A:58:LYS:N | 0.42 | 2.29 | 1 | 2 |
| 1:B:294:LEU:C | 1:B:294:LEU:CD2 | 0.42 | 2.88 | 1 | 2 |
| 1:B:304:ARG:HD3 | 1:B:306:ALA:O | 0.42 | 2.15 | 1 | 2 |
| 1:B:305:ASP:O | 1:B:344:TYR:CE1 | 0.42 | 2.73 | 1 | 2 |
| 1:B:259:LEU:N | 1:B:260:PRO:HD2 | 0.42 | 2.29 | 2 | 1 |
| 1:B:179:PHE:O | 1:B:201:ALA:HB1 | 0.42 | 2.15 | 2 | 2 |
| 1:A:330:ILE:HD13 | 1:A:389:MET:HB2 | 0.41 | 1.92 | 1 | 2 |
| 1:B:115:LEU:O | 1:B:118:LEU:HB2 | 0.41 | 2.15 | 1 | 2 |
| 1:B:167:GLU:OE1 | 1:B:167:GLU:N | 0.41 | 2.52 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:232:THR:HG22 | 1:A:234:GLU:N | 0.41 | 2.27 | 2 | 2 |
| 1:A:214:ASN:O | 1:A:214:ASN:OD1 | 0.41 | 2.38 | 1 | 1 |
| 1:A:67:GLU:H | 1:A:67:GLU:CD | 0.41 | 2.19 | 1 | 1 |
| 1:B:24:ILE:CG1 | 1:B:139:ARG:HH11 | 0.41 | 2.27 | 1 | 2 |
| 1:B:301:PHE:CD1 | 1:B:301:PHE:O | 0.41 | 2.73 | 1 | 2 |
| 1:A:214:ASN:OD1 | 1:A:214:ASN:O | 0.41 | 2.38 | 2 | 1 |
| 1:A:167:GLU:OE1 | 1:A:167:GLU:N | 0.41 | 2.53 | 1 | 1 |
| 1:A:388:ILE:O | 1:A:388:ILE:HG13 | 0.41 | 2.14 | 1 | 1 |
| 1:B:513:LEU:HD22 | 1:B:568:PHE:CD1 | 0.41 | 2.49 | 1 | 2 |
| 1:A:11:ILE:CG2 | 1:A:243:GLN:CB | 0.41 | 2.99 | 2 | 2 |
| 1:A:388:ILE:HG13 | 1:A:388:ILE:O | 0.41 | 2.14 | 2 | 1 |
| 1:A:180:ILE:O | 1:A:180:ILE:HG12 | 0.41 | 2.15 | 1 | 1 |
| 1:A:288:GLY:C | 1:A:530:ILE:CD1 | 0.41 | 2.88 | 1 | 1 |
| 1:A:327:GLN:O | 1:A:327:GLN:OE1 | 0.41 | 2.38 | 1 | 2 |
| 1:B:221:ASP:CA | 1:B:239:MET:HE1 | 0.41 | 2.37 | 1 | 2 |
| 1:A:89:ILE:HG23 | 1:A:90:ILE:N | 0.41 | 2.31 | 2 | 2 |
| 1:A:115:LEU:O | 1:A:118:LEU:HB2 | 0.41 | 2.15 | 2 | 2 |
| 1:A:387:ARG:N | 1:A:387:ARG:CD | 0.41 | 2.83 | 1 | 2 |
| 1:A:392:MET:H | 1:A:429:MET:CE | 0.41 | 2.28 | 1 | 2 |
| 1:B:375:ARG:HH22 | 1:B:418:LYS:NZ | 0.41 | 2.13 | 1 | 2 |
| 1:B:473:LEU:N | 1:B:473:LEU:HD22 | 0.41 | 2.30 | 1 | 1 |
| 1:B:190:THR:O | 1:B:193:MET:HG3 | 0.41 | 2.15 | 2 | 1 |
| 1:B:473:LEU:HD22 | 1:B:473:LEU:N | 0.41 | 2.30 | 2 | 1 |
| 1:B:391:PRO:HA | 1:B:429:MET:CG | 0.41 | 2.41 | 1 | 2 |
| 1:B:221:ASP:C | 1:B:223:VAL:H | 0.41 | 2.19 | 2 | 2 |
| 1:A:180:ILE:HG12 | 1:A:180:ILE:O | 0.41 | 2.15 | 2 | 1 |
| 1:A:177:LEU:HD22 | 1:A:177:LEU:N | 0.41 | 2.31 | 1 | 1 |
| 1:A:32:SER:OG | 1:A:33:ALA:N | 0.41 | 2.52 | 2 | 2 |
| 1:A:167:GLU:N | 1:A:167:GLU:OE1 | 0.41 | 2.53 | 2 | 1 |
| 1:A:177:LEU:N | 1:A:177:LEU:HD22 | 0.41 | 2.31 | 2 | 1 |
| 1:A:265:ASP:CG | 1:A:541:ASN:ND2 | 0.41 | 2.74 | 1 | 2 |
| 1:B:327:GLN:O | 1:B:327:GLN:OE1 | 0.41 | 2.38 | 1 | 1 |
| 1:B:327:GLN:OE1 | 1:B:327:GLN:O | 0.41 | 2.38 | 2 | 1 |
| 1:B:11:ILE:CG2 | 1:B:243:GLN:CB | 0.41 | 2.99 | 1 | 2 |
| 1:B:470:ILE:O | 1:B:470:ILE:HG23 | 0.41 | 2.16 | 1 | 2 |
| 1:A:176:VAL:O | 1:A:176:VAL:CG1 | 0.41 | 2.69 | 1 | 2 |
| 1:A:221:ASP:C | 1:A:223:VAL:H | 0.41 | 2.19 | 1 | 2 |
| 1:B:176:VAL:CG1 | 1:B:176:VAL:O | 0.41 | 2.68 | 1 | 1 |
| 1:B:204:GLY:O | 1:B:205:THR:C | 0.41 | 2.60 | 1 | 1 |
| 1:B:341:GLU:OE2 | 1:B:342:LEU:O | 0.41 | 2.38 | 1 | 2 |
| 1:B:282:GLU:OE2 | 1:B:286:ARG:NH2 | 0.41 | 2.52 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:292:VAL:O | 1:A:330:ILE:CG2 | 0.41 | 2.69 | 1 | 2 |
| 1:A:454:ASN:CG | 1:A:455:ASP:N | 0.41 | 2.74 | 1 | 2 |
| 1:A:456:LEU:HD22 | 1:A:484:LEU:CD1 | 0.41 | 2.38 | 1 | 2 |
| 1:A:484:LEU:CD2 | 1:A:484:LEU:C | 0.41 | 2.86 | 1 | 1 |
| 1:B:11:ILE:CD1 | 1:B:13:PHE:CE1 | 0.41 | 3.01 | 1 | 2 |
| 1:A:484:LEU:C | 1:A:484:LEU:CD2 | 0.41 | 2.86 | 2 | 1 |
| 1:A:130:VAL:HG23 | 1:A:131:ARG:N | 0.40 | 2.31 | 1 | 2 |
| 1:A:205:THR:HG21 | 1:A:208:VAL:CG1 | 0.40 | 2.46 | 1 | 2 |
| 1:A:295:TYR:HB3 | 1:A:331:VAL:HA | 0.40 | 1.94 | 1 | 2 |
| 1:A:367:ARG:O | 1:A:368:GLU:C | 0.40 | 2.60 | 1 | 2 |
| 1:A:274:ASN:HD22 | 1:A:526:SER:N | 0.40 | 2.13 | 1 | 2 |
| 1:B:265:ASP:CG | 1:B:541:ASN:ND2 | 0.40 | 2.74 | 1 | 2 |
| 1:B:86:GLU:O | 1:B:90:ILE:HG12 | 0.40 | 2.15 | 1 | 2 |
| 1:A:186:ARG:C | 1:A:188:SER:H | 0.40 | 2.20 | 2 | 2 |
| 1:B:181:THR:H | 1:B:202:ILE:HD13 | 0.40 | 1.76 | 1 | 1 |
| 1:B:176:VAL:O | 1:B:176:VAL:CG1 | 0.40 | 2.68 | 2 | 1 |
| 1:B:292:VAL:O | 1:B:330:ILE:CG2 | 0.40 | 2.69 | 1 | 2 |
| 1:B:295:TYR:HB3 | 1:B:331:VAL:HA | 0.40 | 1.93 | 1 | 2 |
| 1:B:485:ILE:HG13 | 1:B:486:LYS:N | 0.40 | 2.32 | 1 | 2 |
| 1:A:324:CYS:HB3 | 1:A:327:GLN:NE2 | 0.40 | 2.31 | 1 | 2 |
| 1:A:456:LEU:HD23 | 1:A:456:LEU:HA | 0.40 | 1.80 | 1 | 2 |
| 1:A:470:ILE:O | 1:A:470:ILE:HG23 | 0.40 | 2.16 | 1 | 1 |
| 1:B:367:ARG:O | 1:B:368:GLU:C | 0.40 | 2.60 | 1 | 2 |
| 1:B:538:ARG:C | 1:B:538:ARG:HE | 0.40 | 2.17 | 1 | 1 |
| 1:A:470:ILE:HG23 | 1:A:470:ILE:O | 0.40 | 2.16 | 2 | 1 |
| 1:B:538:ARG:HE | 1:B:538:ARG:C | 0.40 | 2.17 | 2 | 1 |

## 5.2 Torsion angles

### 5.2.1 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 | 571/573 (100%) | 537±1 (94±0%) | 28±1 (5±0%) | 7±0 (1±0%) | 17 | 64 |
| 1 | B | 571/573 (100%) | 537±1 (94±0%) | 27±1 (5±0%) | 8±1 (1±0%) | 16 | 63 |
| All | All | 2284/2292 (100%) | 2146 (94%) | 109 (5%) | 29 (1%) | 16 | 63 |

All 19 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 | 6 | LEU | 2 |
| 1 | A | 148 | ASP | 2 |
| 1 | A | 278 | VAL | 2 |
| 1 | B | 183 | ALA | 2 |
| 1 | B | 278 | VAL | 2 |
| 1 | B | 232 | THR | 2 |
| 1 | A | 232 | THR | 2 |
| 1 | A | 183 | ALA | 2 |
| 1 | B | 6 | LEU | 2 |
| 1 | B | 148 | ASP | 2 |
| 1 | B | 256 | LEU | 1 |
| 1 | A | 255 | LYS | 1 |
| 1 | A | 256 | LEU | 1 |
| 1 | A | 254 | ALA | 1 |
| 1 | B | 254 | ALA | 1 |
| 1 | B | 261 | ALA | 1 |
| 1 | A | 259 | LEU | 1 |
| 1 | B | 259 | LEU | 1 |
| 1 | B | 255 | LYS | 1 |

### 5.2.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 474/474 (100%) | 401±2 (84±0%) | 74±2 (16±0%) | 5 43 |
| 1 | B | 474/474 (100%) | 400±0 (84±0%) | 74±0 (16±0%) | 5 43 |
| All | All | 1896/1896 (100%) | 1601 (84%) | 295 (16%) | 5 43 |

All 155 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 | B | 557 | THR | 2 |
| 1 | B | 216 | ASP | 2 |
| 1 | B | 473 | LEU | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 213 | LYS | 2 |
| 1 | A | 216 | ASP | 2 |
| 1 | A | 269 | VAL | 2 |
| 1 | A | 249 | GLU | 2 |
| 1 | B | 453 | THR | 2 |
| 1 | A | 304 | ARG | 2 |
| 1 | A | 562 | MET | 2 |
| 1 | B | 411 | GLN | 2 |
| 1 | B | 144 | LEU | 2 |
| 1 | A | 205 | THR | 2 |
| 1 | A | 518 | MET | 2 |
| 1 | B | 505 | LEU | 2 |
| 1 | A | 101 | ASP | 2 |
| 1 | A | 28 | ARG | 2 |
| 1 | A | 451 | ILE | 2 |
| 1 | A | 561 | LEU | 2 |
| 1 | A | 89 | ILE | 2 |
| 1 | A | 530 | ILE | 2 |
| 1 | A | 243 | GLN | 2 |
| 1 | B | 205 | THR | 2 |
| 1 | B | 561 | LEU | 2 |
| 1 | A | 464 | ASP | 2 |
| 1 | B | 342 | LEU | 2 |
| 1 | B | 499 | THR | 2 |
| 1 | B | 327 | GLN | 2 |
| 1 | A | 330 | ILE | 2 |
| 1 | A | 327 | GLN | 2 |
| 1 | B | 11 | ILE | 2 |
| 1 | A | 342 | LEU | 2 |
| 1 | A | 484 | LEU | 2 |
| 1 | B | 387 | ARG | 2 |
| 1 | A | 193 | MET | 2 |
| 1 | B | 79 | LEU | 2 |
| 1 | A | 336 | ILE | 2 |
| 1 | A | 485 | ILE | 2 |
| 1 | A | 473 | LEU | 2 |
| 1 | B | 290 | GLU | 2 |
| 1 | A | 54 | LEU | 2 |
| 1 | B | 54 | LEU | 2 |
| 1 | A | 213 | LYS | 2 |
| 1 | A | 534 | LYS | 2 |
| 1 | B | 336 | ILE | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 470 | ILE | 2 |
| 1 | A | 202 | ILE | 2 |
| 1 | B | 28 | ARG | 2 |
| 1 | A | 105 | HIS | 2 |
| 1 | B | 294 | LEU | 2 |
| 1 | B | 70 | GLU | 2 |
| 1 | A | 294 | LEU | 2 |
| 1 | B | 423 | SER | 2 |
| 1 | A | 11 | ILE | 2 |
| 1 | B | 181 | THR | 2 |
| 1 | B | 57 | ILE | 2 |
| 1 | B | 329 | VAL | 2 |
| 1 | A | 242 | VAL | 2 |
| 1 | A | 429 | MET | 2 |
| 1 | B | 538 | ARG | 2 |
| 1 | B | 542 | PHE | 2 |
| 1 | B | 89 | ILE | 2 |
| 1 | B | 249 | GLU | 2 |
| 1 | A | 387 | ARG | 2 |
| 1 | A | 354 | PHE | 2 |
| 1 | A | 377 | ILE | 2 |
| 1 | B | 101 | ASP | 2 |
| 1 | A | 499 | THR | 2 |
| 1 | B | 167 | GLU | 2 |
| 1 | B | 170 | GLN | 2 |
| 1 | B | 180 | ILE | 2 |
| 1 | A | 144 | LEU | 2 |
| 1 | A | 357 | TRP | 2 |
| 1 | A | 215 | ASP | 2 |
| 1 | A | 170 | GLN | 2 |
| 1 | B | 304 | ARG | 2 |
| 1 | A | 209 | THR | 2 |
| 1 | B | 330 | ILE | 2 |
| 1 | B | 105 | HIS | 2 |
| 1 | B | 27 | ASP | 2 |
| 1 | B | 74 | GLU | 2 |
| 1 | A | 167 | GLU | 2 |
| 1 | B | 301 | PHE | 2 |
| 1 | B | 429 | MET | 2 |
| 1 | B | 256 | LEU | 2 |
| 1 | B | 268 | GLN | 2 |
| 1 | A | 182 | ASP | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 70 | GLU | 2 |
| 1 | B | 182 | ASP | 2 |
| 1 | B | 388 | ILE | 2 |
| 1 | B | 372 | ASP | 2 |
| 1 | B | 357 | TRP | 2 |
| 1 | A | 180 | ILE | 2 |
| 1 | B | 451 | ILE | 2 |
| 1 | A | 74 | GLU | 2 |
| 1 | A | 557 | THR | 2 |
| 1 | B | 377 | ILE | 2 |
| 1 | A | 404 | LYS | 2 |
| 1 | B | 485 | ILE | 2 |
| 1 | A | 538 | ARG | 2 |
| 1 | B | 404 | LYS | 2 |
| 1 | B | 209 | THR | 2 |
| 1 | A | 32 | SER | 2 |
| 1 | B | 225 | ASN | 2 |
| 1 | B | 464 | ASP | 2 |
| 1 | A | 423 | SER | 2 |
| 1 | B | 77 | ILE | 2 |
| 1 | B | 32 | SER | 2 |
| 1 | A | 79 | LEU | 2 |
| 1 | A | 372 | ASP | 2 |
| 1 | B | 269 | VAL | 2 |
| 1 | B | 215 | ASP | 2 |
| 1 | A | 505 | LEU | 2 |
| 1 | A | 301 | PHE | 2 |
| 1 | B | 518 | MET | 2 |
| 1 | B | 484 | LEU | 2 |
| 1 | A | 542 | PHE | 2 |
| 1 | A | 329 | VAL | 2 |
| 1 | B | 243 | GLN | 2 |
| 1 | A | 497 | LYS | 2 |
| 1 | A | 465 | ARG | 2 |
| 1 | A | 77 | ILE | 2 |
| 1 | A | 240 | ARG | 2 |
| 1 | A | 453 | THR | 2 |
| 1 | B | 354 | PHE | 2 |
| 1 | B | 534 | LYS | 2 |
| 1 | A | 411 | GLN | 2 |
| 1 | B | 497 | LYS | 2 |
| 1 | B | 202 | ILE | 2 |

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*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 465 | ARG | 2 |
| 1 | B | 242 | VAL | 2 |
| 1 | A | 388 | ILE | 2 |
| 1 | A | 290 | GLU | 2 |
| 1 | A | 57 | ILE | 2 |
| 1 | A | 225 | ASN | 2 |
| 1 | B | 240 | ARG | 2 |
| 1 | A | 181 | THR | 2 |
| 1 | A | 27 | ASP | 2 |
| 1 | B | 562 | MET | 2 |
| 1 | A | 268 | GLN | 2 |
| 1 | B | 186 | ARG | 1 |
| 1 | B | 530 | ILE | 1 |
| 1 | A | 67 | GLU | 1 |
| 1 | B | 193 | MET | 1 |
| 1 | A | 256 | LEU | 1 |
| 1 | A | 258 | ASP | 1 |
| 1 | B | 67 | GLU | 1 |
| 1 | A | 528 | ILE | 1 |
| 1 | A | 186 | ARG | 1 |
| 1 | A | 197 | LEU | 1 |
| 1 | A | 259 | LEU | 1 |
| 1 | B | 259 | LEU | 1 |
| 1 | B | 196 | SER | 1 |
| 1 | B | 190 | THR | 1 |
| 1 | B | 258 | ASP | 1 |

### 5.2.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.4 Carbohydrates

There are no carbohydrates in this entry.

## 5.5 Ligand geometry

There are no ligands in this entry.

## 5.6 Other polymers

There are no such molecules in this entry.

## 5.7 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Chemical shift validation

No chemical shift data were provided