



wwPDB EM Map/Model Validation Report ⓘ

Oct 18, 2016 – 11:30 AM EDT

PDB ID : 5JUY
EMDB ID: : EMD-8178
Title : Active human apoptosome with procaspase-9
Authors : Cheng, T.C.; Hong, C.; Akey, I.V.; Yuan, S.; Akey, C.W.
Deposited on : 2016-05-10
Resolution : 4.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

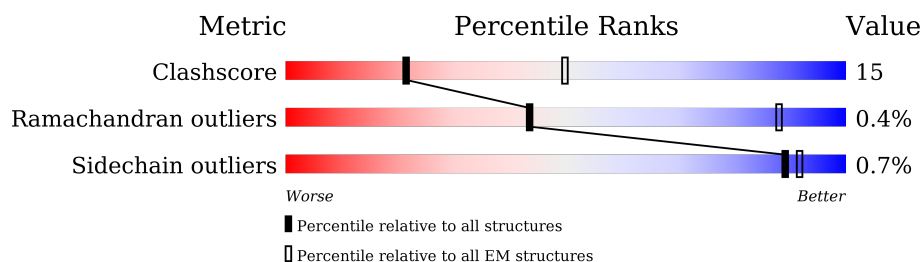
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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












| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 1248 | 65% 26% 9% |
| 1 | B | 1248 | 72% 26% .. |
| 1 | C | 1248 | 65% 26% 9% |
| 1 | D | 1248 | 72% 27% .. |
| 1 | E | 1248 | 72% 27% .. |
| 1 | F | 1248 | 65% 26% 9% |
| 1 | G | 1248 | 72% 26% .. |
| 2 | H | 104 | 57% 43% |
| 2 | I | 104 | 56% 44% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | J | 104 |  58%42% |
| 2 | K | 104 |  58%42% |
| 2 | L | 104 |  58%42% |
| 2 | M | 104 |  59%41% |
| 2 | N | 104 |  60%40% |
| 3 | O | 95 |  76%20%. |
| 3 | P | 95 |  76%19%5% |
| 3 | Q | 95 |  77%19%. |
| 3 | R | 95 |  77%19%. |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 76058 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apoptotic protease-activating factor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 1139 | Total | C | N | O | S | 0 | 0 |
| | | | 9099 | 5764 | 1563 | 1711 | 61 | | |
| 1 | B | 1234 | Total | C | N | O | S | 0 | 0 |
| | | | 9861 | 6243 | 1694 | 1857 | 67 | | |
| 1 | C | 1139 | Total | C | N | O | S | 0 | 0 |
| | | | 9099 | 5764 | 1563 | 1711 | 61 | | |
| 1 | D | 1234 | Total | C | N | O | S | 0 | 0 |
| | | | 9861 | 6243 | 1694 | 1857 | 67 | | |
| 1 | E | 1234 | Total | C | N | O | S | 0 | 0 |
| | | | 9861 | 6243 | 1694 | 1857 | 67 | | |
| 1 | F | 1139 | Total | C | N | O | S | 0 | 0 |
| | | | 9099 | 5764 | 1563 | 1711 | 61 | | |
| 1 | G | 1234 | Total | C | N | O | S | 0 | 0 |
| | | | 9861 | 6243 | 1694 | 1857 | 67 | | |

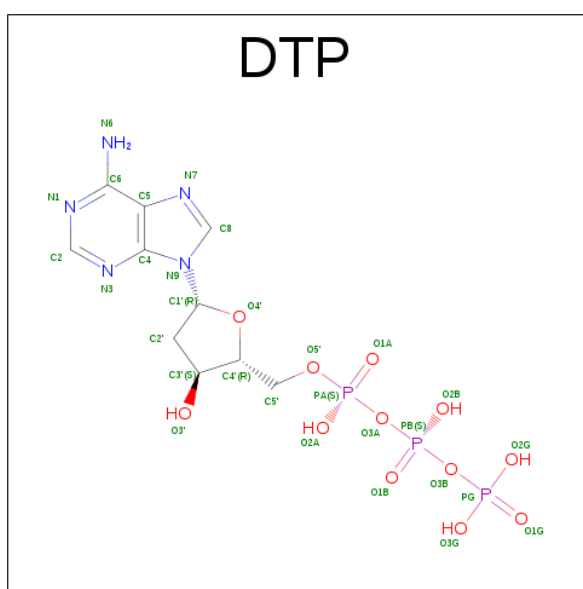
- Molecule 2 is a protein called Cytochrome c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | H | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | I | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | J | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | K | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | L | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | M | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |
| 2 | N | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 517 | 143 | 150 | 4 | | |

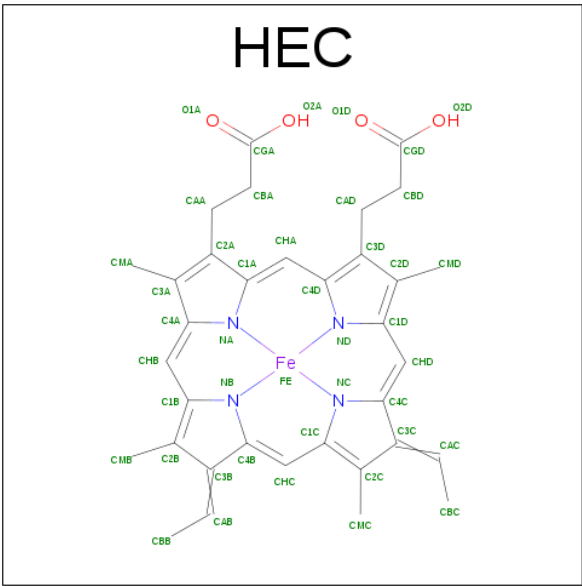
- Molecule 3 is a protein called Caspase-9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | O | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 475 | 152 | 145 | 5 | | |
| 3 | P | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 475 | 152 | 145 | 5 | | |
| 3 | Q | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 475 | 152 | 145 | 5 | | |
| 3 | R | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 475 | 152 | 145 | 5 | | |

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



- Molecule 5 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).

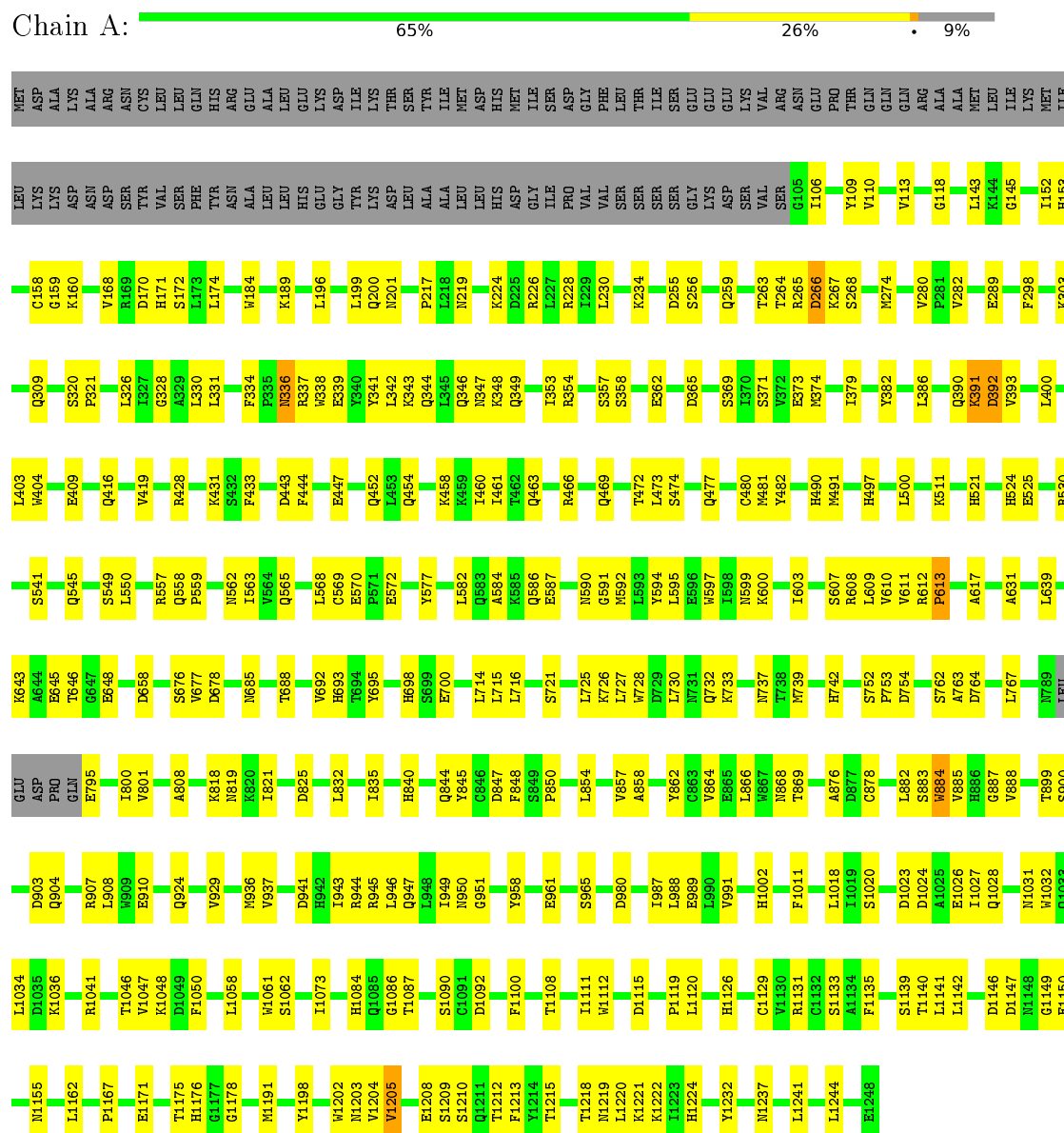


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 5 | H | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | I | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | J | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | K | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | L | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | M | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | N | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

3 Residue-property plots

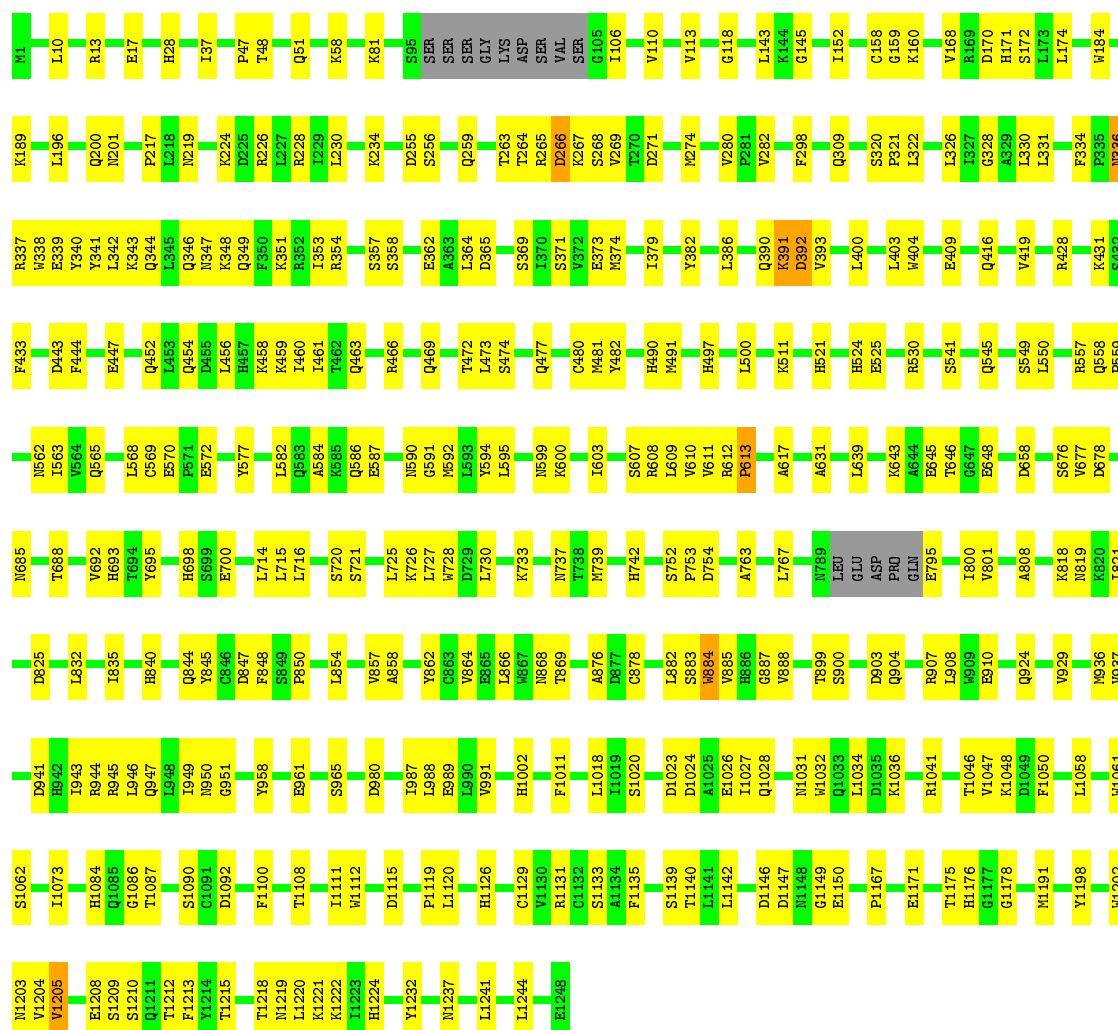
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Apoptotic protease-activating factor 1



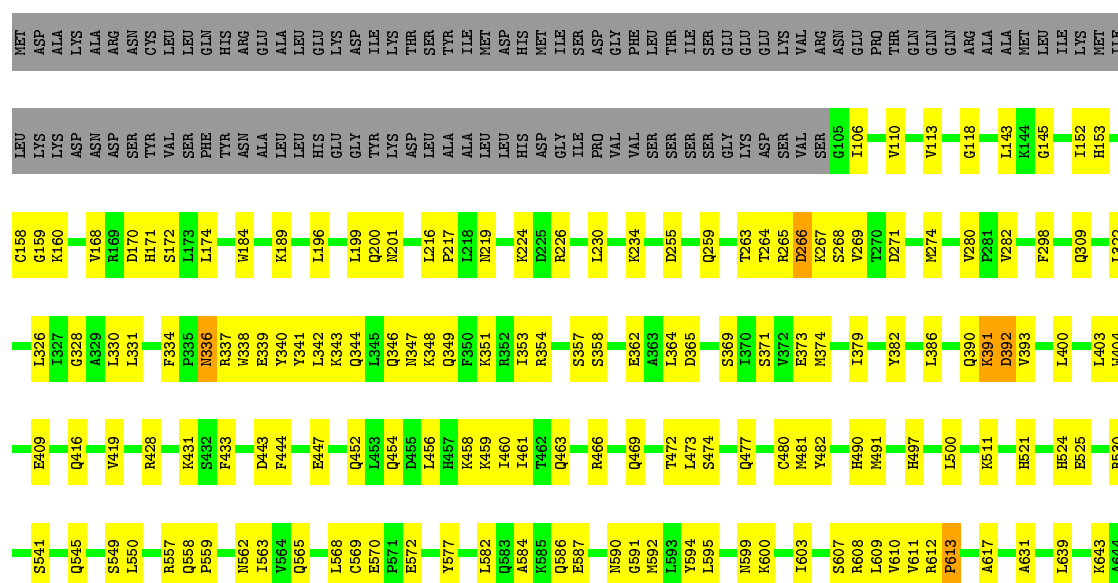
- Molecule 1: Apoptotic protease-activating factor 1





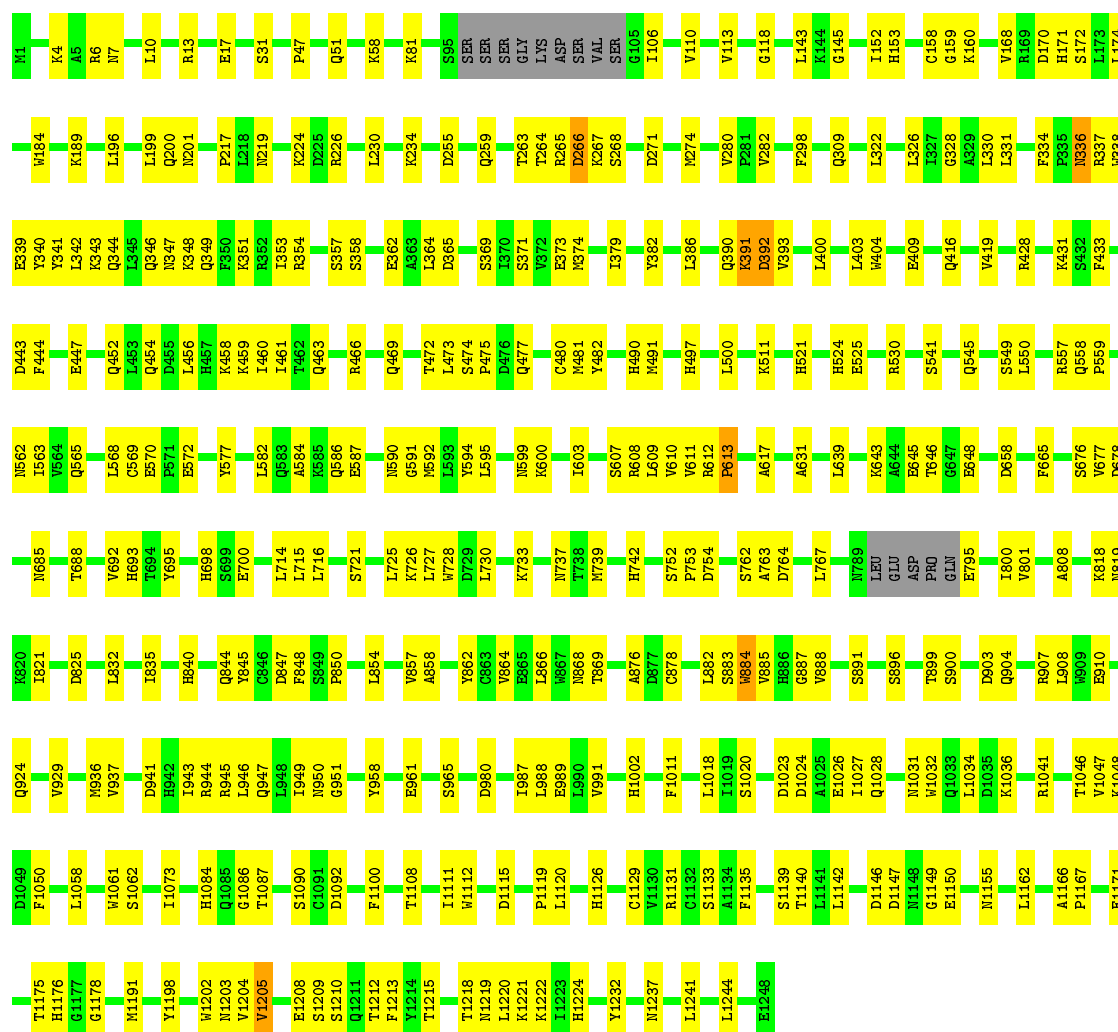
• Molecule 1: Apoptotic protease-activating factor 1

Chain C: 65% 26% 9%



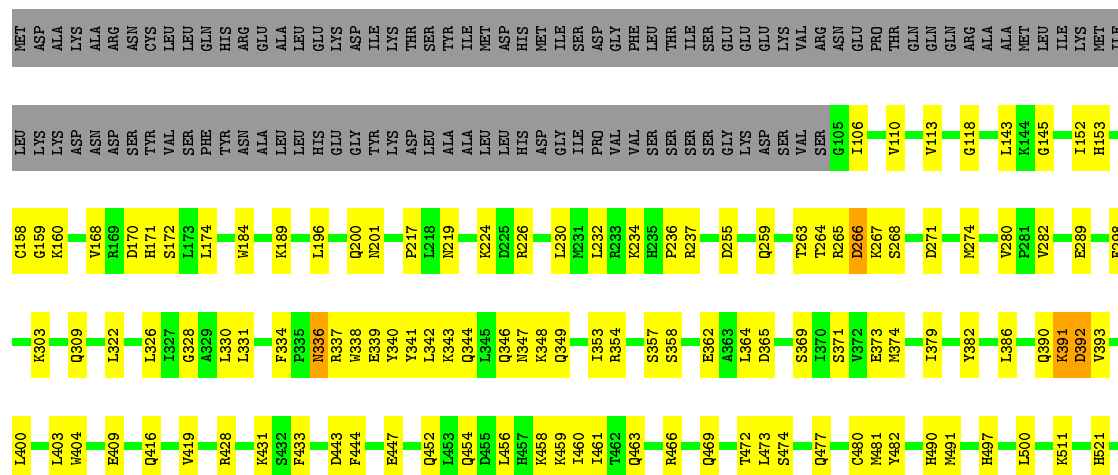


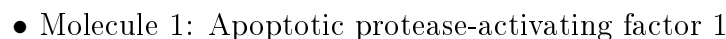
Chain E:  72% 27% ..



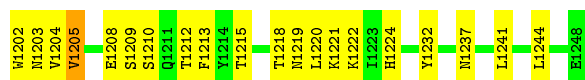
• Molecule 1: Apoptotic protease-activating factor 1

Chain F:  65% 26% 9%



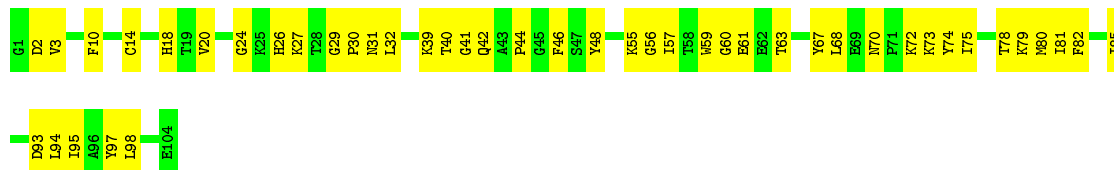


| | | | | | | | | | |
|------------|-------|-------|------|------|------|------|------|------|------|
| Category A | H1084 | H942 | D825 | T888 | Q565 | E447 | E339 | L196 | K1 |
| | H1085 | I943 | L832 | V692 | L568 | L568 | Y340 | L199 | K4 |
| | G1086 | R944 | L832 | H693 | C569 | Q452 | L342 | Q200 | |
| | T1087 | R945 | L835 | T694 | E570 | L453 | K343 | M201 | L10 |
| | S1090 | Q947 | H840 | Y695 | P571 | Q454 | Q344 | P217 | R13 |
| | G1091 | L948 | H848 | H698 | E572 | D485 | L345 | L218 | |
| | D1092 | I949 | Q844 | S699 | V577 | L456 | K346 | M219 | E17 |
| | F1100 | G951 | Y845 | E700 | L582 | K458 | K348 | P47 | |
| | T1108 | Y958 | C846 | L714 | L583 | K459 | Q349 | K224 | |
| | | D847 | D847 | L715 | A584 | I460 | T353 | R226 | E225 |
| Category B | I1111 | E961 | S849 | L716 | K585 | T462 | K354 | L227 | Q51 |
| | W1112 | S965 | P850 | S721 | Q586 | Q463 | R228 | K228 | K58 |
| | | | | | E587 | S357 | L229 | L230 | K81 |
| | D1115 | D980 | L854 | L725 | M590 | R466 | S358 | L230 | K81 |
| | | | | L726 | G591 | Q469 | E362 | K234 | S95 |
| | P1119 | I987 | A858 | L727 | M592 | T472 | L364 | D255 | SER |
| | L1120 | L988 | | W728 | L593 | L473 | D365 | S256 | SER |
| | | E989 | Y862 | D729 | Y594 | S474 | | Q259 | GLY |
| | H1126 | L990 | C983 | L730 | L595 | S369 | | D666 | LVS |
| | | V991 | V864 | K733 | M599 | Q477 | L370 | K267 | G105 |
| Category C | C1129 | E985 | E865 | H742 | R600 | H490 | T379 | S288 | I106 |
| | R1130 | H1002 | L866 | T737 | L603 | C480 | Y382 | D271 | V110 |
| | R1131 | F1011 | H857 | T738 | | M481 | E373 | M274 | V113 |
| | G1132 | S1133 | N868 | W739 | L603 | Y482 | K374 | G118 | |
| | A1134 | L1018 | T869 | | S607 | | Q390 | P281 | L143 |
| | F1135 | I1019 | D877 | H742 | R608 | K511 | K391 | K344 | K143 |
| | | S1020 | C878 | S752 | L609 | H491 | D392 | V282 | G145 |
| | S1139 | D1023 | L882 | D754 | V610 | H497 | V393 | F298 | |
| | L1141 | D1024 | S833 | | R612 | L500 | L400 | Q309 | H152 |
| | L1142 | A1025 | E884 | S762 | P613 | | L403 | S320 | H153 |
| Category D | D1146 | E1026 | H884 | A763 | A617 | K511 | K391 | G159 | C158 |
| | G1147 | I1027 | V885 | D764 | | H521 | D392 | P321 | G159 |
| | G1148 | Q1028 | H886 | A766 | A631 | H521 | K374 | L322 | K160 |
| | I1149 | D1147 | C887 | D764 | | H521 | K374 | L322 | |
| | E1150 | M1031 | V888 | L767 | L639 | H524 | L400 | F298 | |
| | | | | | | E525 | L403 | Q309 | |
| | M1155 | L1034 | T899 | W789 | K643 | R525 | L403 | S320 | C158 |
| | L1162 | D1035 | D903 | GLU | A644 | R630 | N404 | G159 | G159 |
| | P1167 | K1036 | Q904 | ASP | E345 | P80 | E409 | L322 | K160 |
| | | R1041 | R907 | GLU | T646 | S541 | E409 | L322 | |
| Category E | E1171 | T1046 | L908 | E795 | E543 | Q545 | Q416 | L326 | V168 |
| | | V1047 | H909 | | | | | I327 | R169 |
| | T1175 | K1048 | E910 | I800 | D658 | S549 | V419 | G328 | D170 |
| | | D1049 | | V801 | | L550 | | A329 | H171 |
| | F1050 | F1050 | Q924 | | F665 | | R428 | L320 | S172 |
| | | | | | | | | L331 | L173 |
| | G1177 | L1058 | Y929 | A808 | S676 | R557 | K431 | F334 | L174 |
| | G1178 | W1061 | P936 | K818 | V677 | P559 | S432 | P335 | W184 |
| | M1191 | S1062 | Y937 | K820 | D678 | | F433 | N336 | K389 |
| | | | | I821 | N685 | N562 | P335 | R337 | |
| Category F | Y1198 | T1072 | T041 | | | E564 | D443 | P328 | |
| | | | | | | | | | |



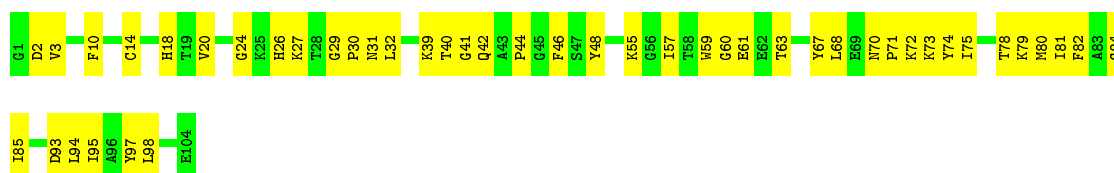
• Molecule 2: Cytochrome c

Chain H: 57% 43%



• Molecule 2: Cytochrome c

Chain I: 56% 44%



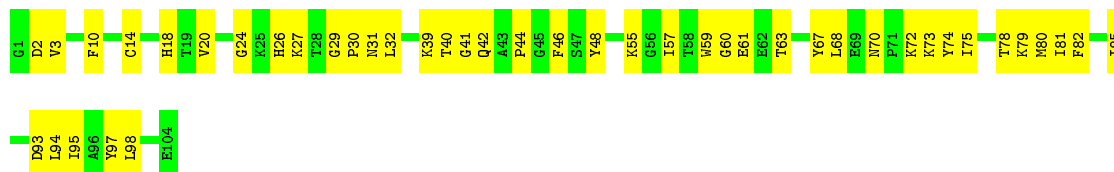
• Molecule 2: Cytochrome c

Chain J: 58% 42%



• Molecule 2: Cytochrome c

Chain K: 58% 42%



• Molecule 2: Cytochrome c

Chain L: 58% 42%





- Molecule 2: Cytochrome c

Chain M: 59% 41%



- Molecule 2: Cytochrome c

Chain N: 60% 40%



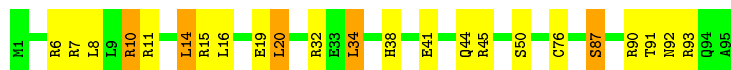
- Molecule 3: Caspase-9

Chain O: 76% 20% .



- Molecule 3: Caspase-9

Chain P: 76% 19% 5%



- Molecule 3: Caspase-9

Chain Q: 77% 19% .



- Molecule 3: Caspase-9

Chain R: 77% 19% .



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 92867 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 2400 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 1 | A | 0.33 | 1/9295 (0.0%) | 0.46 | 0/12575 |
| 1 | B | 0.37 | 1/10068 (0.0%) | 0.47 | 0/13613 |
| 1 | C | 0.33 | 1/9295 (0.0%) | 0.46 | 0/12575 |
| 1 | D | 0.36 | 1/10068 (0.0%) | 0.47 | 0/13613 |
| 1 | E | 0.36 | 1/10068 (0.0%) | 0.47 | 0/13613 |
| 1 | F | 0.33 | 1/9295 (0.0%) | 0.47 | 0/12575 |
| 1 | G | 0.37 | 1/10068 (0.0%) | 0.47 | 0/13613 |
| 2 | H | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | I | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | J | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | K | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | L | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | M | 0.25 | 0/830 | 0.42 | 0/1105 |
| 2 | N | 0.25 | 0/830 | 0.42 | 0/1105 |
| 3 | O | 0.60 | 0/784 | 0.61 | 0/1051 |
| 3 | P | 0.60 | 0/784 | 0.61 | 0/1051 |
| 3 | Q | 0.60 | 0/784 | 0.61 | 0/1051 |
| 3 | R | 0.60 | 0/784 | 0.61 | 0/1051 |
| All | All | 0.36 | 7/77103 (0.0%) | 0.47 | 0/104116 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | F | 0 | 1 |
| 1 | G | 0 | 1 |
| All | All | 0 | 7 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | F | 168 | VAL | C-N | 6.96 | 1.50 | 1.34 |
| 1 | B | 168 | VAL | C-N | 6.94 | 1.50 | 1.34 |
| 1 | A | 168 | VAL | C-N | 6.94 | 1.50 | 1.34 |
| 1 | E | 168 | VAL | C-N | 6.94 | 1.50 | 1.34 |
| 1 | D | 168 | VAL | C-N | 6.93 | 1.50 | 1.34 |
| 1 | G | 168 | VAL | C-N | 6.91 | 1.50 | 1.34 |
| 1 | C | 168 | VAL | C-N | 6.91 | 1.50 | 1.34 |

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 336 | ASN | Peptide |
| 1 | B | 336 | ASN | Peptide |
| 1 | C | 336 | ASN | Peptide |
| 1 | D | 336 | ASN | Peptide |
| 1 | E | 336 | ASN | Peptide |
| 1 | F | 336 | ASN | Peptide |
| 1 | G | 336 | ASN | Peptide |

5.2 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 the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 9099 | 0 | 8967 | 296 | 0 |
| 1 | B | 9861 | 0 | 9736 | 300 | 0 |
| 1 | C | 9099 | 0 | 8968 | 293 | 0 |
| 1 | D | 9861 | 0 | 9736 | 310 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 9861 | 0 | 9736 | 313 | 0 |
| 1 | F | 9099 | 0 | 8968 | 300 | 0 |
| 1 | G | 9861 | 0 | 9736 | 300 | 0 |
| 2 | H | 814 | 0 | 833 | 59 | 0 |
| 2 | I | 814 | 0 | 833 | 58 | 0 |
| 2 | J | 814 | 0 | 833 | 59 | 0 |
| 2 | K | 814 | 0 | 833 | 57 | 0 |
| 2 | L | 814 | 0 | 833 | 58 | 0 |
| 2 | M | 814 | 0 | 833 | 59 | 0 |
| 2 | N | 814 | 0 | 833 | 56 | 0 |
| 3 | O | 777 | 0 | 787 | 21 | 0 |
| 3 | P | 777 | 0 | 787 | 28 | 0 |
| 3 | Q | 777 | 0 | 786 | 39 | 0 |
| 3 | R | 777 | 0 | 787 | 29 | 0 |
| 4 | A | 30 | 0 | 9 | 3 | 0 |
| 4 | B | 30 | 0 | 9 | 3 | 0 |
| 4 | C | 30 | 0 | 9 | 3 | 0 |
| 4 | D | 30 | 0 | 9 | 3 | 0 |
| 4 | E | 30 | 0 | 9 | 3 | 0 |
| 4 | F | 30 | 0 | 9 | 3 | 0 |
| 4 | G | 30 | 0 | 9 | 3 | 0 |
| 5 | H | 43 | 0 | 32 | 4 | 0 |
| 5 | I | 43 | 0 | 32 | 4 | 0 |
| 5 | J | 43 | 0 | 32 | 4 | 0 |
| 5 | K | 43 | 0 | 32 | 4 | 0 |
| 5 | L | 43 | 0 | 32 | 4 | 0 |
| 5 | M | 43 | 0 | 32 | 4 | 0 |
| 5 | N | 43 | 0 | 32 | 4 | 0 |
| All | All | 76058 | 0 | 75112 | 2327 | 0 |

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 15.

All (2327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 3:Q:52:ARG:HD3 | 3:R:38:HIS:CE1 | 1.20 | 1.66 |
| 3:Q:52:ARG:CD | 3:R:38:HIS:CE1 | 2.01 | 1.40 |
| 1:E:884:TRP:CH2 | 2:L:79:LYS:HA | 1.68 | 1.28 |
| 1:D:884:TRP:CH2 | 2:K:79:LYS:HA | 1.68 | 1.28 |
| 1:G:884:TRP:CH2 | 2:N:79:LYS:HA | 1.68 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:884:TRP:CH2 | 2:H:79:LYS:HA | 1.68 | 1.27 |
| 1:E:7:ASN:HB2 | 1:F:236:PRO:CG | 1.63 | 1.26 |
| 1:C:884:TRP:CH2 | 2:J:79:LYS:HA | 1.68 | 1.26 |
| 1:F:884:TRP:CH2 | 2:M:79:LYS:HA | 1.68 | 1.26 |
| 1:B:884:TRP:CH2 | 2:I:79:LYS:HA | 1.68 | 1.26 |
| 1:C:884:TRP:CZ3 | 2:J:79:LYS:HD2 | 1.74 | 1.22 |
| 1:B:884:TRP:CZ3 | 2:I:79:LYS:HD2 | 1.74 | 1.22 |
| 1:D:884:TRP:CZ3 | 2:K:79:LYS:HD2 | 1.74 | 1.21 |
| 1:E:884:TRP:CZ3 | 2:L:79:LYS:HD2 | 1.74 | 1.21 |
| 1:A:884:TRP:CZ3 | 2:H:79:LYS:HD2 | 1.74 | 1.21 |
| 1:F:884:TRP:CZ3 | 2:M:79:LYS:HD2 | 1.74 | 1.21 |
| 1:G:884:TRP:CZ3 | 2:N:79:LYS:HD2 | 1.74 | 1.21 |
| 1:B:884:TRP:CZ3 | 2:I:79:LYS:HA | 1.82 | 1.15 |
| 1:A:884:TRP:CZ3 | 2:H:79:LYS:HA | 1.82 | 1.15 |
| 1:C:884:TRP:CZ3 | 2:J:79:LYS:HA | 1.82 | 1.15 |
| 1:G:884:TRP:CZ3 | 2:N:79:LYS:HA | 1.81 | 1.14 |
| 1:D:884:TRP:CZ3 | 2:K:79:LYS:HA | 1.82 | 1.14 |
| 1:E:884:TRP:CZ3 | 2:L:79:LYS:HA | 1.82 | 1.14 |
| 1:F:884:TRP:CZ3 | 2:M:79:LYS:HA | 1.82 | 1.13 |
| 1:E:7:ASN:HB2 | 1:F:236:PRO:HG3 | 1.28 | 1.10 |
| 1:G:1086:GLY:HA2 | 2:N:39:LYS:HZ1 | 1.22 | 1.04 |
| 1:E:7:ASN:HB2 | 1:F:236:PRO:HG2 | 1.36 | 1.01 |
| 1:G:569:CYS:SG | 1:G:1213:PHE:HE1 | 1.85 | 0.99 |
| 1:A:565:GLN:NE2 | 1:A:1213:PHE:H | 1.60 | 0.99 |
| 1:F:569:CYS:SG | 1:F:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:B:569:CYS:SG | 1:B:600:LYS:NZ | 2.36 | 0.99 |
| 1:C:565:GLN:NE2 | 1:C:1213:PHE:H | 1.60 | 0.99 |
| 1:G:569:CYS:SG | 1:G:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:D:569:CYS:SG | 1:D:1213:PHE:HE1 | 1.85 | 0.99 |
| 1:E:569:CYS:SG | 1:E:600:LYS:NZ | 2.36 | 0.99 |
| 1:F:569:CYS:SG | 1:F:600:LYS:NZ | 2.36 | 0.99 |
| 1:B:569:CYS:SG | 1:B:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:B:569:CYS:SG | 1:B:1213:PHE:HE1 | 1.85 | 0.99 |
| 1:C:569:CYS:SG | 1:C:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:C:569:CYS:SG | 1:C:1213:PHE:HE1 | 1.85 | 0.99 |
| 1:C:569:CYS:SG | 1:C:600:LYS:NZ | 2.36 | 0.99 |
| 1:E:569:CYS:SG | 1:E:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:G:569:CYS:SG | 1:G:600:LYS:NZ | 2.36 | 0.99 |
| 1:A:569:CYS:SG | 1:A:1213:PHE:CE1 | 2.56 | 0.99 |
| 1:B:565:GLN:NE2 | 1:B:1213:PHE:H | 1.60 | 0.99 |
| 1:F:569:CYS:SG | 1:F:1213:PHE:HE1 | 1.85 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:569:CYS:SG | 1:E:1213:PHE:HE1 | 1.85 | 0.98 |
| 1:G:565:GLN:NE2 | 1:G:1213:PHE:H | 1.60 | 0.98 |
| 1:G:884:TRP:HH2 | 2:N:79:LYS:HA | 1.28 | 0.98 |
| 1:D:569:CYS:SG | 1:D:1213:PHE:CE1 | 2.56 | 0.98 |
| 1:A:569:CYS:SG | 1:A:1213:PHE:HE1 | 1.85 | 0.98 |
| 1:A:569:CYS:SG | 1:A:600:LYS:NZ | 2.36 | 0.98 |
| 1:E:565:GLN:NE2 | 1:E:1213:PHE:H | 1.60 | 0.97 |
| 1:D:569:CYS:SG | 1:D:600:LYS:NZ | 2.36 | 0.97 |
| 1:F:565:GLN:NE2 | 1:F:1213:PHE:H | 1.60 | 0.97 |
| 1:A:109:TYR:HE1 | 1:G:4:LYS:NZ | 1.34 | 0.97 |
| 1:A:884:TRP:HH2 | 2:H:79:LYS:HA | 1.28 | 0.97 |
| 1:D:565:GLN:NE2 | 1:D:1213:PHE:H | 1.60 | 0.97 |
| 3:O:52:ARG:CB | 3:P:38:HIS:CE1 | 2.48 | 0.96 |
| 3:Q:52:ARG:HD3 | 3:R:38:HIS:ND1 | 1.79 | 0.96 |
| 1:E:884:TRP:HH2 | 2:L:79:LYS:HA | 1.28 | 0.95 |
| 1:E:565:GLN:CD | 1:E:1213:PHE:H | 1.71 | 0.94 |
| 1:F:565:GLN:CD | 1:F:1213:PHE:H | 1.71 | 0.94 |
| 1:D:565:GLN:CD | 1:D:1213:PHE:H | 1.71 | 0.94 |
| 1:G:565:GLN:CD | 1:G:1213:PHE:H | 1.71 | 0.94 |
| 1:E:7:ASN:CB | 1:F:236:PRO:HG2 | 1.97 | 0.94 |
| 1:C:565:GLN:CD | 1:C:1213:PHE:H | 1.71 | 0.93 |
| 1:D:884:TRP:HH2 | 2:K:79:LYS:HA | 1.28 | 0.93 |
| 1:A:565:GLN:CD | 1:A:1213:PHE:H | 1.71 | 0.93 |
| 1:C:884:TRP:HH2 | 2:J:79:LYS:HA | 1.28 | 0.93 |
| 1:B:565:GLN:CD | 1:B:1213:PHE:H | 1.71 | 0.93 |
| 1:B:1086:GLY:HA2 | 2:I:39:LYS:HZ1 | 1.30 | 0.93 |
| 1:D:30:ILE:CG2 | 3:Q:10:ARG:HB3 | 1.97 | 0.93 |
| 1:F:884:TRP:HH2 | 2:M:79:LYS:HA | 1.28 | 0.93 |
| 1:C:1086:GLY:HA2 | 2:J:39:LYS:HZ1 | 1.34 | 0.93 |
| 1:F:1086:GLY:HA2 | 2:M:39:LYS:HZ1 | 1.30 | 0.93 |
| 1:E:550:LEU:CD2 | 1:E:607:SER:HB2 | 2.00 | 0.92 |
| 1:E:7:ASN:CB | 1:F:236:PRO:CG | 2.46 | 0.92 |
| 1:G:550:LEU:CD2 | 1:G:607:SER:HB2 | 2.00 | 0.92 |
| 1:B:884:TRP:HH2 | 2:I:79:LYS:HA | 1.28 | 0.92 |
| 1:B:550:LEU:CD2 | 1:B:607:SER:HB2 | 2.00 | 0.92 |
| 1:F:550:LEU:CD2 | 1:F:607:SER:HB2 | 2.00 | 0.92 |
| 1:D:1086:GLY:HA2 | 2:K:39:LYS:HZ1 | 1.32 | 0.92 |
| 1:A:550:LEU:CD2 | 1:A:607:SER:HB2 | 2.00 | 0.91 |
| 1:A:1086:GLY:HA2 | 2:H:39:LYS:HZ1 | 1.32 | 0.91 |
| 1:D:524:HIS:HB2 | 1:D:646:THR:HG21 | 1.52 | 0.91 |
| 1:C:1086:GLY:HA2 | 2:J:39:LYS:NZ | 1.85 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:550:LEU:CD2 | 1:C:607:SER:HB2 | 2.00 | 0.91 |
| 1:B:1086:GLY:HA2 | 2:I:39:LYS:NZ | 1.86 | 0.91 |
| 1:C:524:HIS:HB2 | 1:C:646:THR:HG21 | 1.52 | 0.91 |
| 1:D:1086:GLY:HA2 | 2:K:39:LYS:NZ | 1.85 | 0.91 |
| 1:A:1086:GLY:HA2 | 2:H:39:LYS:NZ | 1.86 | 0.90 |
| 3:O:52:ARG:HB2 | 3:P:38:HIS:CE1 | 2.06 | 0.90 |
| 1:E:524:HIS:HB2 | 1:E:646:THR:HG21 | 1.52 | 0.90 |
| 1:D:550:LEU:CD2 | 1:D:607:SER:HB2 | 2.00 | 0.90 |
| 3:O:52:ARG:HB3 | 3:P:38:HIS:CE1 | 2.07 | 0.90 |
| 1:B:524:HIS:HB2 | 1:B:646:THR:HG21 | 1.52 | 0.90 |
| 1:E:1086:GLY:HA2 | 2:L:39:LYS:NZ | 1.85 | 0.90 |
| 1:G:1086:GLY:HA2 | 2:N:39:LYS:NZ | 1.85 | 0.90 |
| 1:G:524:HIS:HB2 | 1:G:646:THR:HG21 | 1.52 | 0.89 |
| 1:F:1086:GLY:HA2 | 2:M:39:LYS:NZ | 1.85 | 0.89 |
| 1:A:524:HIS:HB2 | 1:A:646:THR:HG21 | 1.52 | 0.89 |
| 1:F:524:HIS:HB2 | 1:F:646:THR:HG21 | 1.52 | 0.88 |
| 1:F:884:TRP:CZ3 | 2:M:79:LYS:CD | 2.57 | 0.88 |
| 1:B:884:TRP:CZ3 | 2:I:79:LYS:CD | 2.57 | 0.88 |
| 1:A:884:TRP:CZ3 | 2:H:79:LYS:CD | 2.57 | 0.88 |
| 1:E:884:TRP:CZ3 | 2:L:79:LYS:CD | 2.57 | 0.88 |
| 1:C:884:TRP:CZ3 | 2:J:79:LYS:CD | 2.57 | 0.87 |
| 1:A:109:TYR:CE1 | 1:G:4:LYS:NZ | 2.04 | 0.87 |
| 1:D:884:TRP:CZ3 | 2:K:79:LYS:CD | 2.57 | 0.87 |
| 1:A:109:TYR:CE1 | 1:G:4:LYS:HD2 | 2.11 | 0.86 |
| 3:Q:52:ARG:CD | 3:R:38:HIS:HE1 | 1.89 | 0.86 |
| 3:Q:52:ARG:CB | 3:R:38:HIS:HE1 | 1.88 | 0.86 |
| 3:P:50:SER:CB | 3:Q:45:ARG:HH12 | 1.89 | 0.85 |
| 1:A:884:TRP:CH2 | 2:H:79:LYS:CA | 2.59 | 0.85 |
| 3:Q:52:ARG:HD3 | 3:R:38:HIS:NE2 | 1.88 | 0.85 |
| 1:B:884:TRP:CH2 | 2:I:79:LYS:CA | 2.59 | 0.85 |
| 1:E:885:VAL:HG11 | 1:E:888:VAL:HG13 | 1.59 | 0.85 |
| 1:G:885:VAL:HG11 | 1:G:888:VAL:HG13 | 1.59 | 0.85 |
| 1:G:884:TRP:CH2 | 2:N:79:LYS:CA | 2.59 | 0.85 |
| 1:G:884:TRP:CZ3 | 2:N:79:LYS:CD | 2.57 | 0.85 |
| 1:E:1086:GLY:HA2 | 2:L:39:LYS:HZ1 | 1.41 | 0.85 |
| 1:A:885:VAL:HG11 | 1:A:888:VAL:HG13 | 1.59 | 0.85 |
| 1:D:885:VAL:HG11 | 1:D:888:VAL:HG13 | 1.59 | 0.85 |
| 1:F:885:VAL:HG11 | 1:F:888:VAL:HG13 | 1.59 | 0.85 |
| 1:B:882:LEU:HB2 | 1:B:903:ASP:HB3 | 1.59 | 0.84 |
| 1:A:882:LEU:HB2 | 1:A:903:ASP:HB3 | 1.59 | 0.84 |
| 1:B:885:VAL:HG11 | 1:B:888:VAL:HG13 | 1.59 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:884:TRP:CH2 | 2:J:79:LYS:CA | 2.58 | 0.84 |
| 1:G:550:LEU:HD21 | 1:G:607:SER:HB2 | 1.60 | 0.84 |
| 1:C:885:VAL:HG11 | 1:C:888:VAL:HG13 | 1.59 | 0.84 |
| 1:A:550:LEU:HD21 | 1:A:607:SER:HB2 | 1.60 | 0.83 |
| 1:F:884:TRP:CH2 | 2:M:79:LYS:CA | 2.59 | 0.83 |
| 1:F:550:LEU:HD21 | 1:F:607:SER:HB2 | 1.60 | 0.83 |
| 1:G:882:LEU:HB2 | 1:G:903:ASP:HB3 | 1.59 | 0.83 |
| 1:C:882:LEU:HB2 | 1:C:903:ASP:HB3 | 1.59 | 0.83 |
| 1:F:565:GLN:NE2 | 1:F:1213:PHE:N | 2.27 | 0.82 |
| 1:C:550:LEU:HD21 | 1:C:607:SER:HB2 | 1.60 | 0.82 |
| 1:E:550:LEU:HD21 | 1:E:607:SER:HB2 | 1.60 | 0.82 |
| 1:B:565:GLN:NE2 | 1:B:1213:PHE:N | 2.27 | 0.82 |
| 1:E:565:GLN:NE2 | 1:E:1213:PHE:N | 2.27 | 0.82 |
| 1:E:882:LEU:HB2 | 1:E:903:ASP:HB3 | 1.59 | 0.82 |
| 1:B:550:LEU:HD21 | 1:B:607:SER:HB2 | 1.60 | 0.82 |
| 1:D:550:LEU:HD21 | 1:D:607:SER:HB2 | 1.60 | 0.82 |
| 1:A:565:GLN:NE2 | 1:A:1213:PHE:N | 2.27 | 0.82 |
| 1:C:565:GLN:NE2 | 1:C:1213:PHE:N | 2.27 | 0.82 |
| 1:F:882:LEU:HB2 | 1:F:903:ASP:HB3 | 1.59 | 0.82 |
| 1:D:565:GLN:NE2 | 1:D:1213:PHE:N | 2.27 | 0.81 |
| 1:D:884:TRP:CH2 | 2:K:79:LYS:CA | 2.59 | 0.81 |
| 1:G:584:ALA:HA | 1:G:594:TYR:CE2 | 2.16 | 0.81 |
| 1:G:565:GLN:NE2 | 1:G:1213:PHE:N | 2.27 | 0.81 |
| 1:E:584:ALA:HA | 1:E:594:TYR:CE2 | 2.16 | 0.81 |
| 1:D:882:LEU:HB2 | 1:D:903:ASP:HB3 | 1.59 | 0.81 |
| 1:D:584:ALA:HA | 1:D:594:TYR:CE2 | 2.16 | 0.81 |
| 1:A:862:TYR:CA | 1:A:884:TRP:HA | 2.11 | 0.80 |
| 1:B:584:ALA:HA | 1:B:594:TYR:CE2 | 2.16 | 0.80 |
| 1:F:584:ALA:HA | 1:F:594:TYR:CE2 | 2.16 | 0.80 |
| 1:F:862:TYR:CA | 1:F:884:TRP:HA | 2.11 | 0.80 |
| 1:C:862:TYR:HA | 1:C:884:TRP:HA | 1.63 | 0.80 |
| 1:E:884:TRP:CH2 | 2:L:79:LYS:CA | 2.59 | 0.80 |
| 1:E:862:TYR:CA | 1:E:884:TRP:HA | 2.11 | 0.80 |
| 1:A:584:ALA:HA | 1:A:594:TYR:CE2 | 2.16 | 0.80 |
| 1:B:862:TYR:HA | 1:B:884:TRP:HA | 1.63 | 0.80 |
| 1:D:862:TYR:HA | 1:D:884:TRP:HA | 1.63 | 0.80 |
| 1:E:862:TYR:HA | 1:E:884:TRP:HA | 1.63 | 0.80 |
| 1:E:7:ASN:CB | 1:F:236:PRO:HG3 | 2.11 | 0.80 |
| 1:A:862:TYR:HA | 1:A:884:TRP:HA | 1.63 | 0.80 |
| 3:Q:52:ARG:CD | 3:R:38:HIS:ND1 | 2.40 | 0.80 |
| 1:D:862:TYR:CA | 1:D:884:TRP:HA | 2.11 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:6:ARG:NH2 | 1:F:232:LEU:O | 2.15 | 0.79 |
| 1:G:862:TYR:CA | 1:G:884:TRP:HA | 2.11 | 0.79 |
| 1:F:882:LEU:HD13 | 1:F:1176:HIS:NE2 | 1.98 | 0.79 |
| 1:F:862:TYR:HA | 1:F:884:TRP:HA | 1.64 | 0.79 |
| 3:O:15:ARG:CD | 3:O:19:GLU:OE2 | 2.30 | 0.79 |
| 1:B:862:TYR:CA | 1:B:884:TRP:HA | 2.11 | 0.79 |
| 1:C:584:ALA:HA | 1:C:594:TYR:CE2 | 2.16 | 0.79 |
| 1:E:1084:HIS:HE2 | 1:E:1108:THR:HG1 | 1.30 | 0.79 |
| 1:B:882:LEU:HD13 | 1:B:1176:HIS:NE2 | 1.98 | 0.79 |
| 1:G:862:TYR:HA | 1:G:884:TRP:HA | 1.63 | 0.79 |
| 3:Q:15:ARG:CD | 3:Q:19:GLU:OE2 | 2.30 | 0.79 |
| 1:C:862:TYR:CA | 1:C:884:TRP:HA | 2.11 | 0.79 |
| 1:D:1084:HIS:HE2 | 1:D:1108:THR:HG1 | 1.31 | 0.79 |
| 3:P:15:ARG:CD | 3:P:19:GLU:OE2 | 2.30 | 0.79 |
| 3:R:15:ARG:CD | 3:R:19:GLU:OE2 | 2.30 | 0.79 |
| 1:D:882:LEU:HD13 | 1:D:1176:HIS:NE2 | 1.98 | 0.78 |
| 1:C:882:LEU:HD13 | 1:C:1176:HIS:NE2 | 1.98 | 0.78 |
| 1:A:882:LEU:HD13 | 1:A:1176:HIS:NE2 | 1.98 | 0.78 |
| 1:G:882:LEU:HD13 | 1:G:1176:HIS:NE2 | 1.98 | 0.78 |
| 1:E:882:LEU:HD13 | 1:E:1176:HIS:NE2 | 1.98 | 0.77 |
| 3:P:50:SER:HB2 | 3:Q:45:ARG:HH12 | 1.48 | 0.77 |
| 1:A:565:GLN:HE22 | 1:A:1213:PHE:H | 1.33 | 0.77 |
| 1:E:349:GLN:HA | 1:E:447:GLU:OE2 | 1.86 | 0.76 |
| 1:A:349:GLN:HA | 1:A:447:GLU:OE2 | 1.85 | 0.76 |
| 1:B:884:TRP:HH2 | 2:I:79:LYS:CA | 1.97 | 0.76 |
| 1:B:349:GLN:HA | 1:B:447:GLU:OE2 | 1.85 | 0.76 |
| 1:F:884:TRP:HH2 | 2:M:79:LYS:CA | 1.97 | 0.76 |
| 1:G:47:PRO:HG2 | 1:G:51:GLN:HE22 | 1.51 | 0.76 |
| 1:C:1084:HIS:HE2 | 1:C:1108:THR:HG1 | 1.33 | 0.76 |
| 1:G:1086:GLY:CA | 2:N:39:LYS:HZ1 | 1.98 | 0.76 |
| 1:C:565:GLN:HE22 | 1:C:1213:PHE:H | 1.33 | 0.76 |
| 1:G:884:TRP:HH2 | 2:N:79:LYS:CA | 1.97 | 0.76 |
| 1:A:1084:HIS:HE2 | 1:A:1108:THR:HG1 | 1.31 | 0.76 |
| 1:F:349:GLN:HA | 1:F:447:GLU:OE2 | 1.85 | 0.76 |
| 1:E:47:PRO:HG2 | 1:E:51:GLN:HE22 | 1.51 | 0.76 |
| 1:B:565:GLN:HE22 | 1:B:1213:PHE:H | 1.33 | 0.75 |
| 1:D:349:GLN:HA | 1:D:447:GLU:OE2 | 1.85 | 0.75 |
| 1:E:7:ASN:CG | 1:F:236:PRO:HG2 | 2.06 | 0.75 |
| 1:C:1112:TRP:HB3 | 1:C:1119:PRO:HA | 1.68 | 0.75 |
| 1:A:882:LEU:CD1 | 1:A:1176:HIS:NE2 | 2.50 | 0.75 |
| 1:F:1084:HIS:HE2 | 1:F:1108:THR:HG1 | 1.33 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:Q:7:ARG:O | 3:Q:11:ARG:HG3 | 1.87 | 0.75 |
| 1:A:557:ARG:NH2 | 1:A:1175:THR:HG23 | 2.02 | 0.75 |
| 1:E:882:LEU:CD1 | 1:E:1176:HIS:NE2 | 2.50 | 0.75 |
| 1:G:882:LEU:CD1 | 1:G:1176:HIS:NE2 | 2.50 | 0.75 |
| 1:B:47:PRO:HG2 | 1:B:51:GLN:HE22 | 1.51 | 0.75 |
| 1:B:557:ARG:NH2 | 1:B:1175:THR:HG23 | 2.01 | 0.75 |
| 1:E:884:TRP:HH2 | 2:L:79:LYS:CA | 1.97 | 0.75 |
| 1:C:349:GLN:HA | 1:C:447:GLU:OE2 | 1.85 | 0.75 |
| 1:D:1112:TRP:HB3 | 1:D:1119:PRO:HA | 1.68 | 0.75 |
| 3:R:7:ARG:O | 3:R:11:ARG:HG3 | 1.87 | 0.75 |
| 1:B:882:LEU:CD1 | 1:B:1176:HIS:NE2 | 2.50 | 0.75 |
| 1:F:882:LEU:CD1 | 1:F:1176:HIS:NE2 | 2.50 | 0.75 |
| 2:N:24:GLY:O | 2:N:31:ASN:ND2 | 2.20 | 0.75 |
| 1:E:1112:TRP:HB3 | 1:E:1119:PRO:HA | 1.68 | 0.75 |
| 1:F:1112:TRP:HB3 | 1:F:1119:PRO:HA | 1.68 | 0.74 |
| 1:G:565:GLN:HE22 | 1:G:1213:PHE:H | 1.33 | 0.74 |
| 2:H:24:GLY:O | 2:H:31:ASN:ND2 | 2.20 | 0.74 |
| 1:D:309:GLN:NE2 | 1:D:339:GLU:OE1 | 2.21 | 0.74 |
| 1:E:309:GLN:NE2 | 1:E:339:GLU:OE1 | 2.21 | 0.74 |
| 1:F:557:ARG:NH2 | 1:F:1175:THR:HG23 | 2.01 | 0.74 |
| 1:G:557:ARG:NH2 | 1:G:1175:THR:HG23 | 2.01 | 0.74 |
| 1:G:349:GLN:HA | 1:G:447:GLU:OE2 | 1.85 | 0.74 |
| 1:B:884:TRP:HZ3 | 2:I:79:LYS:HD2 | 1.51 | 0.74 |
| 3:P:7:ARG:O | 3:P:11:ARG:HG3 | 1.87 | 0.74 |
| 1:B:339:GLU:OE2 | 1:B:343:LYS:NZ | 2.20 | 0.74 |
| 1:F:941:ASP:H | 1:F:946:LEU:HA | 1.53 | 0.74 |
| 1:A:884:TRP:HH2 | 2:H:79:LYS:CA | 1.97 | 0.74 |
| 1:C:309:GLN:NE2 | 1:C:339:GLU:OE1 | 2.21 | 0.74 |
| 1:D:882:LEU:CD1 | 1:D:1176:HIS:NE2 | 2.50 | 0.74 |
| 1:F:309:GLN:NE2 | 1:F:339:GLU:OE1 | 2.21 | 0.74 |
| 1:A:1112:TRP:HB3 | 1:A:1119:PRO:HA | 1.68 | 0.74 |
| 1:C:339:GLU:OE2 | 1:C:343:LYS:NZ | 2.20 | 0.74 |
| 2:L:24:GLY:O | 2:L:31:ASN:ND2 | 2.20 | 0.74 |
| 1:C:557:ARG:NH2 | 1:C:1175:THR:HG23 | 2.01 | 0.74 |
| 1:C:882:LEU:CD1 | 1:C:1176:HIS:NE2 | 2.50 | 0.74 |
| 1:D:47:PRO:HG2 | 1:D:51:GLN:HE22 | 1.51 | 0.74 |
| 1:D:557:ARG:NH2 | 1:D:1175:THR:HG23 | 2.01 | 0.74 |
| 1:D:941:ASP:H | 1:D:946:LEU:HA | 1.53 | 0.74 |
| 1:F:565:GLN:HE22 | 1:F:1213:PHE:H | 1.33 | 0.74 |
| 1:A:274:MET:HE3 | 1:G:358:SER:HB3 | 1.70 | 0.74 |
| 2:I:24:GLY:O | 2:I:31:ASN:ND2 | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:884:TRP:HH2 | 2:J:79:LYS:CA | 1.97 | 0.74 |
| 1:C:941:ASP:H | 1:C:946:LEU:HA | 1.53 | 0.74 |
| 1:E:565:GLN:HE22 | 1:E:1213:PHE:H | 1.33 | 0.74 |
| 1:G:1112:TRP:HB3 | 1:G:1119:PRO:HA | 1.68 | 0.74 |
| 2:K:24:GLY:O | 2:K:31:ASN:ND2 | 2.20 | 0.74 |
| 1:E:884:TRP:HZ3 | 2:L:79:LYS:HD2 | 1.51 | 0.74 |
| 2:M:24:GLY:O | 2:M:31:ASN:ND2 | 2.20 | 0.74 |
| 3:Q:52:ARG:HD2 | 3:R:38:HIS:CE1 | 2.17 | 0.74 |
| 1:B:1112:TRP:HB3 | 1:B:1119:PRO:HA | 1.68 | 0.74 |
| 1:A:274:MET:CE | 1:G:358:SER:HB3 | 2.17 | 0.74 |
| 1:D:339:GLU:OE2 | 1:D:343:LYS:NZ | 2.20 | 0.73 |
| 1:G:941:ASP:H | 1:G:946:LEU:HA | 1.53 | 0.73 |
| 3:O:7:ARG:O | 3:O:11:ARG:HG3 | 1.87 | 0.73 |
| 1:D:884:TRP:HH2 | 2:K:79:LYS:CA | 1.97 | 0.73 |
| 1:E:557:ARG:NH2 | 1:E:1175:THR:HG23 | 2.01 | 0.73 |
| 2:J:24:GLY:O | 2:J:31:ASN:ND2 | 2.20 | 0.73 |
| 1:A:309:GLN:NE2 | 1:A:339:GLU:OE1 | 2.21 | 0.73 |
| 1:C:358:SER:HB3 | 1:D:274:MET:HE3 | 1.71 | 0.73 |
| 1:B:309:GLN:NE2 | 1:B:339:GLU:OE1 | 2.21 | 0.73 |
| 1:C:884:TRP:HZ3 | 2:J:79:LYS:HD2 | 1.51 | 0.73 |
| 1:E:339:GLU:OE2 | 1:E:343:LYS:NZ | 2.20 | 0.73 |
| 1:G:309:GLN:NE2 | 1:G:339:GLU:OE1 | 2.21 | 0.73 |
| 3:Q:52:ARG:CB | 3:R:38:HIS:CE1 | 2.72 | 0.73 |
| 1:A:339:GLU:OE2 | 1:A:343:LYS:NZ | 2.20 | 0.73 |
| 1:D:884:TRP:HZ3 | 2:K:79:LYS:HD2 | 1.52 | 0.73 |
| 3:R:87:SER:O | 3:R:91:THR:HG23 | 1.89 | 0.73 |
| 1:B:1084:HIS:HE2 | 1:B:1108:THR:HG1 | 1.34 | 0.73 |
| 3:Q:87:SER:O | 3:Q:91:THR:HG23 | 1.89 | 0.72 |
| 1:E:941:ASP:H | 1:E:946:LEU:HA | 1.53 | 0.72 |
| 1:G:339:GLU:OE2 | 1:G:343:LYS:NZ | 2.20 | 0.72 |
| 1:A:941:ASP:H | 1:A:946:LEU:HA | 1.53 | 0.72 |
| 1:C:358:SER:HB3 | 1:D:274:MET:CE | 2.19 | 0.72 |
| 1:B:941:ASP:H | 1:B:946:LEU:HA | 1.53 | 0.72 |
| 3:P:87:SER:O | 3:P:91:THR:HG23 | 1.89 | 0.72 |
| 1:B:609:LEU:HB3 | 1:B:908:LEU:HB2 | 1.71 | 0.72 |
| 1:C:609:LEU:HB3 | 1:C:908:LEU:HB2 | 1.71 | 0.72 |
| 1:D:565:GLN:HE22 | 1:D:1213:PHE:H | 1.33 | 0.72 |
| 2:K:26:HIS:NE2 | 2:K:44:PRO:O | 2.23 | 0.72 |
| 1:B:882:LEU:HB2 | 1:B:903:ASP:CB | 2.20 | 0.71 |
| 1:F:339:GLU:OE2 | 1:F:343:LYS:NZ | 2.20 | 0.71 |
| 1:G:882:LEU:HB2 | 1:G:903:ASP:CB | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:1084:HIS:HE2 | 1:G:1108:THR:HG1 | 1.35 | 0.71 |
| 2:I:26:HIS:NE2 | 2:I:44:PRO:O | 2.23 | 0.71 |
| 1:D:609:LEU:HB3 | 1:D:908:LEU:HB2 | 1.71 | 0.71 |
| 2:H:26:HIS:NE2 | 2:H:44:PRO:O | 2.23 | 0.71 |
| 2:J:26:HIS:NE2 | 2:J:44:PRO:O | 2.23 | 0.71 |
| 2:L:26:HIS:NE2 | 2:L:44:PRO:O | 2.23 | 0.71 |
| 1:D:1034:LEU:HB3 | 1:D:1036:LYS:HD3 | 1.73 | 0.71 |
| 1:E:609:LEU:HB3 | 1:E:908:LEU:HB2 | 1.71 | 0.71 |
| 3:O:87:SER:O | 3:O:91:THR:HG23 | 1.89 | 0.71 |
| 1:C:1034:LEU:HB3 | 1:C:1036:LYS:HD3 | 1.73 | 0.71 |
| 1:D:358:SER:HB3 | 1:E:274:MET:CE | 2.19 | 0.71 |
| 2:M:26:HIS:NE2 | 2:M:44:PRO:O | 2.23 | 0.71 |
| 1:A:609:LEU:HB3 | 1:A:908:LEU:HB2 | 1.71 | 0.71 |
| 1:G:565:GLN:HE22 | 1:G:1213:PHE:N | 1.89 | 0.71 |
| 1:A:1034:LEU:HB3 | 1:A:1036:LYS:HD3 | 1.73 | 0.71 |
| 1:G:549:SER:O | 1:G:610:VAL:HB | 1.91 | 0.71 |
| 1:D:30:ILE:HG23 | 3:Q:10:ARG:HB3 | 1.73 | 0.71 |
| 1:A:549:SER:O | 1:A:610:VAL:HB | 1.91 | 0.71 |
| 1:D:882:LEU:HB2 | 1:D:903:ASP:CB | 2.20 | 0.71 |
| 1:E:549:SER:O | 1:E:610:VAL:HB | 1.91 | 0.71 |
| 2:N:26:HIS:NE2 | 2:N:44:PRO:O | 2.23 | 0.71 |
| 3:P:41:GLU:HB3 | 3:P:45:ARG:HH12 | 1.56 | 0.71 |
| 1:B:1034:LEU:HB3 | 1:B:1036:LYS:HD3 | 1.73 | 0.71 |
| 1:B:346:GLN:O | 1:B:348:LYS:HG3 | 1.91 | 0.71 |
| 1:B:549:SER:O | 1:B:610:VAL:HB | 1.91 | 0.71 |
| 1:F:609:LEU:HB3 | 1:F:908:LEU:HB2 | 1.71 | 0.71 |
| 1:G:1034:LEU:HB3 | 1:G:1036:LYS:HD3 | 1.73 | 0.71 |
| 1:B:28:HIS:CE1 | 3:P:14:LEU:HD21 | 2.26 | 0.71 |
| 1:C:346:GLN:O | 1:C:348:LYS:HG3 | 1.91 | 0.70 |
| 1:D:47:PRO:HG2 | 1:D:51:GLN:NE2 | 2.07 | 0.70 |
| 1:E:882:LEU:HB2 | 1:E:903:ASP:CB | 2.20 | 0.70 |
| 1:F:346:GLN:O | 1:F:348:LYS:HG3 | 1.91 | 0.70 |
| 1:G:609:LEU:HB3 | 1:G:908:LEU:HB2 | 1.71 | 0.70 |
| 1:A:882:LEU:HB2 | 1:A:903:ASP:CB | 2.20 | 0.70 |
| 1:C:549:SER:O | 1:C:610:VAL:HB | 1.91 | 0.70 |
| 1:D:569:CYS:SG | 1:D:1213:PHE:CZ | 2.85 | 0.70 |
| 1:D:346:GLN:O | 1:D:348:LYS:HG3 | 1.91 | 0.70 |
| 1:D:403:LEU:HD13 | 1:D:460:ILE:HG22 | 1.73 | 0.70 |
| 1:E:47:PRO:HG2 | 1:E:51:GLN:NE2 | 2.07 | 0.70 |
| 1:F:549:SER:O | 1:F:610:VAL:HB | 1.91 | 0.70 |
| 1:A:569:CYS:SG | 1:A:1213:PHE:CZ | 2.85 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:565:GLN:HE22 | 1:C:1213:PHE:N | 1.89 | 0.70 |
| 1:E:884:TRP:CE3 | 2:L:79:LYS:HD2 | 2.27 | 0.70 |
| 1:A:358:SER:HB3 | 1:B:274:MET:CE | 2.20 | 0.70 |
| 1:E:1034:LEU:HB3 | 1:E:1036:LYS:HD3 | 1.73 | 0.70 |
| 1:E:346:GLN:O | 1:E:348:LYS:HG3 | 1.91 | 0.70 |
| 1:E:358:SER:HB3 | 1:F:274:MET:CE | 2.21 | 0.70 |
| 1:E:189:LYS:NZ | 1:E:374:MET:SD | 2.65 | 0.70 |
| 1:E:403:LEU:HD13 | 1:E:460:ILE:HG22 | 1.73 | 0.70 |
| 1:G:569:CYS:SG | 1:G:1213:PHE:CZ | 2.85 | 0.70 |
| 1:C:569:CYS:SG | 1:C:1213:PHE:CZ | 2.85 | 0.70 |
| 1:B:358:SER:HB3 | 1:C:274:MET:CE | 2.21 | 0.70 |
| 1:C:403:LEU:HD13 | 1:C:460:ILE:HG22 | 1.73 | 0.70 |
| 1:D:189:LYS:NZ | 1:D:374:MET:SD | 2.65 | 0.70 |
| 1:D:854:LEU:HB3 | 1:D:866:LEU:HD11 | 1.74 | 0.70 |
| 1:A:854:LEU:HB3 | 1:A:866:LEU:HD11 | 1.74 | 0.70 |
| 1:G:346:GLN:O | 1:G:348:LYS:HG3 | 1.91 | 0.70 |
| 1:C:854:LEU:HB3 | 1:C:866:LEU:HD11 | 1.74 | 0.70 |
| 1:C:882:LEU:HB2 | 1:C:903:ASP:CB | 2.21 | 0.70 |
| 1:E:569:CYS:SG | 1:E:1213:PHE:CZ | 2.85 | 0.70 |
| 1:D:884:TRP:CE3 | 2:K:79:LYS:HD2 | 2.27 | 0.70 |
| 1:B:565:GLN:HE22 | 1:B:1213:PHE:N | 1.89 | 0.69 |
| 1:G:854:LEU:HB3 | 1:G:866:LEU:HD11 | 1.74 | 0.69 |
| 1:B:884:TRP:CE3 | 2:I:79:LYS:HD2 | 2.27 | 0.69 |
| 1:A:346:GLN:O | 1:A:348:LYS:HG3 | 1.91 | 0.69 |
| 1:D:14:GLU:OE1 | 1:E:31:SER:OG | 2.10 | 0.69 |
| 1:E:854:LEU:HB3 | 1:E:866:LEU:HD11 | 1.74 | 0.69 |
| 1:F:1034:LEU:HB3 | 1:F:1036:LYS:HD3 | 1.73 | 0.69 |
| 1:F:882:LEU:HB2 | 1:F:903:ASP:CB | 2.20 | 0.69 |
| 1:G:884:TRP:CE3 | 2:N:79:LYS:HD2 | 2.27 | 0.69 |
| 3:P:15:ARG:HD3 | 3:P:19:GLU:OE2 | 1.92 | 0.69 |
| 1:G:47:PRO:HG2 | 1:G:51:GLN:NE2 | 2.07 | 0.69 |
| 1:A:844:GLN:HE22 | 2:H:79:LYS:NZ | 1.91 | 0.69 |
| 1:B:854:LEU:HB3 | 1:B:866:LEU:HD11 | 1.74 | 0.69 |
| 1:E:844:GLN:HE22 | 2:L:79:LYS:NZ | 1.91 | 0.69 |
| 1:B:569:CYS:SG | 1:B:1213:PHE:CZ | 2.85 | 0.69 |
| 1:D:549:SER:O | 1:D:610:VAL:HB | 1.91 | 0.69 |
| 1:C:844:GLN:HE22 | 2:J:79:LYS:NZ | 1.91 | 0.69 |
| 3:Q:15:ARG:HD3 | 3:Q:19:GLU:OE2 | 1.92 | 0.69 |
| 1:B:47:PRO:HG2 | 1:B:51:GLN:NE2 | 2.07 | 0.69 |
| 1:F:854:LEU:HB3 | 1:F:866:LEU:HD11 | 1.74 | 0.69 |
| 1:F:569:CYS:SG | 1:F:1213:PHE:CZ | 2.85 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:189:LYS:NZ | 1:F:374:MET:SD | 2.65 | 0.69 |
| 1:F:403:LEU:HD13 | 1:F:460:ILE:HG22 | 1.74 | 0.69 |
| 1:B:844:GLN:HE22 | 2:I:79:LYS:NZ | 1.90 | 0.69 |
| 1:D:844:GLN:HE22 | 2:K:79:LYS:NZ | 1.91 | 0.69 |
| 1:G:844:GLN:HE22 | 2:N:79:LYS:NZ | 1.91 | 0.69 |
| 1:F:565:GLN:HE22 | 1:F:1213:PHE:N | 1.89 | 0.68 |
| 1:B:403:LEU:HD13 | 1:B:460:ILE:HG22 | 1.73 | 0.68 |
| 1:F:844:GLN:HE22 | 2:M:79:LYS:NZ | 1.91 | 0.68 |
| 1:A:403:LEU:HD13 | 1:A:460:ILE:HG22 | 1.73 | 0.68 |
| 1:B:37:ILE:HG13 | 3:P:10:ARG:NH1 | 2.08 | 0.68 |
| 1:B:590:ASN:C | 1:B:592:MET:H | 1.97 | 0.68 |
| 1:C:189:LYS:NZ | 1:C:374:MET:SD | 2.65 | 0.68 |
| 1:G:403:LEU:HD13 | 1:G:460:ILE:HG22 | 1.74 | 0.68 |
| 2:I:61:GLU:HA | 2:I:95:ILE:HG21 | 1.76 | 0.68 |
| 3:R:15:ARG:HD3 | 3:R:19:GLU:OE2 | 1.93 | 0.68 |
| 1:F:884:TRP:CE3 | 2:M:79:LYS:HD2 | 2.27 | 0.68 |
| 2:J:61:GLU:HA | 2:J:95:ILE:HG21 | 1.76 | 0.68 |
| 1:B:611:VAL:HG12 | 1:B:613:PRO:HD3 | 1.75 | 0.68 |
| 2:H:61:GLU:HA | 2:H:95:ILE:HG21 | 1.75 | 0.68 |
| 1:C:590:ASN:C | 1:C:592:MET:H | 1.97 | 0.68 |
| 1:D:565:GLN:HE22 | 1:D:1213:PHE:N | 1.89 | 0.68 |
| 1:F:611:VAL:HG12 | 1:F:613:PRO:HD3 | 1.75 | 0.68 |
| 1:G:611:VAL:HG12 | 1:G:613:PRO:HD3 | 1.75 | 0.68 |
| 1:D:1204:VAL:HG12 | 1:D:1205:VAL:HG23 | 1.76 | 0.68 |
| 1:G:189:LYS:NZ | 1:G:374:MET:SD | 2.65 | 0.68 |
| 1:E:565:GLN:HE22 | 1:E:1213:PHE:N | 1.89 | 0.67 |
| 2:H:20:VAL:HG12 | 2:H:32:LEU:HB2 | 1.77 | 0.67 |
| 1:C:1204:VAL:HG12 | 1:C:1205:VAL:HG23 | 1.76 | 0.67 |
| 1:C:611:VAL:HG12 | 1:C:613:PRO:HD3 | 1.75 | 0.67 |
| 1:D:590:ASN:C | 1:D:592:MET:H | 1.97 | 0.67 |
| 1:A:884:TRP:CE3 | 2:H:79:LYS:HD2 | 2.27 | 0.67 |
| 1:C:884:TRP:CE3 | 2:J:79:LYS:HD2 | 2.27 | 0.67 |
| 1:G:565:GLN:CD | 1:G:1213:PHE:N | 2.48 | 0.67 |
| 1:C:1086:GLY:HA2 | 2:J:39:LYS:CE | 2.24 | 0.67 |
| 2:K:61:GLU:HA | 2:K:95:ILE:HG21 | 1.75 | 0.67 |
| 2:N:61:GLU:HA | 2:N:95:ILE:HG21 | 1.75 | 0.67 |
| 3:O:15:ARG:HD3 | 3:O:19:GLU:OE2 | 1.93 | 0.67 |
| 3:O:52:ARG:CB | 3:P:38:HIS:HE1 | 2.07 | 0.67 |
| 1:A:590:ASN:C | 1:A:592:MET:H | 1.97 | 0.67 |
| 2:I:20:VAL:HG12 | 2:I:32:LEU:HB2 | 1.77 | 0.67 |
| 1:E:1204:VAL:HG12 | 1:E:1205:VAL:HG23 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:20:VAL:HG12 | 2:N:32:LEU:HB2 | 1.77 | 0.67 |
| 1:D:358:SER:HB3 | 1:E:274:MET:HE2 | 1.76 | 0.67 |
| 1:E:590:ASN:C | 1:E:592:MET:H | 1.97 | 0.67 |
| 1:F:565:GLN:CD | 1:F:1213:PHE:N | 2.48 | 0.67 |
| 1:B:1086:GLY:HA2 | 2:I:39:LYS:CE | 2.24 | 0.67 |
| 1:A:189:LYS:NZ | 1:A:374:MET:SD | 2.65 | 0.67 |
| 2:J:18:HIS:NE2 | 5:J:500:HEC:NB | 2.43 | 0.67 |
| 2:K:18:HIS:NE2 | 5:K:500:HEC:NB | 2.43 | 0.67 |
| 2:M:61:GLU:HA | 2:M:95:ILE:HG21 | 1.76 | 0.67 |
| 3:O:6:ARG:O | 3:O:10:ARG:HG2 | 1.95 | 0.67 |
| 1:A:611:VAL:HG12 | 1:A:613:PRO:HD3 | 1.75 | 0.67 |
| 2:L:61:GLU:HA | 2:L:95:ILE:HG21 | 1.75 | 0.67 |
| 1:A:565:GLN:CD | 1:A:1213:PHE:N | 2.48 | 0.67 |
| 1:B:189:LYS:NZ | 1:B:374:MET:SD | 2.65 | 0.67 |
| 2:L:18:HIS:NE2 | 5:L:500:HEC:NB | 2.43 | 0.67 |
| 1:B:1204:VAL:HG12 | 1:B:1205:VAL:HG23 | 1.76 | 0.66 |
| 1:D:611:VAL:HG12 | 1:D:613:PRO:HD3 | 1.75 | 0.66 |
| 2:N:18:HIS:NE2 | 5:N:500:HEC:NB | 2.43 | 0.66 |
| 1:E:611:VAL:HG12 | 1:E:613:PRO:HD3 | 1.75 | 0.66 |
| 1:E:1086:GLY:HA2 | 2:L:39:LYS:CE | 2.24 | 0.66 |
| 3:Q:6:ARG:O | 3:Q:10:ARG:HG2 | 1.95 | 0.66 |
| 1:A:569:CYS:HG | 1:A:1213:PHE:HE1 | 1.43 | 0.66 |
| 1:B:474:SER:HB2 | 1:B:477:GLN:HG2 | 1.78 | 0.66 |
| 1:E:565:GLN:CD | 1:E:1213:PHE:N | 2.48 | 0.66 |
| 1:F:590:ASN:C | 1:F:592:MET:H | 1.97 | 0.66 |
| 1:B:565:GLN:CD | 1:B:1213:PHE:N | 2.48 | 0.66 |
| 1:A:1086:GLY:HA2 | 2:H:39:LYS:CE | 2.24 | 0.66 |
| 2:H:18:HIS:NE2 | 5:H:500:HEC:NB | 2.43 | 0.66 |
| 1:F:1086:GLY:HA2 | 2:M:39:LYS:CE | 2.25 | 0.66 |
| 1:C:565:GLN:CD | 1:C:1213:PHE:N | 2.48 | 0.66 |
| 1:D:1027:ILE:HD11 | 1:D:1047:VAL:HG11 | 1.78 | 0.66 |
| 1:D:565:GLN:CD | 1:D:1213:PHE:N | 2.48 | 0.66 |
| 1:E:1027:ILE:HD11 | 1:E:1047:VAL:HG11 | 1.78 | 0.66 |
| 1:F:1027:ILE:HD11 | 1:F:1047:VAL:HG11 | 1.78 | 0.66 |
| 1:G:1086:GLY:HA2 | 2:N:39:LYS:CE | 2.24 | 0.66 |
| 1:F:358:SER:HB3 | 1:G:274:MET:CE | 2.25 | 0.66 |
| 1:A:474:SER:HB2 | 1:A:477:GLN:HG2 | 1.78 | 0.66 |
| 1:G:590:ASN:C | 1:G:592:MET:H | 1.97 | 0.66 |
| 2:I:18:HIS:NE2 | 5:I:500:HEC:NB | 2.43 | 0.66 |
| 2:L:20:VAL:HG12 | 2:L:32:LEU:HB2 | 1.77 | 0.66 |
| 1:F:1204:VAL:HG12 | 1:F:1205:VAL:HG23 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:844:GLN:NE2 | 2:L:79:LYS:HE3 | 2.11 | 0.66 |
| 3:R:6:ARG:O | 3:R:10:ARG:HG2 | 1.95 | 0.66 |
| 2:J:20:VAL:HG12 | 2:J:32:LEU:HB2 | 1.77 | 0.66 |
| 1:D:1086:GLY:HA2 | 2:K:39:LYS:CE | 2.24 | 0.66 |
| 1:F:844:GLN:NE2 | 2:M:79:LYS:HE3 | 2.11 | 0.66 |
| 3:P:6:ARG:O | 3:P:10:ARG:HG2 | 1.95 | 0.66 |
| 1:D:844:GLN:NE2 | 2:K:79:LYS:HE3 | 2.11 | 0.65 |
| 1:F:354:ARG:NH1 | 1:F:362:GLU:OE1 | 2.30 | 0.65 |
| 1:G:1027:ILE:HD11 | 1:G:1047:VAL:HG11 | 1.78 | 0.65 |
| 1:G:844:GLN:NE2 | 2:N:79:LYS:HE3 | 2.11 | 0.65 |
| 2:K:20:VAL:HG12 | 2:K:32:LEU:HB2 | 1.77 | 0.65 |
| 2:M:18:HIS:NE2 | 5:M:500:HEC:NB | 2.43 | 0.65 |
| 1:E:391:LYS:O | 1:E:392:ASP:HB2 | 1.96 | 0.65 |
| 1:F:391:LYS:O | 1:F:392:ASP:HB2 | 1.96 | 0.65 |
| 1:A:1204:VAL:HG12 | 1:A:1205:VAL:HG23 | 1.76 | 0.65 |
| 1:B:354:ARG:NH1 | 1:B:362:GLU:OE1 | 2.30 | 0.65 |
| 1:C:474:SER:HB2 | 1:C:477:GLN:HG2 | 1.78 | 0.65 |
| 1:D:943:ILE:HG22 | 1:D:944:ARG:HG2 | 1.78 | 0.65 |
| 1:E:569:CYS:HG | 1:E:1213:PHE:HE1 | 1.42 | 0.65 |
| 1:E:943:ILE:HG22 | 1:E:944:ARG:HG2 | 1.78 | 0.65 |
| 1:F:201:ASN:HD21 | 1:G:219:ASN:HD21 | 1.44 | 0.65 |
| 1:F:943:ILE:HG22 | 1:F:944:ARG:HG2 | 1.78 | 0.65 |
| 1:G:1204:VAL:HG12 | 1:G:1205:VAL:HG23 | 1.76 | 0.65 |
| 1:A:866:LEU:HB3 | 1:A:876:ALA:HB3 | 1.77 | 0.65 |
| 1:B:590:ASN:O | 1:B:592:MET:N | 2.30 | 0.65 |
| 1:C:1027:ILE:HD11 | 1:C:1047:VAL:HG11 | 1.78 | 0.65 |
| 1:C:590:ASN:O | 1:C:592:MET:N | 2.30 | 0.65 |
| 1:E:354:ARG:NH1 | 1:E:362:GLU:OE1 | 2.30 | 0.65 |
| 1:F:590:ASN:O | 1:F:592:MET:N | 2.30 | 0.65 |
| 1:G:354:ARG:NH1 | 1:G:362:GLU:OE1 | 2.30 | 0.65 |
| 1:C:943:ILE:HG22 | 1:C:944:ARG:HG2 | 1.78 | 0.65 |
| 1:G:866:LEU:HB3 | 1:G:876:ALA:HB3 | 1.77 | 0.65 |
| 1:G:943:ILE:HG22 | 1:G:944:ARG:HG2 | 1.78 | 0.65 |
| 1:C:844:GLN:NE2 | 2:J:79:LYS:HE3 | 2.11 | 0.65 |
| 2:M:20:VAL:HG12 | 2:M:32:LEU:HB2 | 1.77 | 0.65 |
| 1:A:943:ILE:HG22 | 1:A:944:ARG:HG2 | 1.78 | 0.65 |
| 1:B:391:LYS:O | 1:B:392:ASP:HB2 | 1.96 | 0.65 |
| 1:C:354:ARG:NH1 | 1:C:362:GLU:OE1 | 2.30 | 0.65 |
| 1:B:884:TRP:HZ3 | 2:I:79:LYS:HA | 1.56 | 0.65 |
| 1:C:266:ASP:OD2 | 1:C:268:SER:OG | 2.16 | 0.64 |
| 1:D:866:LEU:HB3 | 1:D:876:ALA:HB3 | 1.77 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:565:GLN:HE22 | 1:A:1213:PHE:N | 1.89 | 0.64 |
| 1:B:943:ILE:HG22 | 1:B:944:ARG:HG2 | 1.78 | 0.64 |
| 1:D:160:LYS:N | 4:D:1301:DTP:O1A | 2.21 | 0.64 |
| 1:D:266:ASP:OD2 | 1:D:268:SER:OG | 2.16 | 0.64 |
| 1:D:391:LYS:O | 1:D:392:ASP:HB2 | 1.96 | 0.64 |
| 1:F:1133:SER:HB2 | 1:F:1142:LEU:HD11 | 1.79 | 0.64 |
| 1:F:469:GLN:HB2 | 1:F:472:THR:HB | 1.79 | 0.64 |
| 1:G:474:SER:HB2 | 1:G:477:GLN:HG2 | 1.78 | 0.64 |
| 1:A:1133:SER:HB2 | 1:A:1142:LEU:HD11 | 1.79 | 0.64 |
| 1:A:590:ASN:O | 1:A:592:MET:N | 2.30 | 0.64 |
| 1:C:866:LEU:HB3 | 1:C:876:ALA:HB3 | 1.77 | 0.64 |
| 1:D:643:LYS:HE3 | 1:D:645:GLU:HB3 | 1.79 | 0.64 |
| 1:D:715:LEU:HD13 | 1:D:727:LEU:HD21 | 1.79 | 0.64 |
| 1:G:1133:SER:HB2 | 1:G:1142:LEU:HD11 | 1.79 | 0.64 |
| 2:J:2:ASP:N | 2:J:93:ASP:OD1 | 2.28 | 0.64 |
| 1:A:160:LYS:N | 4:A:1301:DTP:O1A | 2.21 | 0.64 |
| 1:A:643:LYS:HE3 | 1:A:645:GLU:HB3 | 1.79 | 0.64 |
| 1:B:266:ASP:OD2 | 1:B:268:SER:OG | 2.16 | 0.64 |
| 1:D:590:ASN:O | 1:D:592:MET:N | 2.30 | 0.64 |
| 1:E:469:GLN:HB2 | 1:E:472:THR:HB | 1.79 | 0.64 |
| 2:N:2:ASP:N | 2:N:93:ASP:OD1 | 2.28 | 0.64 |
| 1:A:354:ARG:NH1 | 1:A:362:GLU:OE1 | 2.30 | 0.64 |
| 1:B:866:LEU:HB3 | 1:B:876:ALA:HB3 | 1.77 | 0.64 |
| 1:F:866:LEU:HB3 | 1:F:876:ALA:HB3 | 1.77 | 0.64 |
| 1:B:844:GLN:NE2 | 2:I:79:LYS:HE3 | 2.11 | 0.64 |
| 1:A:1027:ILE:HD11 | 1:A:1047:VAL:HG11 | 1.78 | 0.64 |
| 1:C:643:LYS:HE3 | 1:C:645:GLU:HB3 | 1.79 | 0.64 |
| 1:D:354:ARG:NH1 | 1:D:362:GLU:OE1 | 2.30 | 0.64 |
| 1:A:844:GLN:NE2 | 2:H:79:LYS:HE3 | 2.11 | 0.64 |
| 1:E:715:LEU:HD13 | 1:E:727:LEU:HD21 | 1.79 | 0.64 |
| 1:G:391:LYS:O | 1:G:392:ASP:HB2 | 1.96 | 0.64 |
| 1:G:884:TRP:HZ3 | 2:N:79:LYS:HD2 | 1.52 | 0.64 |
| 1:A:1232:TYR:HB2 | 1:A:1244:LEU:HB2 | 1.80 | 0.64 |
| 1:B:1027:ILE:HD11 | 1:B:1047:VAL:HG11 | 1.78 | 0.64 |
| 1:B:1232:TYR:HB2 | 1:B:1244:LEU:HB2 | 1.80 | 0.64 |
| 1:C:1232:TYR:HB2 | 1:C:1244:LEU:HB2 | 1.80 | 0.64 |
| 1:E:160:LYS:N | 4:E:1301:DTP:O1A | 2.21 | 0.64 |
| 1:E:643:LYS:HE3 | 1:E:645:GLU:HB3 | 1.79 | 0.64 |
| 1:A:884:TRP:HZ3 | 2:H:79:LYS:HA | 1.56 | 0.64 |
| 1:E:474:SER:HB2 | 1:E:477:GLN:HG2 | 1.78 | 0.64 |
| 2:I:2:ASP:N | 2:I:93:ASP:OD1 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:1086:GLY:CA | 2:M:39:LYS:HZ1 | 2.07 | 0.64 |
| 1:B:643:LYS:HE3 | 1:B:645:GLU:HB3 | 1.79 | 0.64 |
| 1:D:474:SER:HB2 | 1:D:477:GLN:HG2 | 1.78 | 0.64 |
| 1:E:866:LEU:HB3 | 1:E:876:ALA:HB3 | 1.77 | 0.64 |
| 1:A:391:LYS:O | 1:A:392:ASP:HB2 | 1.96 | 0.63 |
| 1:B:1133:SER:HB2 | 1:B:1142:LEU:HD11 | 1.79 | 0.63 |
| 1:C:715:LEU:HD13 | 1:C:727:LEU:HD21 | 1.79 | 0.63 |
| 1:G:1232:TYR:HB2 | 1:G:1244:LEU:HB2 | 1.80 | 0.63 |
| 1:G:469:GLN:HB2 | 1:G:472:THR:HB | 1.79 | 0.63 |
| 1:G:643:LYS:HE3 | 1:G:645:GLU:HB3 | 1.79 | 0.63 |
| 1:D:469:GLN:HB2 | 1:D:472:THR:HB | 1.79 | 0.63 |
| 1:E:1133:SER:HB2 | 1:E:1142:LEU:HD11 | 1.79 | 0.63 |
| 1:E:945:ARG:HH22 | 1:E:988:LEU:HD22 | 1.64 | 0.63 |
| 1:F:474:SER:HB2 | 1:F:477:GLN:HG2 | 1.78 | 0.63 |
| 1:C:1133:SER:HB2 | 1:C:1142:LEU:HD11 | 1.79 | 0.63 |
| 1:C:391:LYS:O | 1:C:392:ASP:HB2 | 1.96 | 0.63 |
| 1:A:266:ASP:OD2 | 1:A:268:SER:OG | 2.16 | 0.63 |
| 1:C:884:TRP:HZ3 | 2:J:79:LYS:HA | 1.56 | 0.63 |
| 1:G:715:LEU:HD13 | 1:G:727:LEU:HD21 | 1.79 | 0.63 |
| 1:D:1133:SER:HB2 | 1:D:1142:LEU:HD11 | 1.79 | 0.63 |
| 1:D:1232:TYR:HB2 | 1:D:1244:LEU:HB2 | 1.80 | 0.63 |
| 1:A:109:TYR:HE1 | 1:G:4:LYS:HZ3 | 0.70 | 0.63 |
| 1:F:565:GLN:OE1 | 1:F:1213:PHE:N | 2.32 | 0.63 |
| 1:F:1232:TYR:HB2 | 1:F:1244:LEU:HB2 | 1.80 | 0.63 |
| 1:F:715:LEU:HD13 | 1:F:727:LEU:HD21 | 1.79 | 0.63 |
| 1:G:565:GLN:OE1 | 1:G:1213:PHE:N | 2.32 | 0.63 |
| 1:D:565:GLN:OE1 | 1:D:1213:PHE:N | 2.32 | 0.63 |
| 1:A:715:LEU:HD13 | 1:A:727:LEU:HD21 | 1.79 | 0.62 |
| 1:D:945:ARG:HH22 | 1:D:988:LEU:HD22 | 1.64 | 0.62 |
| 1:E:590:ASN:O | 1:E:592:MET:N | 2.30 | 0.62 |
| 1:F:643:LYS:HE3 | 1:F:645:GLU:HB3 | 1.79 | 0.62 |
| 1:G:945:ARG:HH22 | 1:G:988:LEU:HD22 | 1.64 | 0.62 |
| 1:B:715:LEU:HD13 | 1:B:727:LEU:HD21 | 1.79 | 0.62 |
| 1:C:903:ASP:OD2 | 1:C:907:ARG:NH1 | 2.28 | 0.62 |
| 1:E:1232:TYR:HB2 | 1:E:1244:LEU:HB2 | 1.80 | 0.62 |
| 1:G:590:ASN:O | 1:G:592:MET:N | 2.30 | 0.62 |
| 3:O:52:ARG:HB2 | 3:P:38:HIS:HE1 | 1.61 | 0.62 |
| 1:A:945:ARG:HH22 | 1:A:988:LEU:HD22 | 1.64 | 0.62 |
| 1:B:469:GLN:HB2 | 1:B:472:THR:HB | 1.79 | 0.62 |
| 1:B:945:ARG:HH22 | 1:B:988:LEU:HD22 | 1.64 | 0.62 |
| 1:G:160:LYS:N | 4:G:1301:DTP:O1A | 2.21 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:K:2:ASP:N | 2:K:93:ASP:OD1 | 2.28 | 0.62 |
| 1:A:1031:ASN:HB2 | 1:A:1036:LYS:HB2 | 1.82 | 0.62 |
| 1:A:565:GLN:OE1 | 1:A:1213:PHE:N | 2.32 | 0.62 |
| 1:C:945:ARG:HH22 | 1:C:988:LEU:HD22 | 1.64 | 0.62 |
| 1:F:569:CYS:HG | 1:F:1213:PHE:HE1 | 1.47 | 0.62 |
| 1:F:266:ASP:OD2 | 1:F:268:SER:OG | 2.16 | 0.62 |
| 1:A:557:ARG:HH22 | 1:A:1175:THR:HG23 | 1.64 | 0.62 |
| 1:C:565:GLN:OE1 | 1:C:1213:PHE:N | 2.32 | 0.62 |
| 1:F:945:ARG:HH22 | 1:F:988:LEU:HD22 | 1.64 | 0.62 |
| 2:M:2:ASP:N | 2:M:93:ASP:OD1 | 2.28 | 0.62 |
| 1:A:469:GLN:HB2 | 1:A:472:THR:HB | 1.79 | 0.62 |
| 1:B:1031:ASN:HB2 | 1:B:1036:LYS:HB2 | 1.82 | 0.62 |
| 1:B:924:GLN:NE2 | 1:B:965:SER:O | 2.33 | 0.62 |
| 1:C:469:GLN:HB2 | 1:C:472:THR:HB | 1.79 | 0.62 |
| 1:G:1031:ASN:HB2 | 1:G:1036:LYS:HB2 | 1.82 | 0.62 |
| 1:G:569:CYS:HG | 1:G:1213:PHE:HE1 | 1.44 | 0.62 |
| 1:B:557:ARG:HH22 | 1:B:1175:THR:HG23 | 1.64 | 0.62 |
| 1:B:565:GLN:OE1 | 1:B:1213:PHE:N | 2.32 | 0.62 |
| 1:C:924:GLN:NE2 | 1:C:965:SER:O | 2.33 | 0.62 |
| 1:D:862:TYR:HB3 | 1:D:884:TRP:HA | 1.82 | 0.62 |
| 1:F:924:GLN:NE2 | 1:F:965:SER:O | 2.33 | 0.62 |
| 1:A:1086:GLY:CA | 2:H:39:LYS:HZ1 | 2.10 | 0.62 |
| 1:A:924:GLN:NE2 | 1:A:965:SER:O | 2.33 | 0.62 |
| 1:E:924:GLN:NE2 | 1:E:965:SER:O | 2.33 | 0.62 |
| 1:E:587:GLU:OE1 | 1:E:594:TYR:OH | 2.18 | 0.62 |
| 1:G:559:PRO:HD3 | 1:G:1171:GLU:OE1 | 2.00 | 0.62 |
| 1:G:714:LEU:HB3 | 1:G:730:LEU:HD12 | 1.82 | 0.62 |
| 1:A:145:GLY:HA2 | 1:A:259:GLN:NE2 | 2.15 | 0.61 |
| 1:D:569:CYS:HG | 1:D:1213:PHE:HE1 | 1.48 | 0.61 |
| 1:E:565:GLN:OE1 | 1:E:1213:PHE:N | 2.32 | 0.61 |
| 1:G:266:ASP:OD2 | 1:G:268:SER:OG | 2.16 | 0.61 |
| 1:G:587:GLU:OE1 | 1:G:594:TYR:OH | 2.17 | 0.61 |
| 1:A:358:SER:HB3 | 1:B:274:MET:HE3 | 1.81 | 0.61 |
| 1:C:1031:ASN:HB2 | 1:C:1036:LYS:HB2 | 1.82 | 0.61 |
| 1:G:557:ARG:HH22 | 1:G:1175:THR:HG23 | 1.64 | 0.61 |
| 1:D:559:PRO:HD3 | 1:D:1171:GLU:OE1 | 2.00 | 0.61 |
| 1:F:714:LEU:HB3 | 1:F:730:LEU:HD12 | 1.82 | 0.61 |
| 1:G:924:GLN:NE2 | 1:G:965:SER:O | 2.33 | 0.61 |
| 2:L:2:ASP:N | 2:L:93:ASP:OD1 | 2.28 | 0.61 |
| 1:G:884:TRP:HZ3 | 2:N:79:LYS:HA | 1.56 | 0.61 |
| 1:A:274:MET:HG2 | 1:G:358:SER:OG | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:559:PRO:HD3 | 1:C:1171:GLU:OE1 | 2.00 | 0.61 |
| 1:C:862:TYR:HB3 | 1:C:884:TRP:HA | 1.82 | 0.61 |
| 1:D:924:GLN:NE2 | 1:D:965:SER:O | 2.33 | 0.61 |
| 1:E:145:GLY:HA2 | 1:E:259:GLN:NE2 | 2.15 | 0.61 |
| 1:F:559:PRO:HD3 | 1:F:1171:GLU:OE1 | 2.00 | 0.61 |
| 1:A:587:GLU:OE1 | 1:A:594:TYR:OH | 2.18 | 0.61 |
| 1:D:145:GLY:HA2 | 1:D:259:GLN:NE2 | 2.15 | 0.61 |
| 1:E:862:TYR:HB3 | 1:E:884:TRP:HA | 1.82 | 0.61 |
| 1:F:1031:ASN:HB2 | 1:F:1036:LYS:HB2 | 1.82 | 0.61 |
| 1:F:587:GLU:OE1 | 1:F:594:TYR:OH | 2.18 | 0.61 |
| 1:F:882:LEU:HD12 | 1:F:903:ASP:HB2 | 1.83 | 0.61 |
| 1:A:884:TRP:HZ3 | 2:H:79:LYS:HD2 | 1.52 | 0.61 |
| 2:H:2:ASP:N | 2:H:93:ASP:OD1 | 2.28 | 0.61 |
| 1:A:862:TYR:HB3 | 1:A:884:TRP:HA | 1.82 | 0.61 |
| 1:B:160:LYS:N | 4:B:1301:DTP:O1A | 2.21 | 0.61 |
| 1:B:882:LEU:HD13 | 1:B:1176:HIS:CE1 | 2.36 | 0.61 |
| 1:A:882:LEU:HD13 | 1:A:1176:HIS:CE1 | 2.36 | 0.61 |
| 1:A:882:LEU:HD12 | 1:A:903:ASP:HB2 | 1.83 | 0.61 |
| 1:D:882:LEU:HD13 | 1:D:1176:HIS:CE1 | 2.36 | 0.61 |
| 1:D:599:ASN:ND2 | 1:D:1241:LEU:O | 2.34 | 0.61 |
| 1:E:714:LEU:HB3 | 1:E:730:LEU:HD12 | 1.82 | 0.61 |
| 1:E:882:LEU:HD12 | 1:E:903:ASP:HB2 | 1.83 | 0.61 |
| 1:F:1092:ASP:OD2 | 1:F:1133:SER:OG | 2.17 | 0.61 |
| 1:F:145:GLY:HA2 | 1:F:259:GLN:NE2 | 2.15 | 0.61 |
| 1:F:862:TYR:CB | 1:F:884:TRP:HA | 2.31 | 0.61 |
| 1:G:145:GLY:HA2 | 1:G:259:GLN:NE2 | 2.16 | 0.61 |
| 1:A:752:SER:OG | 1:A:754:ASP:O | 2.19 | 0.61 |
| 1:B:145:GLY:HA2 | 1:B:259:GLN:NE2 | 2.16 | 0.61 |
| 1:B:599:ASN:ND2 | 1:B:1241:LEU:O | 2.34 | 0.61 |
| 1:E:559:PRO:HD3 | 1:E:1171:GLU:OE1 | 2.00 | 0.61 |
| 1:G:599:ASN:ND2 | 1:G:1241:LEU:O | 2.34 | 0.61 |
| 1:A:714:LEU:HB3 | 1:A:730:LEU:HD12 | 1.82 | 0.61 |
| 1:B:882:LEU:HD12 | 1:B:903:ASP:HB2 | 1.83 | 0.61 |
| 1:C:265:ARG:NH2 | 4:C:1301:DTP:O2G | 2.31 | 0.61 |
| 1:E:266:ASP:OD2 | 1:E:268:SER:OG | 2.16 | 0.61 |
| 1:E:358:SER:HB3 | 1:F:274:MET:HE3 | 1.82 | 0.61 |
| 1:G:862:TYR:HB3 | 1:G:884:TRP:HA | 1.82 | 0.61 |
| 1:F:844:GLN:HE22 | 2:M:79:LYS:CE | 2.14 | 0.61 |
| 1:C:557:ARG:HH22 | 1:C:1175:THR:HG23 | 1.64 | 0.61 |
| 1:C:714:LEU:HB3 | 1:C:730:LEU:HD12 | 1.82 | 0.61 |
| 1:C:882:LEU:HD13 | 1:C:1176:HIS:CE1 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:844:GLN:HE22 | 2:K:79:LYS:CE | 2.14 | 0.61 |
| 1:F:482:TYR:HH | 1:F:490:HIS:HE2 | 1.45 | 0.61 |
| 1:B:844:GLN:HE22 | 2:I:79:LYS:CE | 2.14 | 0.61 |
| 3:Q:52:ARG:HB2 | 3:R:38:HIS:HE1 | 1.65 | 0.61 |
| 1:C:160:LYS:N | 4:C:1301:DTP:O1A | 2.21 | 0.60 |
| 1:B:358:SER:HB3 | 1:C:274:MET:HE2 | 1.82 | 0.60 |
| 1:D:1031:ASN:HB2 | 1:D:1036:LYS:HB2 | 1.82 | 0.60 |
| 1:G:752:SER:OG | 1:G:754:ASP:O | 2.19 | 0.60 |
| 1:G:882:LEU:HD12 | 1:G:903:ASP:HB2 | 1.83 | 0.60 |
| 1:A:559:PRO:HD3 | 1:A:1171:GLU:OE1 | 2.00 | 0.60 |
| 1:B:714:LEU:HB3 | 1:B:730:LEU:HD12 | 1.82 | 0.60 |
| 1:C:1092:ASP:OD2 | 1:C:1133:SER:OG | 2.17 | 0.60 |
| 1:D:882:LEU:HD12 | 1:D:903:ASP:HB2 | 1.83 | 0.60 |
| 1:E:1031:ASN:HB2 | 1:E:1036:LYS:HB2 | 1.82 | 0.60 |
| 1:E:557:ARG:HH22 | 1:E:1175:THR:HG23 | 1.64 | 0.60 |
| 1:E:201:ASN:HD21 | 1:F:219:ASN:HD21 | 1.49 | 0.60 |
| 1:E:752:SER:OG | 1:E:754:ASP:O | 2.19 | 0.60 |
| 1:G:265:ARG:NH2 | 4:G:1301:DTP:O2G | 2.31 | 0.60 |
| 1:F:358:SER:HB3 | 1:G:274:MET:HE3 | 1.83 | 0.60 |
| 1:D:1086:GLY:CA | 2:K:39:LYS:HZ1 | 2.10 | 0.60 |
| 1:D:844:GLN:NE2 | 2:K:79:LYS:CE | 2.64 | 0.60 |
| 1:E:844:GLN:NE2 | 2:L:79:LYS:CE | 2.64 | 0.60 |
| 1:B:903:ASP:OD2 | 1:B:907:ARG:NH1 | 2.28 | 0.60 |
| 1:D:1092:ASP:OD2 | 1:D:1133:SER:OG | 2.17 | 0.60 |
| 1:F:599:ASN:ND2 | 1:F:1241:LEU:O | 2.34 | 0.60 |
| 1:B:1086:GLY:CA | 2:I:39:LYS:HZ1 | 2.07 | 0.60 |
| 1:E:844:GLN:HE22 | 2:L:79:LYS:CE | 2.14 | 0.60 |
| 1:G:844:GLN:HE22 | 2:N:79:LYS:CE | 2.14 | 0.60 |
| 1:C:882:LEU:HD12 | 1:C:903:ASP:HB2 | 1.83 | 0.60 |
| 1:C:862:TYR:CB | 1:C:884:TRP:HA | 2.31 | 0.60 |
| 1:E:1087:THR:N | 2:L:39:LYS:HZ3 | 2.00 | 0.60 |
| 1:G:844:GLN:NE2 | 2:N:79:LYS:CE | 2.65 | 0.60 |
| 1:C:844:GLN:NE2 | 2:J:79:LYS:CE | 2.65 | 0.60 |
| 1:D:884:TRP:HZ3 | 2:K:79:LYS:HA | 1.56 | 0.60 |
| 1:B:559:PRO:HD3 | 1:B:1171:GLU:OE1 | 2.00 | 0.60 |
| 1:B:862:TYR:HB3 | 1:B:884:TRP:HA | 1.82 | 0.60 |
| 1:D:714:LEU:HB3 | 1:D:730:LEU:HD12 | 1.82 | 0.60 |
| 1:D:752:SER:OG | 1:D:754:ASP:O | 2.19 | 0.60 |
| 1:E:862:TYR:CB | 1:E:884:TRP:HA | 2.31 | 0.60 |
| 1:F:557:ARG:HH22 | 1:F:1175:THR:HG23 | 1.64 | 0.60 |
| 1:F:1210:SER:HB2 | 1:F:1212:THR:HG23 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:599:ASN:ND2 | 1:A:1241:LEU:O | 2.34 | 0.60 |
| 1:B:569:CYS:HG | 1:B:1213:PHE:HE1 | 1.50 | 0.60 |
| 1:B:862:TYR:CB | 1:B:884:TRP:HA | 2.31 | 0.60 |
| 1:C:145:GLY:HA2 | 1:C:259:GLN:NE2 | 2.15 | 0.60 |
| 1:D:557:ARG:HH22 | 1:D:1175:THR:HG23 | 1.64 | 0.60 |
| 1:E:882:LEU:HD13 | 1:E:1176:HIS:CE1 | 2.36 | 0.60 |
| 1:F:862:TYR:HB3 | 1:F:884:TRP:HA | 1.82 | 0.60 |
| 1:F:884:TRP:HZ3 | 2:M:79:LYS:HD2 | 1.51 | 0.60 |
| 1:B:587:GLU:OE1 | 1:B:594:TYR:OH | 2.18 | 0.60 |
| 1:B:752:SER:OG | 1:B:754:ASP:O | 2.19 | 0.60 |
| 1:D:862:TYR:CB | 1:D:884:TRP:HA | 2.31 | 0.60 |
| 1:A:862:TYR:CB | 1:A:884:TRP:HA | 2.31 | 0.60 |
| 1:B:844:GLN:NE2 | 2:I:79:LYS:CE | 2.65 | 0.60 |
| 1:G:1210:SER:HB2 | 1:G:1212:THR:HG23 | 1.84 | 0.60 |
| 1:A:844:GLN:HE22 | 2:H:79:LYS:CE | 2.14 | 0.60 |
| 1:A:844:GLN:NE2 | 2:H:79:LYS:CE | 2.65 | 0.60 |
| 1:E:265:ARG:NH2 | 4:E:1301:DTP:O2G | 2.31 | 0.60 |
| 1:F:882:LEU:HD13 | 1:F:1176:HIS:CE1 | 2.36 | 0.60 |
| 1:G:882:LEU:HD13 | 1:G:1176:HIS:CE1 | 2.36 | 0.60 |
| 1:G:862:TYR:CB | 1:G:884:TRP:HA | 2.31 | 0.60 |
| 1:C:358:SER:OG | 1:D:274:MET:HG2 | 2.02 | 0.60 |
| 1:D:1210:SER:HB2 | 1:D:1212:THR:HG23 | 1.84 | 0.60 |
| 1:E:599:ASN:ND2 | 1:E:1241:LEU:O | 2.34 | 0.60 |
| 1:F:844:GLN:NE2 | 2:M:79:LYS:CE | 2.64 | 0.60 |
| 1:C:599:ASN:ND2 | 1:C:1241:LEU:O | 2.34 | 0.59 |
| 1:E:1115:ASP:HB2 | 1:E:1120:LEU:HD11 | 1.84 | 0.59 |
| 1:F:882:LEU:HD13 | 1:F:1176:HIS:CD2 | 2.37 | 0.59 |
| 1:A:1115:ASP:HB2 | 1:A:1120:LEU:HD11 | 1.84 | 0.59 |
| 1:A:903:ASP:OD2 | 1:A:907:ARG:NH1 | 2.28 | 0.59 |
| 1:B:201:ASN:HD21 | 1:C:219:ASN:HD21 | 1.50 | 0.59 |
| 1:E:1210:SER:HB2 | 1:E:1212:THR:HG23 | 1.84 | 0.59 |
| 1:F:752:SER:OG | 1:F:754:ASP:O | 2.19 | 0.59 |
| 1:F:903:ASP:OD2 | 1:F:907:ARG:NH1 | 2.28 | 0.59 |
| 1:B:1115:ASP:HB2 | 1:B:1120:LEU:HD11 | 1.84 | 0.59 |
| 1:G:903:ASP:OD2 | 1:G:907:ARG:NH1 | 2.28 | 0.59 |
| 1:A:882:LEU:HD13 | 1:A:1176:HIS:CD2 | 2.38 | 0.59 |
| 1:A:201:ASN:HD21 | 1:B:219:ASN:HD21 | 1.50 | 0.59 |
| 1:C:844:GLN:HE22 | 2:J:79:LYS:CE | 2.14 | 0.59 |
| 1:D:1115:ASP:HB2 | 1:D:1120:LEU:HD11 | 1.84 | 0.59 |
| 1:E:715:LEU:HB3 | 1:E:727:LEU:HD11 | 1.85 | 0.59 |
| 1:B:882:LEU:HD13 | 1:B:1176:HIS:CD2 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1210:SER:HB2 | 1:C:1212:THR:HG23 | 1.84 | 0.59 |
| 1:C:752:SER:OG | 1:C:754:ASP:O | 2.19 | 0.59 |
| 1:D:1131:ARG:NH2 | 1:D:1147:ASP:OD1 | 2.36 | 0.59 |
| 1:D:482:TYR:HH | 1:D:490:HIS:HE2 | 1.50 | 0.59 |
| 1:D:715:LEU:HB3 | 1:D:727:LEU:HD11 | 1.85 | 0.59 |
| 1:E:903:ASP:OD2 | 1:E:907:ARG:NH1 | 2.28 | 0.59 |
| 1:F:1115:ASP:HB2 | 1:F:1120:LEU:HD11 | 1.84 | 0.59 |
| 3:Q:52:ARG:CG | 3:R:38:HIS:CE1 | 2.82 | 0.59 |
| 1:F:715:LEU:HB3 | 1:F:727:LEU:HD11 | 1.85 | 0.59 |
| 1:A:1210:SER:HB2 | 1:A:1212:THR:HG23 | 1.84 | 0.59 |
| 1:C:1131:ARG:NH2 | 1:C:1147:ASP:OD1 | 2.36 | 0.59 |
| 1:E:1131:ARG:NH2 | 1:E:1147:ASP:OD1 | 2.36 | 0.59 |
| 1:G:1115:ASP:HB2 | 1:G:1120:LEU:HD11 | 1.84 | 0.59 |
| 3:P:41:GLU:HB3 | 3:P:45:ARG:NH1 | 2.17 | 0.59 |
| 1:B:358:SER:HB3 | 1:C:274:MET:HE3 | 1.84 | 0.59 |
| 1:D:882:LEU:HD13 | 1:D:1176:HIS:CD2 | 2.37 | 0.59 |
| 1:C:1031:ASN:HB3 | 1:C:1034:LEU:HD12 | 1.85 | 0.59 |
| 1:C:521:HIS:NE2 | 1:C:525:GLU:OE2 | 2.36 | 0.59 |
| 1:E:882:LEU:HD13 | 1:E:1176:HIS:CD2 | 2.37 | 0.59 |
| 1:G:463:GLN:OE1 | 1:G:466:ARG:NH2 | 2.28 | 0.59 |
| 1:A:358:SER:HB3 | 1:B:274:MET:HE2 | 1.84 | 0.58 |
| 1:A:521:HIS:NE2 | 1:A:525:GLU:OE2 | 2.36 | 0.58 |
| 1:F:160:LYS:N | 4:F:1301:DTP:O1A | 2.20 | 0.58 |
| 1:G:882:LEU:HD13 | 1:G:1176:HIS:CD2 | 2.38 | 0.58 |
| 1:D:358:SER:OG | 1:E:274:MET:HG2 | 2.03 | 0.58 |
| 1:E:1202:TRP:HA | 1:E:1208:GLU:HB2 | 1.85 | 0.58 |
| 1:F:1202:TRP:HA | 1:F:1208:GLU:HB2 | 1.85 | 0.58 |
| 1:B:1031:ASN:HB3 | 1:B:1034:LEU:HD12 | 1.85 | 0.58 |
| 1:B:1210:SER:HB2 | 1:B:1212:THR:HG23 | 1.84 | 0.58 |
| 1:B:48:THR:HG22 | 1:D:45:ASN:OD1 | 2.04 | 0.58 |
| 1:C:1115:ASP:HB2 | 1:C:1120:LEU:HD11 | 1.84 | 0.58 |
| 1:C:715:LEU:HB3 | 1:C:727:LEU:HD11 | 1.85 | 0.58 |
| 1:C:201:ASN:HD21 | 1:D:219:ASN:HD21 | 1.51 | 0.58 |
| 1:D:903:ASP:OD2 | 1:D:907:ARG:NH1 | 2.28 | 0.58 |
| 1:E:4:LYS:HA | 1:F:237:ARG:HH21 | 1.68 | 0.58 |
| 2:J:67:TYR:OH | 2:J:80:MET:SD | 2.57 | 0.58 |
| 1:F:884:TRP:HZ3 | 2:M:79:LYS:HA | 1.56 | 0.58 |
| 3:Q:52:ARG:HB3 | 3:R:38:HIS:CE1 | 2.37 | 0.58 |
| 1:C:1202:TRP:HA | 1:C:1208:GLU:HB2 | 1.85 | 0.58 |
| 1:C:882:LEU:HD13 | 1:C:1176:HIS:CD2 | 2.38 | 0.58 |
| 1:D:1202:TRP:HA | 1:D:1208:GLU:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1086:GLY:CA | 2:J:39:LYS:HZ1 | 2.12 | 0.58 |
| 1:B:1131:ARG:NH2 | 1:B:1147:ASP:OD1 | 2.36 | 0.58 |
| 1:F:1131:ARG:NH2 | 1:F:1147:ASP:OD1 | 2.36 | 0.58 |
| 1:G:884:TRP:CZ3 | 2:N:79:LYS:CA | 2.74 | 0.58 |
| 1:E:884:TRP:HZ3 | 2:L:79:LYS:HA | 1.56 | 0.58 |
| 1:A:1031:ASN:HB3 | 1:A:1034:LEU:HD12 | 1.85 | 0.58 |
| 1:B:265:ARG:NH2 | 4:B:1301:DTP:O2G | 2.31 | 0.58 |
| 1:B:482:TYR:HH | 1:B:490:HIS:HE2 | 1.50 | 0.58 |
| 1:D:265:ARG:NH2 | 4:D:1301:DTP:O2G | 2.31 | 0.58 |
| 1:F:1031:ASN:HB3 | 1:F:1034:LEU:HD12 | 1.85 | 0.58 |
| 1:G:1131:ARG:NH2 | 1:G:1147:ASP:OD1 | 2.36 | 0.58 |
| 1:A:1131:ARG:NH2 | 1:A:1147:ASP:OD1 | 2.36 | 0.58 |
| 1:C:884:TRP:CH2 | 2:J:78:THR:O | 2.57 | 0.58 |
| 1:D:1031:ASN:HB3 | 1:D:1034:LEU:HD12 | 1.85 | 0.58 |
| 1:E:358:SER:HB3 | 1:F:274:MET:HE2 | 1.85 | 0.58 |
| 1:G:1048:LYS:H | 1:G:1062:SER:HA | 1.69 | 0.58 |
| 1:B:1202:TRP:HA | 1:B:1208:GLU:HB2 | 1.85 | 0.58 |
| 1:C:587:GLU:OE1 | 1:C:594:TYR:OH | 2.18 | 0.58 |
| 1:E:482:TYR:HH | 1:E:490:HIS:HE2 | 1.48 | 0.58 |
| 1:F:1048:LYS:H | 1:F:1062:SER:HA | 1.69 | 0.58 |
| 1:G:715:LEU:HB3 | 1:G:727:LEU:HD11 | 1.85 | 0.58 |
| 1:B:521:HIS:NE2 | 1:B:525:GLU:OE2 | 2.36 | 0.57 |
| 1:D:521:HIS:NE2 | 1:D:525:GLU:OE2 | 2.36 | 0.57 |
| 1:E:482:TYR:OH | 1:E:490:HIS:NE2 | 2.35 | 0.57 |
| 1:F:521:HIS:NE2 | 1:F:525:GLU:OE2 | 2.36 | 0.57 |
| 1:G:482:TYR:OH | 1:G:490:HIS:NE2 | 2.36 | 0.57 |
| 1:A:715:LEU:HB3 | 1:A:727:LEU:HD11 | 1.85 | 0.57 |
| 1:B:884:TRP:CH2 | 2:I:78:THR:O | 2.57 | 0.57 |
| 1:G:1202:TRP:HA | 1:G:1208:GLU:HB2 | 1.86 | 0.57 |
| 1:D:884:TRP:CH2 | 2:K:78:THR:O | 2.57 | 0.57 |
| 1:B:715:LEU:HB3 | 1:B:727:LEU:HD11 | 1.85 | 0.57 |
| 1:D:201:ASN:HD21 | 1:E:219:ASN:HD21 | 1.52 | 0.57 |
| 1:B:454:GLN:OE1 | 1:B:458:LYS:NZ | 2.38 | 0.57 |
| 1:D:454:GLN:OE1 | 1:D:458:LYS:NZ | 2.38 | 0.57 |
| 1:E:521:HIS:NE2 | 1:E:525:GLU:OE2 | 2.36 | 0.57 |
| 1:E:358:SER:OG | 1:F:274:MET:HG2 | 2.04 | 0.57 |
| 1:B:1048:LYS:H | 1:B:1062:SER:HA | 1.69 | 0.57 |
| 1:C:454:GLN:OE1 | 1:C:458:LYS:NZ | 2.38 | 0.57 |
| 1:E:454:GLN:OE1 | 1:E:458:LYS:NZ | 2.38 | 0.57 |
| 1:G:521:HIS:NE2 | 1:G:525:GLU:OE2 | 2.36 | 0.57 |
| 1:F:884:TRP:CH2 | 2:M:78:THR:O | 2.57 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:454:GLN:OE1 | 1:A:458:LYS:NZ | 2.38 | 0.57 |
| 1:B:884:TRP:CZ3 | 2:I:79:LYS:CA | 2.74 | 0.57 |
| 1:D:1048:LYS:H | 1:D:1062:SER:HA | 1.69 | 0.57 |
| 1:E:1048:LYS:H | 1:E:1062:SER:HA | 1.69 | 0.57 |
| 1:G:1031:ASN:HB3 | 1:G:1034:LEU:HD12 | 1.85 | 0.57 |
| 1:G:884:TRP:CH2 | 2:N:78:THR:O | 2.57 | 0.57 |
| 1:A:1202:TRP:HA | 1:A:1208:GLU:HB2 | 1.85 | 0.57 |
| 1:B:358:SER:OG | 1:C:274:MET:HG2 | 2.04 | 0.57 |
| 1:D:482:TYR:OH | 1:D:490:HIS:NE2 | 2.35 | 0.57 |
| 1:G:454:GLN:OE1 | 1:G:458:LYS:NZ | 2.38 | 0.57 |
| 1:A:884:TRP:CH2 | 2:H:78:THR:O | 2.57 | 0.57 |
| 1:D:1139:SER:O | 1:D:1140:THR:HG22 | 2.05 | 0.57 |
| 1:G:264:THR:OG1 | 1:G:265:ARG:N | 2.37 | 0.57 |
| 1:A:358:SER:OG | 1:B:274:MET:HG2 | 2.04 | 0.57 |
| 1:C:1048:LYS:H | 1:C:1062:SER:HA | 1.69 | 0.57 |
| 1:C:763:ALA:HA | 1:C:801:VAL:H | 1.70 | 0.57 |
| 1:D:264:THR:OG1 | 1:D:265:ARG:N | 2.37 | 0.57 |
| 1:E:1031:ASN:HB3 | 1:E:1034:LEU:HD12 | 1.85 | 0.57 |
| 1:E:763:ALA:HA | 1:E:801:VAL:H | 1.70 | 0.57 |
| 1:F:265:ARG:NH2 | 4:F:1301:DTP:O2G | 2.31 | 0.57 |
| 1:F:454:GLN:OE1 | 1:F:458:LYS:NZ | 2.38 | 0.57 |
| 1:G:1092:ASP:OD2 | 1:G:1133:SER:OG | 2.17 | 0.57 |
| 1:G:1139:SER:O | 1:G:1140:THR:HG22 | 2.05 | 0.57 |
| 1:B:264:THR:OG1 | 1:B:265:ARG:N | 2.37 | 0.56 |
| 1:B:524:HIS:HB2 | 1:B:646:THR:CG2 | 2.32 | 0.56 |
| 1:F:264:THR:OG1 | 1:F:265:ARG:N | 2.38 | 0.56 |
| 1:A:1139:SER:O | 1:A:1140:THR:HG22 | 2.05 | 0.56 |
| 1:C:1139:SER:O | 1:C:1140:THR:HG22 | 2.05 | 0.56 |
| 1:C:482:TYR:HH | 1:C:490:HIS:HE2 | 1.53 | 0.56 |
| 1:D:587:GLU:OE1 | 1:D:594:TYR:OH | 2.18 | 0.56 |
| 1:E:1092:ASP:OD2 | 1:E:1133:SER:OG | 2.17 | 0.56 |
| 1:B:1139:SER:O | 1:B:1140:THR:HG22 | 2.05 | 0.56 |
| 1:E:524:HIS:HB2 | 1:E:646:THR:CG2 | 2.32 | 0.56 |
| 1:B:1023:ASP:OD1 | 1:B:1046:THR:OG1 | 2.24 | 0.56 |
| 1:C:482:TYR:OH | 1:C:490:HIS:NE2 | 2.35 | 0.56 |
| 1:C:884:TRP:CZ3 | 2:J:79:LYS:CA | 2.74 | 0.56 |
| 1:D:569:CYS:HB3 | 1:D:600:LYS:HZ3 | 1.71 | 0.56 |
| 1:E:884:TRP:CH2 | 2:L:78:THR:O | 2.57 | 0.56 |
| 1:A:264:THR:OG1 | 1:A:265:ARG:N | 2.37 | 0.56 |
| 1:C:716:LEU:HB3 | 1:C:728:TRP:HB2 | 1.87 | 0.56 |
| 1:D:463:GLN:OE1 | 1:D:466:ARG:NH2 | 2.28 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:264:THR:OG1 | 1:E:265:ARG:N | 2.37 | 0.56 |
| 1:A:1048:LYS:H | 1:A:1062:SER:HA | 1.69 | 0.56 |
| 1:A:565:GLN:NE2 | 1:A:1213:PHE:CA | 2.69 | 0.56 |
| 1:A:524:HIS:HB2 | 1:A:646:THR:CG2 | 2.32 | 0.56 |
| 1:F:1139:SER:O | 1:F:1140:THR:HG22 | 2.05 | 0.56 |
| 1:C:1087:THR:N | 2:J:39:LYS:HZ3 | 2.04 | 0.56 |
| 1:G:565:GLN:NE2 | 1:G:1213:PHE:CA | 2.69 | 0.56 |
| 1:G:716:LEU:HB3 | 1:G:728:TRP:HB2 | 1.87 | 0.56 |
| 1:C:1086:GLY:CA | 2:J:39:LYS:NZ | 2.66 | 0.56 |
| 1:A:1023:ASP:OD1 | 1:A:1046:THR:OG1 | 2.24 | 0.56 |
| 1:B:763:ALA:HA | 1:B:801:VAL:H | 1.70 | 0.56 |
| 1:D:716:LEU:HB3 | 1:D:728:TRP:HB2 | 1.87 | 0.56 |
| 1:E:1139:SER:O | 1:E:1140:THR:HG22 | 2.05 | 0.56 |
| 1:A:844:GLN:HE22 | 2:H:79:LYS:HE3 | 1.71 | 0.56 |
| 2:M:67:TYR:OH | 2:M:80:MET:SD | 2.57 | 0.56 |
| 1:A:170:ASP:OD1 | 1:A:171:HIS:N | 2.39 | 0.56 |
| 1:B:143:LEU:C | 1:B:145:GLY:H | 2.09 | 0.56 |
| 1:C:264:THR:OG1 | 1:C:265:ARG:N | 2.37 | 0.56 |
| 1:C:326:LEU:HD13 | 1:C:353:ILE:CG2 | 2.37 | 0.56 |
| 1:D:326:LEU:HD13 | 1:D:353:ILE:CG2 | 2.36 | 0.56 |
| 1:F:143:LEU:C | 1:F:145:GLY:H | 2.09 | 0.56 |
| 1:B:844:GLN:HE22 | 2:I:79:LYS:HE3 | 1.71 | 0.56 |
| 3:P:50:SER:CB | 3:Q:45:ARG:NH1 | 2.64 | 0.56 |
| 1:C:1023:ASP:OD1 | 1:C:1046:THR:OG1 | 2.24 | 0.55 |
| 1:D:884:TRP:CZ3 | 2:K:79:LYS:CA | 2.74 | 0.55 |
| 1:E:326:LEU:HD13 | 1:E:353:ILE:CG2 | 2.36 | 0.55 |
| 1:F:336:ASN:HB2 | 1:G:431:LYS:HE3 | 1.87 | 0.55 |
| 1:G:844:GLN:HE22 | 2:N:79:LYS:HE3 | 1.71 | 0.55 |
| 1:A:463:GLN:OE1 | 1:A:466:ARG:NH2 | 2.28 | 0.55 |
| 1:B:1092:ASP:OD2 | 1:B:1133:SER:OG | 2.17 | 0.55 |
| 1:B:170:ASP:OD1 | 1:B:171:HIS:N | 2.39 | 0.55 |
| 1:B:326:LEU:HD13 | 1:B:353:ILE:CG2 | 2.37 | 0.55 |
| 1:G:170:ASP:OD1 | 1:G:171:HIS:N | 2.39 | 0.55 |
| 1:A:326:LEU:HD13 | 1:A:353:ILE:CG2 | 2.37 | 0.55 |
| 1:A:716:LEU:HB3 | 1:A:728:TRP:HB2 | 1.87 | 0.55 |
| 1:A:884:TRP:CZ3 | 2:H:79:LYS:CA | 2.74 | 0.55 |
| 1:B:845:TYR:HB3 | 1:B:858:ALA:HB3 | 1.89 | 0.55 |
| 1:C:217:PRO:HG3 | 1:C:226:ARG:HH12 | 1.72 | 0.55 |
| 1:C:844:GLN:HE22 | 2:J:79:LYS:HE3 | 1.71 | 0.55 |
| 1:D:217:PRO:HG3 | 1:D:226:ARG:HH12 | 1.71 | 0.55 |
| 1:A:763:ALA:HA | 1:A:801:VAL:H | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:845:TYR:HB3 | 1:C:858:ALA:HB3 | 1.89 | 0.55 |
| 1:C:617:ALA:HA | 1:C:904:GLN:HG2 | 1.89 | 0.55 |
| 1:D:572:GLU:HA | 1:D:577:TYR:CD2 | 2.42 | 0.55 |
| 1:E:884:TRP:CD1 | 1:E:884:TRP:N | 2.73 | 0.55 |
| 1:F:572:GLU:HA | 1:F:577:TYR:CD2 | 2.42 | 0.55 |
| 1:F:716:LEU:HB3 | 1:F:728:TRP:HB2 | 1.87 | 0.55 |
| 1:F:763:ALA:HA | 1:F:801:VAL:H | 1.70 | 0.55 |
| 1:G:763:ALA:HA | 1:G:801:VAL:H | 1.70 | 0.55 |
| 1:A:845:TYR:HB3 | 1:A:858:ALA:HB3 | 1.89 | 0.55 |
| 1:B:572:GLU:HA | 1:B:577:TYR:CD2 | 2.42 | 0.55 |
| 1:C:170:ASP:OD1 | 1:C:171:HIS:N | 2.39 | 0.55 |
| 1:C:463:GLN:OE1 | 1:C:466:ARG:NH2 | 2.28 | 0.55 |
| 1:C:572:GLU:HA | 1:C:577:TYR:CD2 | 2.42 | 0.55 |
| 1:D:763:ALA:HA | 1:D:801:VAL:H | 1.70 | 0.55 |
| 1:E:572:GLU:HA | 1:E:577:TYR:CD2 | 2.42 | 0.55 |
| 1:F:326:LEU:HD13 | 1:F:353:ILE:CG2 | 2.36 | 0.55 |
| 1:A:572:GLU:HA | 1:A:577:TYR:CD2 | 2.42 | 0.55 |
| 1:B:28:HIS:CE1 | 3:P:14:LEU:CD2 | 2.90 | 0.55 |
| 1:B:565:GLN:NE2 | 1:B:1213:PHE:CA | 2.69 | 0.55 |
| 1:C:565:GLN:NE2 | 1:C:1213:PHE:CA | 2.69 | 0.55 |
| 1:D:143:LEU:C | 1:D:145:GLY:H | 2.09 | 0.55 |
| 1:D:617:ALA:HA | 1:D:904:GLN:HG2 | 1.89 | 0.55 |
| 1:F:217:PRO:HG3 | 1:F:226:ARG:HH12 | 1.71 | 0.55 |
| 1:G:326:LEU:HD13 | 1:G:353:ILE:CG2 | 2.36 | 0.55 |
| 1:G:572:GLU:HA | 1:G:577:TYR:CD2 | 2.42 | 0.55 |
| 1:B:1086:GLY:CA | 2:I:39:LYS:NZ | 2.66 | 0.55 |
| 1:D:844:GLN:HE22 | 2:K:79:LYS:HE3 | 1.71 | 0.55 |
| 1:E:716:LEU:HB3 | 1:E:728:TRP:HB2 | 1.87 | 0.55 |
| 3:O:27:ASP:OD1 | 3:R:13:ARG:HG2 | 2.06 | 0.55 |
| 1:A:1092:ASP:OD2 | 1:A:1133:SER:OG | 2.17 | 0.55 |
| 1:D:565:GLN:NE2 | 1:D:1213:PHE:CA | 2.69 | 0.55 |
| 1:D:170:ASP:OD1 | 1:D:171:HIS:N | 2.39 | 0.55 |
| 1:E:565:GLN:NE2 | 1:E:1213:PHE:CA | 2.69 | 0.55 |
| 1:F:844:GLN:HE22 | 2:M:79:LYS:HE3 | 1.71 | 0.55 |
| 1:G:845:TYR:HB3 | 1:G:858:ALA:HB3 | 1.89 | 0.55 |
| 3:R:15:ARG:HD2 | 3:R:19:GLU:OE2 | 2.07 | 0.55 |
| 3:R:8:LEU:HD23 | 3:R:8:LEU:C | 2.27 | 0.55 |
| 1:F:170:ASP:OD1 | 1:F:171:HIS:N | 2.39 | 0.55 |
| 1:D:1086:GLY:CA | 2:K:39:LYS:NZ | 2.66 | 0.55 |
| 2:N:60:GLY:N | 2:N:63:THR:OG1 | 2.34 | 0.55 |
| 3:P:8:LEU:C | 3:P:8:LEU:HD23 | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:617:ALA:HA | 1:B:904:GLN:HG2 | 1.89 | 0.55 |
| 1:D:845:TYR:HB3 | 1:D:858:ALA:HB3 | 1.89 | 0.55 |
| 1:D:884:TRP:CD1 | 1:D:884:TRP:N | 2.73 | 0.55 |
| 1:F:524:HIS:HB2 | 1:F:646:THR:CG2 | 2.32 | 0.55 |
| 1:A:482:TYR:HH | 1:A:490:HIS:HE2 | 1.47 | 0.54 |
| 1:E:143:LEU:C | 1:E:145:GLY:H | 2.09 | 0.54 |
| 1:F:565:GLN:NE2 | 1:F:1213:PHE:CA | 2.69 | 0.54 |
| 1:A:550:LEU:HD21 | 1:A:607:SER:CB | 2.35 | 0.54 |
| 1:B:1219:ASN:HB2 | 1:B:1237:ASN:HB3 | 1.89 | 0.54 |
| 1:B:716:LEU:HB3 | 1:B:728:TRP:HB2 | 1.87 | 0.54 |
| 1:E:170:ASP:OD1 | 1:E:171:HIS:N | 2.39 | 0.54 |
| 1:G:1023:ASP:OD1 | 1:G:1046:THR:OG1 | 2.24 | 0.54 |
| 1:G:265:ARG:HH11 | 1:G:371:SER:HG | 1.52 | 0.54 |
| 1:E:844:GLN:HE22 | 2:L:79:LYS:HE3 | 1.71 | 0.54 |
| 1:C:1219:ASN:HB2 | 1:C:1237:ASN:HB3 | 1.89 | 0.54 |
| 1:F:550:LEU:HD21 | 1:F:607:SER:CB | 2.35 | 0.54 |
| 1:F:884:TRP:CD1 | 1:F:884:TRP:N | 2.73 | 0.54 |
| 3:Q:8:LEU:HD23 | 3:Q:8:LEU:C | 2.27 | 0.54 |
| 1:B:482:TYR:OH | 1:B:490:HIS:NE2 | 2.35 | 0.54 |
| 1:C:727:LEU:HB3 | 1:C:737:ASN:HB2 | 1.90 | 0.54 |
| 1:D:1087:THR:N | 2:K:39:LYS:HZ3 | 2.06 | 0.54 |
| 1:D:800:ILE:H | 1:D:818:LYS:HE2 | 1.73 | 0.54 |
| 1:E:217:PRO:HG3 | 1:E:226:ARG:HH12 | 1.71 | 0.54 |
| 1:E:617:ALA:HA | 1:E:904:GLN:HG2 | 1.89 | 0.54 |
| 1:A:143:LEU:C | 1:A:145:GLY:H | 2.09 | 0.54 |
| 1:A:217:PRO:HG3 | 1:A:226:ARG:HH12 | 1.71 | 0.54 |
| 1:D:1023:ASP:OD1 | 1:D:1046:THR:OG1 | 2.24 | 0.54 |
| 1:D:727:LEU:HB3 | 1:D:737:ASN:HB2 | 1.90 | 0.54 |
| 1:F:800:ILE:H | 1:F:818:LYS:HE2 | 1.73 | 0.54 |
| 1:G:143:LEU:C | 1:G:145:GLY:H | 2.09 | 0.54 |
| 1:A:219:ASN:HD21 | 1:G:201:ASN:HD21 | 1.54 | 0.54 |
| 1:B:800:ILE:H | 1:B:818:LYS:HE2 | 1.73 | 0.54 |
| 1:E:884:TRP:CZ3 | 2:L:79:LYS:CA | 2.74 | 0.54 |
| 3:O:15:ARG:HD2 | 3:O:19:GLU:OE2 | 2.07 | 0.54 |
| 1:B:217:PRO:HG3 | 1:B:226:ARG:HH12 | 1.72 | 0.54 |
| 1:B:727:LEU:HB3 | 1:B:737:ASN:HB2 | 1.90 | 0.54 |
| 1:C:143:LEU:C | 1:C:145:GLY:H | 2.09 | 0.54 |
| 1:C:800:ILE:H | 1:C:818:LYS:HE2 | 1.73 | 0.54 |
| 1:D:558:GLN:HA | 1:D:559:PRO:C | 2.28 | 0.54 |
| 1:D:612:ARG:NH2 | 1:D:903:ASP:O | 2.41 | 0.54 |
| 1:E:727:LEU:HB3 | 1:E:737:ASN:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:612:ARG:NH2 | 1:F:903:ASP:O | 2.41 | 0.54 |
| 1:F:845:TYR:HB3 | 1:F:858:ALA:HB3 | 1.89 | 0.54 |
| 2:I:40:THR:HA | 2:I:59:TRP:HE1 | 1.73 | 0.54 |
| 1:E:1086:GLY:CA | 2:L:39:LYS:NZ | 2.66 | 0.54 |
| 1:A:1219:ASN:HB2 | 1:A:1237:ASN:HB3 | 1.89 | 0.54 |
| 1:A:800:ILE:H | 1:A:818:LYS:HE2 | 1.73 | 0.54 |
| 1:C:265:ARG:NH1 | 1:C:371:SER:OG | 2.37 | 0.54 |
| 1:D:30:ILE:CG2 | 3:Q:10:ARG:CB | 2.80 | 0.54 |
| 1:A:265:ARG:HH11 | 1:A:371:SER:HG | 1.55 | 0.54 |
| 1:E:558:GLN:HA | 1:E:559:PRO:C | 2.28 | 0.54 |
| 1:F:558:GLN:HA | 1:F:559:PRO:C | 2.28 | 0.54 |
| 1:G:482:TYR:HH | 1:G:490:HIS:HE2 | 1.52 | 0.54 |
| 1:G:550:LEU:HD21 | 1:G:607:SER:CB | 2.35 | 0.54 |
| 2:L:40:THR:HA | 2:L:59:TRP:HE1 | 1.73 | 0.54 |
| 1:A:558:GLN:HA | 1:A:559:PRO:C | 2.28 | 0.54 |
| 1:A:617:ALA:HA | 1:A:904:GLN:HG2 | 1.89 | 0.54 |
| 1:A:864:VAL:CG2 | 1:A:885:VAL:HG21 | 2.38 | 0.54 |
| 1:B:336:ASN:HB2 | 1:C:431:LYS:HE3 | 1.90 | 0.54 |
| 1:D:1219:ASN:HB2 | 1:D:1237:ASN:HB3 | 1.89 | 0.54 |
| 1:F:987:ILE:HD11 | 1:F:1018:LEU:HD22 | 1.90 | 0.54 |
| 1:F:1219:ASN:HB2 | 1:F:1237:ASN:HB3 | 1.89 | 0.54 |
| 1:F:265:ARG:HH11 | 1:F:371:SER:HG | 1.55 | 0.54 |
| 1:G:217:PRO:HG3 | 1:G:226:ARG:HH12 | 1.72 | 0.54 |
| 1:G:612:ARG:NH2 | 1:G:903:ASP:O | 2.41 | 0.54 |
| 3:Q:15:ARG:HD2 | 3:Q:19:GLU:OE2 | 2.07 | 0.54 |
| 1:B:13:ARG:O | 1:B:17:GLU:HG3 | 2.09 | 0.53 |
| 1:B:558:GLN:HA | 1:B:559:PRO:C | 2.28 | 0.53 |
| 1:B:612:ARG:NH2 | 1:B:903:ASP:O | 2.41 | 0.53 |
| 1:C:558:GLN:HA | 1:C:559:PRO:C | 2.28 | 0.53 |
| 1:F:727:LEU:HB3 | 1:F:737:ASN:HB2 | 1.90 | 0.53 |
| 1:D:358:SER:HB3 | 1:E:274:MET:HE3 | 1.89 | 0.53 |
| 1:D:524:HIS:HB2 | 1:D:646:THR:CG2 | 2.32 | 0.53 |
| 1:E:987:ILE:HD11 | 1:E:1018:LEU:HD22 | 1.90 | 0.53 |
| 1:E:845:TYR:HB3 | 1:E:858:ALA:HB3 | 1.89 | 0.53 |
| 1:F:266:ASP:OD1 | 1:F:267:LYS:N | 2.41 | 0.53 |
| 1:G:800:ILE:H | 1:G:818:LYS:HE2 | 1.73 | 0.53 |
| 3:O:8:LEU:C | 3:O:8:LEU:HD23 | 2.27 | 0.53 |
| 1:A:266:ASP:OD1 | 1:A:267:LYS:N | 2.41 | 0.53 |
| 1:C:1061:TRP:CE2 | 1:C:1090:SER:HA | 2.43 | 0.53 |
| 1:C:266:ASP:OD1 | 1:C:267:LYS:N | 2.42 | 0.53 |
| 1:E:1023:ASP:OD1 | 1:E:1046:THR:OG1 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:266:ASP:OD1 | 1:E:267:LYS:N | 2.42 | 0.53 |
| 1:E:612:ARG:NH2 | 1:E:903:ASP:O | 2.41 | 0.53 |
| 1:F:1023:ASP:OD1 | 1:F:1046:THR:OG1 | 2.24 | 0.53 |
| 2:K:40:THR:HA | 2:K:59:TRP:HE1 | 1.73 | 0.53 |
| 2:N:40:THR:HA | 2:N:59:TRP:HE1 | 1.73 | 0.53 |
| 1:C:864:VAL:CG2 | 1:C:885:VAL:HG21 | 2.38 | 0.53 |
| 1:D:1061:TRP:CE2 | 1:D:1090:SER:HA | 2.43 | 0.53 |
| 1:D:13:ARG:O | 1:D:17:GLU:HG3 | 2.09 | 0.53 |
| 1:E:1061:TRP:CE2 | 1:E:1090:SER:HA | 2.43 | 0.53 |
| 1:E:698:HIS:CE1 | 1:E:726:LYS:HD2 | 2.44 | 0.53 |
| 1:E:864:VAL:CG2 | 1:E:885:VAL:HG21 | 2.38 | 0.53 |
| 1:F:358:SER:OG | 1:G:274:MET:HG2 | 2.09 | 0.53 |
| 1:G:266:ASP:OD1 | 1:G:267:LYS:N | 2.41 | 0.53 |
| 1:G:558:GLN:HA | 1:G:559:PRO:C | 2.28 | 0.53 |
| 1:G:864:VAL:CG2 | 1:G:885:VAL:HG21 | 2.38 | 0.53 |
| 1:G:987:ILE:HD11 | 1:G:1018:LEU:HD22 | 1.91 | 0.53 |
| 1:A:884:TRP:N | 1:A:884:TRP:CD1 | 2.73 | 0.53 |
| 1:A:612:ARG:NH2 | 1:A:903:ASP:O | 2.41 | 0.53 |
| 1:B:1061:TRP:CE2 | 1:B:1090:SER:HA | 2.43 | 0.53 |
| 1:B:267:LYS:HZ1 | 1:B:419:VAL:HG12 | 1.74 | 0.53 |
| 1:E:13:ARG:O | 1:E:17:GLU:HG3 | 2.09 | 0.53 |
| 1:E:800:ILE:H | 1:E:818:LYS:HE2 | 1.73 | 0.53 |
| 1:F:617:ALA:HA | 1:F:904:GLN:HG2 | 1.89 | 0.53 |
| 1:B:584:ALA:HB1 | 1:B:594:TYR:CD2 | 2.44 | 0.53 |
| 1:B:884:TRP:CD1 | 1:B:884:TRP:N | 2.73 | 0.53 |
| 1:C:612:ARG:NH2 | 1:C:903:ASP:O | 2.41 | 0.53 |
| 1:D:1149:GLY:HA3 | 1:D:1178:GLY:HA2 | 1.91 | 0.53 |
| 1:E:1149:GLY:HA3 | 1:E:1178:GLY:HA2 | 1.91 | 0.53 |
| 2:M:40:THR:HA | 2:M:59:TRP:HE1 | 1.73 | 0.53 |
| 1:A:1087:THR:N | 2:H:39:LYS:HZ3 | 2.06 | 0.53 |
| 1:A:698:HIS:CE1 | 1:A:726:LYS:HD2 | 2.44 | 0.53 |
| 1:B:463:GLN:OE1 | 1:B:466:ARG:NH2 | 2.28 | 0.53 |
| 1:C:884:TRP:N | 1:C:884:TRP:CD1 | 2.73 | 0.53 |
| 1:D:987:ILE:HD11 | 1:D:1018:LEU:HD22 | 1.90 | 0.53 |
| 1:D:864:VAL:CG2 | 1:D:885:VAL:HG21 | 2.38 | 0.53 |
| 1:G:1149:GLY:HA3 | 1:G:1178:GLY:HA2 | 1.91 | 0.53 |
| 1:G:727:LEU:HB3 | 1:G:737:ASN:HB2 | 1.90 | 0.53 |
| 1:A:1086:GLY:CA | 2:H:39:LYS:NZ | 2.66 | 0.53 |
| 2:I:67:TYR:OH | 2:I:80:MET:SD | 2.57 | 0.53 |
| 2:J:40:THR:HA | 2:J:59:TRP:HE1 | 1.73 | 0.53 |
| 1:A:1149:GLY:HA3 | 1:A:1178:GLY:HA2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:336:ASN:HB2 | 1:B:431:LYS:HE3 | 1.90 | 0.53 |
| 1:B:266:ASP:OD1 | 1:B:267:LYS:N | 2.41 | 0.53 |
| 1:B:864:VAL:CG2 | 1:B:885:VAL:HG21 | 2.38 | 0.53 |
| 1:F:864:VAL:CG2 | 1:F:885:VAL:HG21 | 2.38 | 0.53 |
| 1:G:524:HIS:HB2 | 1:G:646:THR:CG2 | 2.32 | 0.53 |
| 1:A:267:LYS:HZ1 | 1:A:419:VAL:HG12 | 1.74 | 0.53 |
| 1:A:727:LEU:HB3 | 1:A:737:ASN:HB2 | 1.90 | 0.53 |
| 1:C:267:LYS:HZ1 | 1:C:419:VAL:HG12 | 1.74 | 0.53 |
| 1:D:584:ALA:HB1 | 1:D:594:TYR:CD2 | 2.44 | 0.53 |
| 1:F:698:HIS:CE1 | 1:F:726:LYS:HD2 | 2.44 | 0.53 |
| 1:G:1219:ASN:HB2 | 1:G:1237:ASN:HB3 | 1.90 | 0.53 |
| 1:G:698:HIS:CE1 | 1:G:726:LYS:HD2 | 2.44 | 0.53 |
| 1:G:617:ALA:HA | 1:G:904:GLN:HG2 | 1.89 | 0.53 |
| 1:C:524:HIS:HB2 | 1:C:646:THR:CG2 | 2.32 | 0.53 |
| 1:C:584:ALA:HB1 | 1:C:594:TYR:CD2 | 2.44 | 0.53 |
| 1:D:698:HIS:CE1 | 1:D:726:LYS:HD2 | 2.44 | 0.53 |
| 1:F:1061:TRP:CE2 | 1:F:1090:SER:HA | 2.43 | 0.53 |
| 1:F:1149:GLY:HA3 | 1:F:1178:GLY:HA2 | 1.91 | 0.53 |
| 1:F:1191:MET:SD | 1:F:1209:SER:OG | 2.63 | 0.53 |
| 1:F:631:ALA:HB1 | 1:F:639:LEU:HD11 | 1.91 | 0.53 |
| 2:H:40:THR:HA | 2:H:59:TRP:HE1 | 1.73 | 0.53 |
| 1:D:266:ASP:OD1 | 1:D:267:LYS:N | 2.41 | 0.52 |
| 1:D:267:LYS:HZ1 | 1:D:419:VAL:HG12 | 1.74 | 0.52 |
| 1:E:1219:ASN:HB2 | 1:E:1237:ASN:HB3 | 1.89 | 0.52 |
| 1:E:844:GLN:HE22 | 2:L:79:LYS:HZ2 | 1.56 | 0.52 |
| 1:G:13:ARG:O | 1:G:17:GLU:HG3 | 2.08 | 0.52 |
| 1:A:274:MET:HE2 | 1:G:358:SER:HB3 | 1.91 | 0.52 |
| 1:G:884:TRP:CD1 | 1:G:884:TRP:N | 2.73 | 0.52 |
| 1:A:1061:TRP:CE2 | 1:A:1090:SER:HA | 2.43 | 0.52 |
| 1:A:844:GLN:HE22 | 2:H:79:LYS:HZ2 | 1.56 | 0.52 |
| 1:C:1149:GLY:HA3 | 1:C:1178:GLY:HA2 | 1.91 | 0.52 |
| 1:D:609:LEU:HD23 | 1:D:908:LEU:HD13 | 1.91 | 0.52 |
| 1:E:336:ASN:HB2 | 1:F:431:LYS:HE3 | 1.91 | 0.52 |
| 1:F:1087:THR:N | 2:M:39:LYS:HZ3 | 2.07 | 0.52 |
| 1:G:584:ALA:HB1 | 1:G:594:TYR:CD2 | 2.44 | 0.52 |
| 1:A:987:ILE:HD11 | 1:A:1018:LEU:HD22 | 1.90 | 0.52 |
| 1:B:1126:HIS:CE1 | 1:B:1129:CYS:H | 2.28 | 0.52 |
| 1:B:1149:GLY:HA3 | 1:B:1178:GLY:HA2 | 1.91 | 0.52 |
| 1:B:326:LEU:HD13 | 1:B:353:ILE:HG22 | 1.92 | 0.52 |
| 1:C:698:HIS:CE1 | 1:C:726:LYS:HD2 | 2.44 | 0.52 |
| 1:E:631:ALA:HB1 | 1:E:639:LEU:HD11 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:1061:TRP:CE2 | 1:G:1090:SER:HA | 2.43 | 0.52 |
| 1:G:945:ARG:HD2 | 1:G:961:GLU:HB2 | 1.92 | 0.52 |
| 2:K:67:TYR:OH | 2:K:80:MET:SD | 2.57 | 0.52 |
| 1:A:365:ASP:OD1 | 1:A:444:PHE:CE1 | 2.63 | 0.52 |
| 1:B:1087:THR:N | 2:I:39:LYS:HZ3 | 2.07 | 0.52 |
| 1:C:265:ARG:HH11 | 1:C:371:SER:HG | 1.57 | 0.52 |
| 1:E:267:LYS:HZ1 | 1:E:419:VAL:HG12 | 1.74 | 0.52 |
| 1:E:609:LEU:HD23 | 1:E:908:LEU:HD13 | 1.91 | 0.52 |
| 1:G:365:ASP:OD1 | 1:G:444:PHE:CE1 | 2.63 | 0.52 |
| 3:P:50:SER:HB3 | 3:Q:45:ARG:NH1 | 2.24 | 0.52 |
| 1:A:584:ALA:HB1 | 1:A:594:TYR:CD2 | 2.44 | 0.52 |
| 1:C:336:ASN:HB2 | 1:D:431:LYS:HE3 | 1.91 | 0.52 |
| 1:D:326:LEU:HD13 | 1:D:353:ILE:HG22 | 1.92 | 0.52 |
| 1:F:945:ARG:HD2 | 1:F:961:GLU:HB2 | 1.92 | 0.52 |
| 1:F:358:SER:HB3 | 1:G:274:MET:HE2 | 1.92 | 0.52 |
| 2:M:60:GLY:N | 2:M:63:THR:OG1 | 2.34 | 0.52 |
| 1:A:945:ARG:HD2 | 1:A:961:GLU:HB2 | 1.92 | 0.52 |
| 1:C:326:LEU:HD13 | 1:C:353:ILE:HG22 | 1.92 | 0.52 |
| 1:E:326:LEU:HD13 | 1:E:353:ILE:HG22 | 1.92 | 0.52 |
| 1:E:584:ALA:HB1 | 1:E:594:TYR:CD2 | 2.44 | 0.52 |
| 1:G:631:ALA:HB1 | 1:G:639:LEU:HD11 | 1.91 | 0.52 |
| 2:H:67:TYR:OH | 2:H:80:MET:SD | 2.57 | 0.52 |
| 1:F:1086:GLY:CA | 2:M:39:LYS:NZ | 2.66 | 0.52 |
| 1:G:844:GLN:NE2 | 2:N:79:LYS:NZ | 2.58 | 0.52 |
| 1:B:987:ILE:HD11 | 1:B:1018:LEU:HD22 | 1.90 | 0.52 |
| 1:C:987:ILE:HD11 | 1:C:1018:LEU:HD22 | 1.90 | 0.52 |
| 1:D:37:ILE:HG12 | 3:Q:10:ARG:CD | 2.40 | 0.52 |
| 1:D:725:LEU:HB2 | 1:D:739:MET:HB2 | 1.92 | 0.52 |
| 1:F:365:ASP:OD1 | 1:F:444:PHE:CE1 | 2.63 | 0.52 |
| 1:A:882:LEU:HD12 | 1:A:1176:HIS:NE2 | 2.25 | 0.52 |
| 1:A:326:LEU:HD13 | 1:A:353:ILE:HG22 | 1.92 | 0.52 |
| 1:A:609:LEU:HD23 | 1:A:908:LEU:HD13 | 1.91 | 0.52 |
| 1:B:550:LEU:HD21 | 1:B:607:SER:CB | 2.35 | 0.52 |
| 1:C:1126:HIS:CE1 | 1:C:1129:CYS:H | 2.28 | 0.52 |
| 1:D:14:GLU:HB2 | 1:E:31:SER:OG | 2.09 | 0.52 |
| 1:D:864:VAL:HG23 | 1:D:885:VAL:HG21 | 1.92 | 0.52 |
| 1:E:945:ARG:HD2 | 1:E:961:GLU:HB2 | 1.92 | 0.52 |
| 2:N:67:TYR:OH | 2:N:80:MET:SD | 2.57 | 0.52 |
| 1:A:1126:HIS:CE1 | 1:A:1129:CYS:H | 2.28 | 0.52 |
| 1:B:365:ASP:OD1 | 1:B:444:PHE:CE1 | 2.63 | 0.52 |
| 1:E:365:ASP:OD1 | 1:E:444:PHE:CE1 | 2.63 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:267:LYS:HZ1 | 1:F:419:VAL:HG12 | 1.75 | 0.52 |
| 1:F:326:LEU:HD13 | 1:F:353:ILE:HG22 | 1.92 | 0.52 |
| 1:A:265:ARG:NH2 | 4:A:1301:DTP:O2G | 2.31 | 0.52 |
| 1:A:530:ARG:HD2 | 1:A:545:GLN:HE22 | 1.75 | 0.52 |
| 1:B:698:HIS:CE1 | 1:B:726:LYS:HD2 | 2.44 | 0.52 |
| 1:B:945:ARG:HD2 | 1:B:961:GLU:HB2 | 1.92 | 0.52 |
| 1:C:864:VAL:HG23 | 1:C:885:VAL:HG21 | 1.92 | 0.52 |
| 1:D:1126:HIS:CE1 | 1:D:1129:CYS:H | 2.28 | 0.52 |
| 1:D:882:LEU:HD12 | 1:D:1176:HIS:NE2 | 2.25 | 0.52 |
| 1:D:844:GLN:NE2 | 2:K:79:LYS:NZ | 2.57 | 0.52 |
| 1:E:864:VAL:HG23 | 1:E:885:VAL:HG21 | 1.92 | 0.52 |
| 1:F:584:ALA:HB1 | 1:F:594:TYR:CD2 | 2.44 | 0.52 |
| 1:A:416:GLN:HE21 | 1:G:334:PHE:HE1 | 1.57 | 0.52 |
| 1:G:609:LEU:HD23 | 1:G:908:LEU:HD13 | 1.91 | 0.52 |
| 1:B:844:GLN:NE2 | 2:I:79:LYS:NZ | 2.57 | 0.51 |
| 1:C:609:LEU:HD23 | 1:C:908:LEU:HD13 | 1.91 | 0.51 |
| 1:E:600:LYS:HZ1 | 1:E:1213:PHE:HZ | 1.58 | 0.51 |
| 1:E:550:LEU:HD21 | 1:E:607:SER:CB | 2.35 | 0.51 |
| 1:G:265:ARG:NH1 | 1:G:371:SER:OG | 2.37 | 0.51 |
| 1:E:725:LEU:HB2 | 1:E:739:MET:HB2 | 1.92 | 0.51 |
| 1:F:882:LEU:HD12 | 1:F:1176:HIS:NE2 | 2.25 | 0.51 |
| 1:G:267:LYS:HZ1 | 1:G:419:VAL:HG12 | 1.74 | 0.51 |
| 1:A:844:GLN:NE2 | 2:H:79:LYS:NZ | 2.58 | 0.51 |
| 2:J:60:GLY:N | 2:J:63:THR:OG1 | 2.34 | 0.51 |
| 1:C:550:LEU:HD21 | 1:C:607:SER:CB | 2.35 | 0.51 |
| 1:C:725:LEU:HB2 | 1:C:739:MET:HB2 | 1.92 | 0.51 |
| 1:F:337:ARG:NH1 | 1:G:409:GLU:OE2 | 2.44 | 0.51 |
| 1:G:326:LEU:HD13 | 1:G:353:ILE:HG22 | 1.92 | 0.51 |
| 1:B:400:LEU:HB3 | 1:B:404:TRP:CZ3 | 2.46 | 0.51 |
| 1:C:334:PHE:HE1 | 1:D:416:GLN:HE21 | 1.57 | 0.51 |
| 1:C:400:LEU:HB3 | 1:C:404:TRP:CZ3 | 2.46 | 0.51 |
| 1:D:365:ASP:OD1 | 1:D:444:PHE:CE1 | 2.63 | 0.51 |
| 1:D:530:ARG:HD2 | 1:D:545:GLN:HE22 | 1.75 | 0.51 |
| 1:D:550:LEU:HD21 | 1:D:607:SER:CB | 2.35 | 0.51 |
| 1:D:631:ALA:HB1 | 1:D:639:LEU:HD11 | 1.91 | 0.51 |
| 1:E:530:ARG:HD2 | 1:E:545:GLN:HE22 | 1.76 | 0.51 |
| 1:F:482:TYR:OH | 1:F:490:HIS:NE2 | 2.35 | 0.51 |
| 1:F:692:VAL:HG12 | 1:F:693:HIS:ND1 | 2.26 | 0.51 |
| 1:F:884:TRP:CZ3 | 2:M:79:LYS:CA | 2.74 | 0.51 |
| 1:F:609:LEU:HD23 | 1:F:908:LEU:HD13 | 1.91 | 0.51 |
| 1:G:864:VAL:HG23 | 1:G:885:VAL:HG21 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:590:ASN:C | 1:A:592:MET:N | 2.64 | 0.51 |
| 1:A:692:VAL:HG12 | 1:A:693:HIS:ND1 | 2.25 | 0.51 |
| 1:A:725:LEU:HB2 | 1:A:739:MET:HB2 | 1.92 | 0.51 |
| 1:B:609:LEU:HD23 | 1:B:908:LEU:HD13 | 1.91 | 0.51 |
| 1:D:1191:MET:SD | 1:D:1209:SER:OG | 2.63 | 0.51 |
| 1:E:882:LEU:HD12 | 1:E:1176:HIS:NE2 | 2.25 | 0.51 |
| 1:F:844:GLN:NE2 | 2:M:79:LYS:NZ | 2.57 | 0.51 |
| 2:K:60:GLY:N | 2:K:63:THR:OG1 | 2.34 | 0.51 |
| 3:P:50:SER:HB3 | 3:Q:45:ARG:HH12 | 1.74 | 0.51 |
| 1:B:692:VAL:HG12 | 1:B:693:HIS:ND1 | 2.26 | 0.51 |
| 1:C:692:VAL:HG12 | 1:C:693:HIS:ND1 | 2.26 | 0.51 |
| 1:F:1126:HIS:CE1 | 1:F:1129:CYS:H | 2.28 | 0.51 |
| 1:F:530:ARG:HD2 | 1:F:545:GLN:HE22 | 1.75 | 0.51 |
| 1:E:1086:GLY:HA2 | 2:L:39:LYS:HE2 | 1.92 | 0.51 |
| 1:C:365:ASP:OD1 | 1:C:444:PHE:CE1 | 2.63 | 0.51 |
| 1:D:590:ASN:C | 1:D:592:MET:N | 2.64 | 0.51 |
| 1:F:590:ASN:C | 1:F:592:MET:N | 2.64 | 0.51 |
| 1:G:1086:GLY:HA2 | 2:N:39:LYS:HE2 | 1.92 | 0.51 |
| 1:G:1126:HIS:CE1 | 1:G:1129:CYS:H | 2.28 | 0.51 |
| 2:L:60:GLY:N | 2:L:63:THR:OG1 | 2.34 | 0.51 |
| 1:G:1086:GLY:CA | 2:N:39:LYS:NZ | 2.66 | 0.51 |
| 1:A:400:LEU:HB3 | 1:A:404:TRP:CZ3 | 2.46 | 0.51 |
| 1:A:631:ALA:HB1 | 1:A:639:LEU:HD11 | 1.91 | 0.51 |
| 1:B:265:ARG:HH11 | 1:B:371:SER:HG | 1.54 | 0.51 |
| 1:B:725:LEU:HB2 | 1:B:739:MET:HB2 | 1.92 | 0.51 |
| 1:B:864:VAL:HG23 | 1:B:885:VAL:HG21 | 1.92 | 0.51 |
| 1:C:945:ARG:HD2 | 1:C:961:GLU:HB2 | 1.92 | 0.51 |
| 1:D:336:ASN:HB2 | 1:E:431:LYS:HE3 | 1.93 | 0.51 |
| 1:D:400:LEU:HB3 | 1:D:404:TRP:CZ3 | 2.46 | 0.51 |
| 1:F:265:ARG:NH1 | 1:F:371:SER:OG | 2.37 | 0.51 |
| 1:G:590:ASN:C | 1:G:592:MET:N | 2.64 | 0.51 |
| 2:H:60:GLY:N | 2:H:63:THR:OG1 | 2.34 | 0.51 |
| 2:H:94:LEU:HD21 | 5:H:500:HEC:HMB1 | 1.93 | 0.51 |
| 2:M:94:LEU:HD21 | 5:M:500:HEC:HMB1 | 1.93 | 0.51 |
| 1:B:590:ASN:C | 1:B:592:MET:N | 2.64 | 0.51 |
| 1:C:530:ARG:HD2 | 1:C:545:GLN:HE22 | 1.76 | 0.51 |
| 1:E:1126:HIS:CE1 | 1:E:1129:CYS:H | 2.28 | 0.51 |
| 1:G:152:ILE:HD11 | 1:G:263:THR:HG22 | 1.92 | 0.51 |
| 2:I:94:LEU:HD21 | 5:I:500:HEC:HMB1 | 1.93 | 0.51 |
| 2:N:94:LEU:HD21 | 5:N:500:HEC:HMB1 | 1.93 | 0.51 |
| 3:P:32:ARG:HD2 | 3:P:76:CYS:SG | 2.51 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1002:HIS:ND1 | 1:B:1024:ASP:OD2 | 2.44 | 0.51 |
| 1:B:530:ARG:HD2 | 1:B:545:GLN:HE22 | 1.76 | 0.51 |
| 1:C:562:ASN:HB2 | 1:C:565:GLN:HG2 | 1.93 | 0.51 |
| 1:F:725:LEU:HB2 | 1:F:739:MET:HB2 | 1.92 | 0.51 |
| 1:G:882:LEU:HD12 | 1:G:1176:HIS:NE2 | 2.25 | 0.51 |
| 1:F:334:PHE:HE1 | 1:G:416:GLN:HE21 | 1.58 | 0.51 |
| 1:G:530:ARG:HD2 | 1:G:545:GLN:HE22 | 1.76 | 0.51 |
| 1:G:725:LEU:HB2 | 1:G:739:MET:HB2 | 1.92 | 0.51 |
| 1:A:152:ILE:HD11 | 1:A:263:THR:HG22 | 1.92 | 0.50 |
| 1:A:864:VAL:HG23 | 1:A:885:VAL:HG21 | 1.92 | 0.50 |
| 1:B:608:ARG:HD2 | 1:B:910:GLU:HB2 | 1.94 | 0.50 |
| 1:C:844:GLN:NE2 | 2:J:79:LYS:NZ | 2.57 | 0.50 |
| 1:D:562:ASN:HB2 | 1:D:565:GLN:HG2 | 1.94 | 0.50 |
| 1:D:945:ARG:HD2 | 1:D:961:GLU:HB2 | 1.92 | 0.50 |
| 1:E:692:VAL:HG12 | 1:E:693:HIS:ND1 | 2.26 | 0.50 |
| 1:F:864:VAL:HG23 | 1:F:885:VAL:HG21 | 1.92 | 0.50 |
| 2:I:60:GLY:N | 2:I:63:THR:OG1 | 2.34 | 0.50 |
| 3:O:32:ARG:HD2 | 3:O:76:CYS:SG | 2.51 | 0.50 |
| 1:B:700:GLU:HG3 | 1:B:721:SER:HB2 | 1.94 | 0.50 |
| 1:C:1002:HIS:ND1 | 1:C:1024:ASP:OD2 | 2.45 | 0.50 |
| 1:D:1002:HIS:ND1 | 1:D:1024:ASP:OD2 | 2.44 | 0.50 |
| 1:E:400:LEU:HB3 | 1:E:404:TRP:CZ3 | 2.46 | 0.50 |
| 1:F:1002:HIS:ND1 | 1:F:1024:ASP:OD2 | 2.44 | 0.50 |
| 1:F:862:TYR:HB3 | 1:F:884:TRP:CA | 2.42 | 0.50 |
| 1:A:1002:HIS:ND1 | 1:A:1024:ASP:OD2 | 2.44 | 0.50 |
| 1:A:334:PHE:HE1 | 1:B:416:GLN:HE21 | 1.58 | 0.50 |
| 1:A:608:ARG:HD2 | 1:A:910:GLU:HB2 | 1.94 | 0.50 |
| 1:B:344:GLN:OE1 | 1:B:349:GLN:NE2 | 2.44 | 0.50 |
| 1:B:562:ASN:HB2 | 1:B:565:GLN:HG2 | 1.94 | 0.50 |
| 1:C:1086:GLY:HA2 | 2:J:39:LYS:HE2 | 1.92 | 0.50 |
| 1:G:819:ASN:ND2 | 1:G:840:HIS:O | 2.45 | 0.50 |
| 1:C:348:LYS:NZ | 1:C:443:ASP:OD1 | 2.45 | 0.50 |
| 1:G:1002:HIS:ND1 | 1:G:1024:ASP:OD2 | 2.44 | 0.50 |
| 1:G:692:VAL:HG12 | 1:G:693:HIS:ND1 | 2.26 | 0.50 |
| 2:L:94:LEU:HD21 | 5:L:500:HEC:HMB1 | 1.93 | 0.50 |
| 3:P:15:ARG:HD2 | 3:P:19:GLU:OE2 | 2.07 | 0.50 |
| 1:A:482:TYR:OH | 1:A:490:HIS:NE2 | 2.35 | 0.50 |
| 1:A:762:SER:OG | 1:A:764:ASP:OD1 | 2.26 | 0.50 |
| 1:B:631:ALA:HB1 | 1:B:639:LEU:HD11 | 1.91 | 0.50 |
| 1:E:562:ASN:HB2 | 1:E:565:GLN:HG2 | 1.94 | 0.50 |
| 1:E:862:TYR:HB3 | 1:E:884:TRP:CA | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:152:ILE:HD11 | 1:F:263:THR:HG22 | 1.92 | 0.50 |
| 1:A:431:LYS:HE3 | 1:G:336:ASN:HB2 | 1.92 | 0.50 |
| 1:G:400:LEU:HB3 | 1:G:404:TRP:CZ3 | 2.46 | 0.50 |
| 3:Q:52:ARG:HD2 | 3:R:38:HIS:ND1 | 2.22 | 0.50 |
| 1:B:152:ILE:HD11 | 1:B:263:THR:HG22 | 1.92 | 0.50 |
| 1:B:348:LYS:NZ | 1:B:443:ASP:OD1 | 2.45 | 0.50 |
| 1:C:882:LEU:HD12 | 1:C:1176:HIS:NE2 | 2.25 | 0.50 |
| 1:D:348:LYS:NZ | 1:D:443:ASP:OD1 | 2.45 | 0.50 |
| 1:D:265:ARG:NH1 | 1:D:371:SER:OG | 2.37 | 0.50 |
| 1:E:463:GLN:OE1 | 1:E:466:ARG:NH2 | 2.28 | 0.50 |
| 1:F:562:ASN:HB2 | 1:F:565:GLN:HG2 | 1.93 | 0.50 |
| 1:F:819:ASN:ND2 | 1:F:840:HIS:O | 2.45 | 0.50 |
| 1:G:646:THR:HG23 | 1:G:648:GLU:HG3 | 1.94 | 0.50 |
| 1:A:700:GLU:HG3 | 1:A:721:SER:HB2 | 1.94 | 0.50 |
| 1:A:819:ASN:ND2 | 1:A:840:HIS:O | 2.45 | 0.50 |
| 1:C:631:ALA:HB1 | 1:C:639:LEU:HD11 | 1.91 | 0.50 |
| 1:C:700:GLU:HG3 | 1:C:721:SER:HB2 | 1.94 | 0.50 |
| 1:D:692:VAL:HG12 | 1:D:693:HIS:ND1 | 2.26 | 0.50 |
| 1:F:862:TYR:OH | 1:F:1237:ASN:O | 2.30 | 0.50 |
| 3:R:32:ARG:HD2 | 3:R:76:CYS:SG | 2.51 | 0.50 |
| 1:C:152:ILE:HD11 | 1:C:263:THR:HG22 | 1.92 | 0.50 |
| 1:C:825:ASP:HB2 | 1:C:832:LEU:HD22 | 1.93 | 0.50 |
| 1:D:1222:LYS:HB3 | 1:D:1224:HIS:HE1 | 1.77 | 0.50 |
| 1:E:1002:HIS:ND1 | 1:E:1024:ASP:OD2 | 2.44 | 0.50 |
| 1:F:400:LEU:HB3 | 1:F:404:TRP:CZ3 | 2.46 | 0.50 |
| 1:D:1086:GLY:HA2 | 2:K:39:LYS:HE2 | 1.92 | 0.50 |
| 1:A:298:PHE:HD2 | 1:A:328:GLY:HA3 | 1.77 | 0.50 |
| 1:A:562:ASN:HB2 | 1:A:565:GLN:HG2 | 1.93 | 0.50 |
| 1:B:825:ASP:HB2 | 1:B:832:LEU:HD22 | 1.93 | 0.50 |
| 1:C:608:ARG:HD2 | 1:C:910:GLU:HB2 | 1.94 | 0.50 |
| 1:C:819:ASN:ND2 | 1:C:840:HIS:O | 2.45 | 0.50 |
| 1:C:358:SER:HB3 | 1:D:274:MET:HE2 | 1.93 | 0.50 |
| 1:D:819:ASN:ND2 | 1:D:840:HIS:O | 2.45 | 0.50 |
| 1:E:348:LYS:NZ | 1:E:443:ASP:OD1 | 2.45 | 0.50 |
| 1:E:862:TYR:OH | 1:E:1237:ASN:O | 2.30 | 0.50 |
| 1:G:348:LYS:NZ | 1:G:443:ASP:OD1 | 2.45 | 0.50 |
| 1:A:1222:LYS:HB3 | 1:A:1224:HIS:HE1 | 1.77 | 0.49 |
| 1:A:365:ASP:OD1 | 1:A:444:PHE:HE1 | 1.95 | 0.49 |
| 1:A:646:THR:HG23 | 1:A:648:GLU:HG3 | 1.94 | 0.49 |
| 1:B:819:ASN:ND2 | 1:B:840:HIS:O | 2.45 | 0.49 |
| 1:D:152:ILE:HD11 | 1:D:263:THR:HG22 | 1.92 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:365:ASP:OD1 | 1:D:444:PHE:HE1 | 1.95 | 0.49 |
| 1:F:646:THR:HG23 | 1:F:648:GLU:HG3 | 1.94 | 0.49 |
| 1:G:862:TYR:OH | 1:G:1237:ASN:O | 2.30 | 0.49 |
| 1:G:298:PHE:HD2 | 1:G:328:GLY:HA3 | 1.77 | 0.49 |
| 1:G:862:TYR:HB3 | 1:G:884:TRP:CA | 2.42 | 0.49 |
| 2:I:41:GLY:HA2 | 2:I:48:TYR:CE1 | 2.47 | 0.49 |
| 2:J:41:GLY:HA2 | 2:J:48:TYR:CE1 | 2.47 | 0.49 |
| 3:Q:16:LEU:O | 3:Q:20:LEU:HB2 | 2.12 | 0.49 |
| 1:B:1222:LYS:HB3 | 1:B:1224:HIS:HE1 | 1.77 | 0.49 |
| 1:E:819:ASN:ND2 | 1:E:840:HIS:O | 2.45 | 0.49 |
| 1:E:884:TRP:CE3 | 2:L:81:ILE:HD11 | 2.48 | 0.49 |
| 1:F:1222:LYS:HB3 | 1:F:1224:HIS:HE1 | 1.77 | 0.49 |
| 1:F:298:PHE:HD2 | 1:F:328:GLY:HA3 | 1.77 | 0.49 |
| 1:F:463:GLN:OE1 | 1:F:466:ARG:NH2 | 2.28 | 0.49 |
| 1:G:562:ASN:HB2 | 1:G:565:GLN:HG2 | 1.94 | 0.49 |
| 1:A:1086:GLY:HA2 | 2:H:39:LYS:HE2 | 1.92 | 0.49 |
| 2:H:41:GLY:HA2 | 2:H:48:TYR:CE1 | 2.47 | 0.49 |
| 1:E:1086:GLY:CA | 2:L:39:LYS:HZ1 | 2.20 | 0.49 |
| 3:R:16:LEU:O | 3:R:20:LEU:HB2 | 2.12 | 0.49 |
| 1:C:365:ASP:OD1 | 1:C:444:PHE:HE1 | 1.96 | 0.49 |
| 1:C:862:TYR:HB3 | 1:C:884:TRP:CA | 2.42 | 0.49 |
| 1:D:762:SER:OG | 1:D:764:ASP:OD1 | 2.26 | 0.49 |
| 1:F:600:LYS:HZ1 | 1:F:1213:PHE:HZ | 1.60 | 0.49 |
| 1:G:1020:SER:HB2 | 1:G:1028:GLN:HE21 | 1.77 | 0.49 |
| 2:J:94:LEU:HD21 | 5:J:500:HEC:HMB1 | 1.93 | 0.49 |
| 1:C:884:TRP:CE3 | 2:J:81:ILE:HD11 | 2.48 | 0.49 |
| 2:K:41:GLY:HA2 | 2:K:48:TYR:CE1 | 2.47 | 0.49 |
| 1:F:884:TRP:CE3 | 2:M:81:ILE:HD11 | 2.47 | 0.49 |
| 1:A:331:LEU:HD13 | 1:A:338:TRP:CH2 | 2.48 | 0.49 |
| 1:A:265:ARG:NH1 | 1:A:371:SER:OG | 2.37 | 0.49 |
| 1:C:1222:LYS:HB3 | 1:C:1224:HIS:HE1 | 1.77 | 0.49 |
| 1:D:825:ASP:HB2 | 1:D:832:LEU:HD22 | 1.93 | 0.49 |
| 1:E:152:ILE:HD11 | 1:E:263:THR:HG22 | 1.92 | 0.49 |
| 1:F:365:ASP:OD1 | 1:F:444:PHE:HE1 | 1.96 | 0.49 |
| 1:F:700:GLU:HG3 | 1:F:721:SER:HB2 | 1.94 | 0.49 |
| 2:N:41:GLY:HA2 | 2:N:48:TYR:CE1 | 2.47 | 0.49 |
| 3:Q:32:ARG:HD2 | 3:Q:76:CYS:SG | 2.52 | 0.49 |
| 1:A:825:ASP:HB2 | 1:A:832:LEU:HD22 | 1.93 | 0.49 |
| 1:B:298:PHE:HD2 | 1:B:328:GLY:HA3 | 1.77 | 0.49 |
| 1:B:885:VAL:HG12 | 1:B:887:GLY:N | 2.28 | 0.49 |
| 1:D:862:TYR:OH | 1:D:1237:ASN:O | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:646:THR:HG23 | 1:D:648:GLU:HG3 | 1.94 | 0.49 |
| 1:D:700:GLU:HG3 | 1:D:721:SER:HB2 | 1.94 | 0.49 |
| 1:E:700:GLU:HG3 | 1:E:721:SER:HB2 | 1.94 | 0.49 |
| 1:B:1086:GLY:HA2 | 2:I:39:LYS:HE2 | 1.92 | 0.49 |
| 2:I:40:THR:HG22 | 2:I:59:TRP:CE2 | 2.48 | 0.49 |
| 1:D:884:TRP:CE3 | 2:K:81:ILE:HD11 | 2.47 | 0.49 |
| 1:B:118:GLY:O | 1:B:184:TRP:HB2 | 2.13 | 0.49 |
| 1:B:862:TYR:HB3 | 1:B:884:TRP:CA | 2.42 | 0.49 |
| 1:D:334:PHE:HE1 | 1:E:416:GLN:HE21 | 1.60 | 0.49 |
| 1:E:590:ASN:C | 1:E:592:MET:N | 2.64 | 0.49 |
| 1:E:885:VAL:HG12 | 1:E:887:GLY:N | 2.28 | 0.49 |
| 1:F:118:GLY:O | 1:F:184:TRP:HB2 | 2.13 | 0.49 |
| 1:F:348:LYS:NZ | 1:F:443:ASP:OD1 | 2.45 | 0.49 |
| 1:F:825:ASP:HB2 | 1:F:832:LEU:HD22 | 1.93 | 0.49 |
| 1:G:608:ARG:HD2 | 1:G:910:GLU:HB2 | 1.94 | 0.49 |
| 1:D:31:SER:HA | 3:Q:11:ARG:HA | 1.95 | 0.49 |
| 1:A:862:TYR:HB3 | 1:A:884:TRP:CA | 2.42 | 0.49 |
| 1:B:334:PHE:HE1 | 1:C:416:GLN:HE21 | 1.60 | 0.49 |
| 1:D:118:GLY:O | 1:D:184:TRP:HB2 | 2.13 | 0.49 |
| 1:D:565:GLN:NE2 | 1:D:1213:PHE:HA | 2.28 | 0.49 |
| 1:E:365:ASP:OD1 | 1:E:444:PHE:HE1 | 1.95 | 0.49 |
| 1:E:265:ARG:NH1 | 1:E:371:SER:OG | 2.37 | 0.49 |
| 1:F:608:ARG:HD2 | 1:F:910:GLU:HB2 | 1.94 | 0.49 |
| 1:G:1222:LYS:HB3 | 1:G:1224:HIS:HE1 | 1.76 | 0.49 |
| 1:G:825:ASP:HB2 | 1:G:832:LEU:HD22 | 1.93 | 0.49 |
| 1:B:884:TRP:CE3 | 2:I:81:ILE:HD11 | 2.48 | 0.49 |
| 1:E:844:GLN:NE2 | 2:L:79:LYS:NZ | 2.57 | 0.49 |
| 1:A:862:TYR:OH | 1:A:1237:ASN:O | 2.30 | 0.49 |
| 1:C:1020:SER:HB2 | 1:C:1028:GLN:HE21 | 1.77 | 0.49 |
| 1:C:118:GLY:O | 1:C:184:TRP:HB2 | 2.13 | 0.49 |
| 1:C:885:VAL:HG12 | 1:C:887:GLY:N | 2.28 | 0.49 |
| 1:D:1020:SER:HB2 | 1:D:1028:GLN:HE21 | 1.77 | 0.49 |
| 1:E:331:LEU:HD13 | 1:E:338:TRP:CH2 | 2.48 | 0.49 |
| 1:E:825:ASP:HB2 | 1:E:832:LEU:HD22 | 1.93 | 0.49 |
| 2:L:41:GLY:HA2 | 2:L:48:TYR:CE1 | 2.47 | 0.49 |
| 2:M:40:THR:HG22 | 2:M:59:TRP:CE2 | 2.48 | 0.49 |
| 3:O:16:LEU:O | 3:O:20:LEU:HB2 | 2.12 | 0.49 |
| 1:B:365:ASP:OD1 | 1:B:444:PHE:HE1 | 1.96 | 0.49 |
| 1:B:929:VAL:HB | 1:B:936:MET:HB2 | 1.95 | 0.49 |
| 1:D:569:CYS:CB | 1:D:600:LYS:HZ3 | 2.25 | 0.49 |
| 1:D:862:TYR:HB3 | 1:D:884:TRP:CA | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:298:PHE:HD2 | 1:E:328:GLY:HA3 | 1.77 | 0.49 |
| 1:E:608:ARG:HD2 | 1:E:910:GLU:HB2 | 1.94 | 0.49 |
| 1:F:565:GLN:NE2 | 1:F:1213:PHE:HA | 2.28 | 0.49 |
| 1:F:331:LEU:HD13 | 1:F:338:TRP:CH2 | 2.47 | 0.49 |
| 2:H:40:THR:HG22 | 2:H:59:TRP:CE2 | 2.48 | 0.49 |
| 2:J:40:THR:HG22 | 2:J:59:TRP:CE2 | 2.48 | 0.49 |
| 2:K:94:LEU:HD21 | 5:K:500:HEC:HMB1 | 1.93 | 0.49 |
| 2:L:40:THR:HG22 | 2:L:59:TRP:CE2 | 2.48 | 0.49 |
| 1:A:885:VAL:HG12 | 1:A:887:GLY:N | 2.28 | 0.49 |
| 1:B:1203:ASN:OD1 | 1:B:1204:VAL:N | 2.46 | 0.49 |
| 1:B:265:ARG:NH1 | 1:B:371:SER:OG | 2.37 | 0.49 |
| 1:C:331:LEU:HD13 | 1:C:338:TRP:CH2 | 2.47 | 0.49 |
| 1:C:646:THR:HG23 | 1:C:648:GLU:HG3 | 1.94 | 0.49 |
| 1:F:1086:GLY:HA2 | 2:M:39:LYS:HE2 | 1.92 | 0.49 |
| 1:G:700:GLU:HG3 | 1:G:721:SER:HB2 | 1.94 | 0.49 |
| 1:B:646:THR:HG23 | 1:B:648:GLU:HG3 | 1.94 | 0.48 |
| 1:C:565:GLN:NE2 | 1:C:1213:PHE:HA | 2.28 | 0.48 |
| 1:D:1026:GLU:HG3 | 1:D:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:D:1203:ASN:OD1 | 1:D:1204:VAL:N | 2.46 | 0.48 |
| 1:D:608:ARG:HD2 | 1:D:910:GLU:HB2 | 1.94 | 0.48 |
| 1:E:1203:ASN:OD1 | 1:E:1204:VAL:N | 2.46 | 0.48 |
| 1:E:646:THR:HG23 | 1:E:648:GLU:HG3 | 1.94 | 0.48 |
| 1:G:118:GLY:O | 1:G:184:TRP:HB2 | 2.13 | 0.48 |
| 1:G:565:GLN:NE2 | 1:G:1213:PHE:HA | 2.28 | 0.48 |
| 1:G:884:TRP:CE3 | 2:N:81:ILE:HD11 | 2.47 | 0.48 |
| 1:A:565:GLN:NE2 | 1:A:1213:PHE:HA | 2.28 | 0.48 |
| 1:A:884:TRP:CE3 | 2:H:81:ILE:HD11 | 2.47 | 0.48 |
| 1:B:565:GLN:NE2 | 1:B:1213:PHE:HA | 2.28 | 0.48 |
| 1:B:862:TYR:OH | 1:B:1237:ASN:O | 2.30 | 0.48 |
| 1:D:113:VAL:HG11 | 1:D:174:LEU:HD21 | 1.95 | 0.48 |
| 1:D:885:VAL:HG12 | 1:D:887:GLY:N | 2.28 | 0.48 |
| 1:E:1026:GLU:HG3 | 1:E:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:E:1222:LYS:HB3 | 1:E:1224:HIS:HE1 | 1.77 | 0.48 |
| 1:E:265:ARG:HH11 | 1:E:371:SER:HG | 1.58 | 0.48 |
| 1:E:568:LEU:HD13 | 1:E:595:LEU:O | 2.13 | 0.48 |
| 1:F:752:SER:HB2 | 1:F:753:PRO:HD2 | 1.95 | 0.48 |
| 1:G:1026:GLU:HG3 | 1:G:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:G:1203:ASN:OD1 | 1:G:1204:VAL:N | 2.46 | 0.48 |
| 2:K:40:THR:HG22 | 2:K:59:TRP:CE2 | 2.48 | 0.48 |
| 2:M:41:GLY:HA2 | 2:M:48:TYR:CE1 | 2.47 | 0.48 |
| 3:P:16:LEU:O | 3:P:20:LEU:HB2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:118:GLY:O | 1:A:184:TRP:HB2 | 2.13 | 0.48 |
| 1:A:568:LEU:HD13 | 1:A:595:LEU:O | 2.13 | 0.48 |
| 1:A:929:VAL:HB | 1:A:936:MET:HB2 | 1.95 | 0.48 |
| 1:E:1020:SER:HB2 | 1:E:1028:GLN:HE21 | 1.77 | 0.48 |
| 1:E:113:VAL:HG11 | 1:E:174:LEU:HD21 | 1.95 | 0.48 |
| 1:F:885:VAL:HG12 | 1:F:887:GLY:N | 2.28 | 0.48 |
| 1:G:752:SER:HB2 | 1:G:753:PRO:HD2 | 1.95 | 0.48 |
| 1:A:1026:GLU:HG3 | 1:A:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:A:196:LEU:HG | 1:A:200:GLN:HE22 | 1.78 | 0.48 |
| 1:B:1198:TYR:HA | 1:B:1215:THR:HB | 1.96 | 0.48 |
| 1:D:568:LEU:HD13 | 1:D:595:LEU:O | 2.13 | 0.48 |
| 1:E:565:GLN:NE2 | 1:E:1213:PHE:HA | 2.28 | 0.48 |
| 1:E:230:LEU:O | 1:E:234:LYS:N | 2.41 | 0.48 |
| 1:F:1026:GLU:HG3 | 1:F:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:F:344:GLN:OE1 | 1:F:349:GLN:NE2 | 2.44 | 0.48 |
| 1:G:550:LEU:HD23 | 1:G:607:SER:HB2 | 1.91 | 0.48 |
| 1:B:1191:MET:SD | 1:B:1209:SER:OG | 2.63 | 0.48 |
| 1:B:331:LEU:HD13 | 1:B:338:TRP:CH2 | 2.48 | 0.48 |
| 1:C:1026:GLU:HG3 | 1:C:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:C:1198:TYR:HA | 1:C:1215:THR:HB | 1.96 | 0.48 |
| 1:C:862:TYR:OH | 1:C:1237:ASN:O | 2.30 | 0.48 |
| 1:C:113:VAL:HG11 | 1:C:174:LEU:HD21 | 1.95 | 0.48 |
| 1:C:929:VAL:HB | 1:C:936:MET:HB2 | 1.95 | 0.48 |
| 1:D:1198:TYR:HA | 1:D:1215:THR:HB | 1.96 | 0.48 |
| 1:G:331:LEU:HD13 | 1:G:338:TRP:CH2 | 2.48 | 0.48 |
| 1:G:885:VAL:HG12 | 1:G:887:GLY:N | 2.28 | 0.48 |
| 2:N:40:THR:HG22 | 2:N:59:TRP:CE2 | 2.48 | 0.48 |
| 1:B:1020:SER:HB2 | 1:B:1028:GLN:HE21 | 1.77 | 0.48 |
| 1:C:298:PHE:HD2 | 1:C:328:GLY:HA3 | 1.77 | 0.48 |
| 1:D:298:PHE:HD2 | 1:D:328:GLY:HA3 | 1.77 | 0.48 |
| 1:F:196:LEU:HG | 1:F:200:GLN:HE22 | 1.78 | 0.48 |
| 1:A:1203:ASN:OD1 | 1:A:1204:VAL:N | 2.46 | 0.48 |
| 1:A:113:VAL:HG11 | 1:A:174:LEU:HD21 | 1.95 | 0.48 |
| 1:B:113:VAL:HG11 | 1:B:174:LEU:HD21 | 1.95 | 0.48 |
| 1:B:752:SER:HB2 | 1:B:753:PRO:HD2 | 1.95 | 0.48 |
| 1:D:331:LEU:HD13 | 1:D:338:TRP:CH2 | 2.48 | 0.48 |
| 1:D:752:SER:HB2 | 1:D:753:PRO:HD2 | 1.95 | 0.48 |
| 1:E:1198:TYR:HA | 1:E:1215:THR:HB | 1.96 | 0.48 |
| 1:F:1203:ASN:OD1 | 1:F:1204:VAL:N | 2.46 | 0.48 |
| 1:C:170:ASP:OD2 | 1:C:172:SER:OG | 2.32 | 0.48 |
| 1:D:326:LEU:HD23 | 1:D:326:LEU:HA | 1.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:497:HIS:HA | 1:E:500:LEU:HB3 | 1.96 | 0.48 |
| 1:F:1020:SER:HB2 | 1:F:1028:GLN:HE21 | 1.77 | 0.48 |
| 1:F:113:VAL:HG11 | 1:F:174:LEU:HD21 | 1.95 | 0.48 |
| 1:F:497:HIS:HA | 1:F:500:LEU:HB3 | 1.96 | 0.48 |
| 1:G:541:SER:O | 1:G:545:GLN:HG3 | 2.14 | 0.48 |
| 1:G:929:VAL:HB | 1:G:936:MET:HB2 | 1.95 | 0.48 |
| 1:A:1198:TYR:HA | 1:A:1215:THR:HB | 1.96 | 0.48 |
| 1:B:1026:GLU:HG3 | 1:B:1041:ARG:HG2 | 1.95 | 0.48 |
| 1:B:497:HIS:HA | 1:B:500:LEU:HB3 | 1.95 | 0.48 |
| 1:B:882:LEU:HD12 | 1:B:1176:HIS:NE2 | 2.25 | 0.48 |
| 1:C:158:CYS:SG | 1:C:159:GLY:N | 2.87 | 0.48 |
| 1:D:14:GLU:OE1 | 1:E:31:SER:CB | 2.62 | 0.48 |
| 1:D:929:VAL:HB | 1:D:936:MET:HB2 | 1.95 | 0.48 |
| 1:E:170:ASP:OD2 | 1:E:172:SER:OG | 2.32 | 0.48 |
| 1:E:118:GLY:O | 1:E:184:TRP:HB2 | 2.13 | 0.48 |
| 1:G:113:VAL:HG11 | 1:G:174:LEU:HD21 | 1.95 | 0.48 |
| 1:G:196:LEU:HG | 1:G:200:GLN:HE22 | 1.78 | 0.48 |
| 1:G:568:LEU:HD13 | 1:G:595:LEU:O | 2.13 | 0.48 |
| 1:G:762:SER:OG | 1:G:764:ASP:OD1 | 2.26 | 0.48 |
| 1:A:330:LEU:HD13 | 1:A:341:TYR:OH | 2.14 | 0.48 |
| 1:B:196:LEU:HG | 1:B:200:GLN:HE22 | 1.78 | 0.48 |
| 1:C:541:SER:O | 1:C:545:GLN:HG3 | 2.14 | 0.48 |
| 1:C:568:LEU:HD13 | 1:C:595:LEU:O | 2.13 | 0.48 |
| 1:C:590:ASN:C | 1:C:592:MET:N | 2.64 | 0.48 |
| 1:D:541:SER:O | 1:D:545:GLN:HG3 | 2.14 | 0.48 |
| 1:D:550:LEU:HD23 | 1:D:607:SER:HB2 | 1.91 | 0.48 |
| 1:E:158:CYS:SG | 1:E:159:GLY:N | 2.87 | 0.48 |
| 1:E:196:LEU:HG | 1:E:200:GLN:HE22 | 1.78 | 0.48 |
| 1:E:929:VAL:HB | 1:E:936:MET:HB2 | 1.95 | 0.48 |
| 1:F:158:CYS:SG | 1:F:159:GLY:N | 2.87 | 0.48 |
| 1:F:568:LEU:HD13 | 1:F:595:LEU:O | 2.13 | 0.48 |
| 1:F:550:LEU:HD23 | 1:F:607:SER:HB2 | 1.91 | 0.48 |
| 1:B:569:CYS:HB3 | 1:B:600:LYS:HZ3 | 1.79 | 0.47 |
| 1:D:330:LEU:HD13 | 1:D:341:TYR:OH | 2.14 | 0.47 |
| 1:E:752:SER:HB2 | 1:E:753:PRO:HD2 | 1.95 | 0.47 |
| 1:G:365:ASP:OD1 | 1:G:444:PHE:HE1 | 1.95 | 0.47 |
| 1:A:344:GLN:OE1 | 1:A:349:GLN:NE2 | 2.44 | 0.47 |
| 1:A:752:SER:HB2 | 1:A:753:PRO:HD2 | 1.95 | 0.47 |
| 1:B:568:LEU:HD13 | 1:B:595:LEU:O | 2.13 | 0.47 |
| 1:C:330:LEU:HD13 | 1:C:341:TYR:OH | 2.14 | 0.47 |
| 1:C:600:LYS:HZ1 | 1:C:1213:PHE:HZ | 1.62 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1020:SER:HB2 | 1:A:1028:GLN:HE21 | 1.77 | 0.47 |
| 1:A:348:LYS:NZ | 1:A:443:ASP:OD1 | 2.45 | 0.47 |
| 1:A:541:SER:O | 1:A:545:GLN:HG3 | 2.14 | 0.47 |
| 1:C:1203:ASN:OD1 | 1:C:1204:VAL:N | 2.46 | 0.47 |
| 1:C:497:HIS:HA | 1:C:500:LEU:HB3 | 1.96 | 0.47 |
| 1:D:344:GLN:OE1 | 1:D:349:GLN:NE2 | 2.44 | 0.47 |
| 1:F:1198:TYR:HA | 1:F:1215:THR:HB | 1.96 | 0.47 |
| 1:F:330:LEU:HD13 | 1:F:341:TYR:OH | 2.14 | 0.47 |
| 1:F:844:GLN:HE22 | 2:M:79:LYS:HZ2 | 1.61 | 0.47 |
| 1:B:821:ILE:HB | 1:B:835:ILE:HB | 1.97 | 0.47 |
| 1:C:344:GLN:OE1 | 1:C:349:GLN:NE2 | 2.44 | 0.47 |
| 1:D:196:LEU:HG | 1:D:200:GLN:HE22 | 1.78 | 0.47 |
| 1:E:1131:ARG:H | 1:E:1146:ASP:HA | 1.80 | 0.47 |
| 1:G:158:CYS:SG | 1:G:159:GLY:N | 2.87 | 0.47 |
| 1:A:109:TYR:CE1 | 1:G:4:LYS:CD | 2.58 | 0.47 |
| 1:A:106:ILE:HA | 1:A:110:VAL:HG21 | 1.97 | 0.47 |
| 1:B:170:ASP:OD2 | 1:B:172:SER:OG | 2.32 | 0.47 |
| 1:C:752:SER:HB2 | 1:C:753:PRO:HD2 | 1.95 | 0.47 |
| 1:C:821:ILE:HB | 1:C:835:ILE:HB | 1.97 | 0.47 |
| 1:E:330:LEU:HD13 | 1:E:341:TYR:OH | 2.14 | 0.47 |
| 1:F:541:SER:O | 1:F:545:GLN:HG3 | 2.14 | 0.47 |
| 1:B:230:LEU:O | 1:B:234:LYS:N | 2.41 | 0.47 |
| 1:C:1131:ARG:H | 1:C:1146:ASP:HA | 1.80 | 0.47 |
| 1:E:160:LYS:HB3 | 4:E:1301:DTP:O1B | 2.15 | 0.47 |
| 1:D:14:GLU:HB2 | 1:E:31:SER:HG | 1.80 | 0.47 |
| 1:G:600:LYS:HZ1 | 1:G:1213:PHE:HZ | 1.63 | 0.47 |
| 2:K:39:LYS:HB2 | 2:K:42:GLN:HG3 | 1.97 | 0.47 |
| 2:L:39:LYS:HB2 | 2:L:42:GLN:HG3 | 1.97 | 0.47 |
| 1:B:1221:LYS:HE3 | 1:B:1222:LYS:HE3 | 1.97 | 0.47 |
| 1:B:330:LEU:HD13 | 1:B:341:TYR:OH | 2.14 | 0.47 |
| 1:A:337:ARG:NH1 | 1:B:409:GLU:OE2 | 2.48 | 0.47 |
| 1:D:497:HIS:HA | 1:D:500:LEU:HB3 | 1.96 | 0.47 |
| 1:D:821:ILE:HB | 1:D:835:ILE:HB | 1.97 | 0.47 |
| 1:E:344:GLN:OE1 | 1:E:349:GLN:NE2 | 2.44 | 0.47 |
| 1:E:541:SER:O | 1:E:545:GLN:HG3 | 2.14 | 0.47 |
| 1:F:106:ILE:HA | 1:F:110:VAL:HG21 | 1.97 | 0.47 |
| 1:F:1131:ARG:H | 1:F:1146:ASP:HA | 1.80 | 0.47 |
| 1:G:497:HIS:HA | 1:G:500:LEU:HB3 | 1.96 | 0.47 |
| 1:A:600:LYS:HZ1 | 1:A:1213:PHE:HZ | 1.63 | 0.47 |
| 1:A:230:LEU:O | 1:A:234:LYS:N | 2.41 | 0.47 |
| 1:A:497:HIS:HA | 1:A:500:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:550:LEU:HD23 | 1:A:607:SER:HB2 | 1.91 | 0.47 |
| 1:B:158:CYS:SG | 1:B:159:GLY:N | 2.87 | 0.47 |
| 1:D:1131:ARG:H | 1:D:1146:ASP:HA | 1.80 | 0.47 |
| 1:F:160:LYS:HB3 | 4:F:1301:DTP:O1B | 2.15 | 0.47 |
| 1:G:106:ILE:HA | 1:G:110:VAL:HG21 | 1.97 | 0.47 |
| 1:G:1198:TYR:HA | 1:G:1215:THR:HB | 1.96 | 0.47 |
| 2:I:39:LYS:HB2 | 2:I:42:GLN:HG3 | 1.97 | 0.47 |
| 1:A:1221:LYS:HE3 | 1:A:1222:LYS:HE3 | 1.97 | 0.47 |
| 1:A:158:CYS:SG | 1:A:159:GLY:N | 2.87 | 0.47 |
| 1:A:170:ASP:OD2 | 1:A:172:SER:OG | 2.32 | 0.47 |
| 1:B:541:SER:O | 1:B:545:GLN:HG3 | 2.14 | 0.47 |
| 1:C:196:LEU:HG | 1:C:200:GLN:HE22 | 1.78 | 0.47 |
| 1:B:337:ARG:NH1 | 1:C:409:GLU:OE2 | 2.48 | 0.47 |
| 1:D:158:CYS:SG | 1:D:159:GLY:N | 2.87 | 0.47 |
| 1:G:170:ASP:OD2 | 1:G:172:SER:OG | 2.32 | 0.47 |
| 1:A:821:ILE:HB | 1:A:835:ILE:HB | 1.97 | 0.47 |
| 1:B:106:ILE:HA | 1:B:110:VAL:HG21 | 1.97 | 0.47 |
| 1:B:1222:LYS:HB3 | 1:B:1224:HIS:CE1 | 2.50 | 0.47 |
| 1:D:170:ASP:OD2 | 1:D:172:SER:OG | 2.32 | 0.47 |
| 1:D:230:LEU:O | 1:D:234:LYS:N | 2.41 | 0.47 |
| 1:E:266:ASP:CG | 1:E:268:SER:HG | 2.18 | 0.47 |
| 1:F:929:VAL:HB | 1:F:936:MET:HB2 | 1.95 | 0.47 |
| 1:A:1131:ARG:H | 1:A:1146:ASP:HA | 1.80 | 0.47 |
| 1:A:1222:LYS:HB3 | 1:A:1224:HIS:CE1 | 2.50 | 0.47 |
| 1:B:570:GLU:HB2 | 1:B:577:TYR:HB2 | 1.97 | 0.47 |
| 1:C:1222:LYS:HB3 | 1:C:1224:HIS:CE1 | 2.50 | 0.47 |
| 1:D:1222:LYS:HB3 | 1:D:1224:HIS:CE1 | 2.50 | 0.47 |
| 1:E:1222:LYS:HB3 | 1:E:1224:HIS:CE1 | 2.50 | 0.47 |
| 1:D:337:ARG:NH1 | 1:E:409:GLU:OE2 | 2.48 | 0.47 |
| 2:J:39:LYS:HB2 | 2:J:42:GLN:HG3 | 1.97 | 0.47 |
| 1:A:570:GLU:HB2 | 1:A:577:TYR:HB2 | 1.97 | 0.46 |
| 1:C:230:LEU:O | 1:C:234:LYS:N | 2.41 | 0.46 |
| 1:C:1221:LYS:HE3 | 1:C:1222:LYS:HE3 | 1.97 | 0.46 |
| 1:C:612:ARG:HG3 | 1:C:904:GLN:O | 2.16 | 0.46 |
| 1:D:160:LYS:HB3 | 4:D:1301:DTP:O1B | 2.15 | 0.46 |
| 1:E:152:ILE:HG22 | 1:E:280:VAL:HB | 1.97 | 0.46 |
| 1:G:330:LEU:HD13 | 1:G:341:TYR:OH | 2.14 | 0.46 |
| 2:H:39:LYS:HB2 | 2:H:42:GLN:HG3 | 1.97 | 0.46 |
| 1:B:160:LYS:HB3 | 4:B:1301:DTP:O1B | 2.15 | 0.46 |
| 1:C:337:ARG:NH1 | 1:D:409:GLU:OE2 | 2.49 | 0.46 |
| 1:E:1221:LYS:HE3 | 1:E:1222:LYS:HE3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:524:HIS:CB | 1:E:646:THR:HG21 | 2.36 | 0.46 |
| 1:E:612:ARG:HG3 | 1:E:904:GLN:O | 2.16 | 0.46 |
| 1:G:1222:LYS:HB3 | 1:G:1224:HIS:CE1 | 2.50 | 0.46 |
| 2:I:70:ASN:HD22 | 2:I:73:LYS:HB2 | 1.81 | 0.46 |
| 2:M:39:LYS:HB2 | 2:M:42:GLN:HG3 | 1.97 | 0.46 |
| 1:A:160:LYS:HB3 | 4:A:1301:DTP:O1B | 2.15 | 0.46 |
| 1:B:862:TYR:HB3 | 1:B:884:TRP:N | 2.31 | 0.46 |
| 1:E:106:ILE:HA | 1:E:110:VAL:HG21 | 1.97 | 0.46 |
| 1:E:862:TYR:HB3 | 1:E:884:TRP:N | 2.31 | 0.46 |
| 1:F:152:ILE:HG22 | 1:F:280:VAL:HB | 1.97 | 0.46 |
| 1:G:1131:ARG:H | 1:G:1146:ASP:HA | 1.80 | 0.46 |
| 2:L:70:ASN:HD22 | 2:L:73:LYS:HB2 | 1.81 | 0.46 |
| 1:A:472:THR:O | 1:A:473:LEU:HD12 | 2.16 | 0.46 |
| 1:A:888:VAL:HG12 | 1:A:899:THR:HA | 1.98 | 0.46 |
| 1:C:524:HIS:CB | 1:C:646:THR:HG21 | 2.36 | 0.46 |
| 1:D:152:ILE:HG22 | 1:D:280:VAL:HB | 1.97 | 0.46 |
| 1:D:862:TYR:HB3 | 1:D:884:TRP:N | 2.31 | 0.46 |
| 1:E:472:THR:O | 1:E:473:LEU:HD12 | 2.16 | 0.46 |
| 1:E:821:ILE:HB | 1:E:835:ILE:HB | 1.97 | 0.46 |
| 1:E:337:ARG:NH1 | 1:F:409:GLU:OE2 | 2.48 | 0.46 |
| 1:G:160:LYS:HB3 | 4:G:1301:DTP:O1B | 2.15 | 0.46 |
| 1:C:950:ASN:OD1 | 1:C:951:GLY:N | 2.49 | 0.46 |
| 1:D:265:ARG:HH11 | 1:D:371:SER:HG | 1.57 | 0.46 |
| 1:D:950:ASN:OD1 | 1:D:951:GLY:N | 2.49 | 0.46 |
| 1:G:821:ILE:HB | 1:G:835:ILE:HB | 1.97 | 0.46 |
| 1:G:888:VAL:HG12 | 1:G:899:THR:HA | 1.98 | 0.46 |
| 2:H:10:PHE:HA | 2:H:14:CYS:HB2 | 1.98 | 0.46 |
| 1:C:570:GLU:HB2 | 1:C:577:TYR:HB2 | 1.97 | 0.46 |
| 1:C:862:TYR:HB3 | 1:C:884:TRP:N | 2.31 | 0.46 |
| 1:F:1221:LYS:HE3 | 1:F:1222:LYS:HE3 | 1.97 | 0.46 |
| 1:F:170:ASP:OD2 | 1:F:172:SER:OG | 2.32 | 0.46 |
| 1:G:1011:PHE:HE1 | 1:G:1018:LEU:HD13 | 1.81 | 0.46 |
| 1:G:152:ILE:HG22 | 1:G:280:VAL:HB | 1.97 | 0.46 |
| 2:N:39:LYS:HB2 | 2:N:42:GLN:HG3 | 1.97 | 0.46 |
| 1:A:1011:PHE:HE1 | 1:A:1018:LEU:HD13 | 1.81 | 0.46 |
| 1:A:643:LYS:HD3 | 1:A:646:THR:HG22 | 1.98 | 0.46 |
| 1:B:888:VAL:HG12 | 1:B:899:THR:HA | 1.98 | 0.46 |
| 1:B:950:ASN:OD1 | 1:B:951:GLY:N | 2.49 | 0.46 |
| 1:D:1011:PHE:HE1 | 1:D:1018:LEU:HD13 | 1.81 | 0.46 |
| 1:G:1191:MET:SD | 1:G:1209:SER:OG | 2.63 | 0.46 |
| 1:B:472:THR:O | 1:B:473:LEU:HD12 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:643:LYS:HD3 | 1:B:646:THR:HG22 | 1.98 | 0.46 |
| 1:D:106:ILE:HA | 1:D:110:VAL:HG21 | 1.97 | 0.46 |
| 1:E:950:ASN:OD1 | 1:E:951:GLY:N | 2.49 | 0.46 |
| 1:F:1222:LYS:HB3 | 1:F:1224:HIS:CE1 | 2.50 | 0.46 |
| 1:F:570:GLU:HB2 | 1:F:577:TYR:HB2 | 1.97 | 0.46 |
| 1:F:821:ILE:HB | 1:F:835:ILE:HB | 1.97 | 0.46 |
| 1:G:570:GLU:HB2 | 1:G:577:TYR:HB2 | 1.97 | 0.46 |
| 1:G:862:TYR:HB3 | 1:G:884:TRP:N | 2.31 | 0.46 |
| 2:M:10:PHE:HA | 2:M:14:CYS:HB2 | 1.98 | 0.46 |
| 2:M:70:ASN:HD22 | 2:M:73:LYS:HB2 | 1.81 | 0.46 |
| 2:N:10:PHE:HA | 2:N:14:CYS:HB2 | 1.98 | 0.46 |
| 3:R:90:ARG:NH2 | 3:R:90:ARG:HG2 | 2.31 | 0.46 |
| 1:A:612:ARG:HG3 | 1:A:904:GLN:O | 2.16 | 0.46 |
| 1:B:152:ILE:HG22 | 1:B:280:VAL:HB | 1.97 | 0.46 |
| 1:F:1215:THR:HG21 | 1:F:1220:LEU:HD21 | 1.98 | 0.46 |
| 1:F:950:ASN:OD1 | 1:F:951:GLY:N | 2.49 | 0.46 |
| 1:G:1215:THR:HG21 | 1:G:1220:LEU:HD21 | 1.98 | 0.46 |
| 2:H:70:ASN:HD22 | 2:H:73:LYS:HB2 | 1.81 | 0.46 |
| 1:A:1215:THR:HG21 | 1:A:1220:LEU:HD21 | 1.98 | 0.45 |
| 1:A:950:ASN:OD1 | 1:A:951:GLY:N | 2.49 | 0.45 |
| 1:B:1215:THR:HG21 | 1:B:1220:LEU:HD21 | 1.99 | 0.45 |
| 1:C:1215:THR:HG21 | 1:C:1220:LEU:HD21 | 1.98 | 0.45 |
| 1:C:160:LYS:HB3 | 4:C:1301:DTP:O1B | 2.15 | 0.45 |
| 1:C:472:THR:O | 1:C:473:LEU:HD12 | 2.16 | 0.45 |
| 1:D:1221:LYS:HE3 | 1:D:1222:LYS:HE3 | 1.97 | 0.45 |
| 1:E:1011:PHE:HE1 | 1:E:1018:LEU:HD13 | 1.81 | 0.45 |
| 1:E:550:LEU:HD23 | 1:E:607:SER:HB2 | 1.91 | 0.45 |
| 1:F:862:TYR:HB3 | 1:F:884:TRP:N | 2.31 | 0.45 |
| 1:G:472:THR:O | 1:G:473:LEU:HD12 | 2.16 | 0.45 |
| 1:C:1011:PHE:HE1 | 1:C:1018:LEU:HD13 | 1.81 | 0.45 |
| 1:C:106:ILE:HA | 1:C:110:VAL:HG21 | 1.97 | 0.45 |
| 1:C:844:GLN:HE22 | 2:J:79:LYS:HZ2 | 1.62 | 0.45 |
| 1:D:472:THR:O | 1:D:473:LEU:HD12 | 2.16 | 0.45 |
| 1:D:570:GLU:HB2 | 1:D:577:TYR:HB2 | 1.97 | 0.45 |
| 1:G:1221:LYS:HE3 | 1:G:1222:LYS:HE3 | 1.97 | 0.45 |
| 2:J:68:LEU:HB3 | 2:J:85:ILE:HD12 | 1.98 | 0.45 |
| 2:K:68:LEU:HB3 | 2:K:85:ILE:HD12 | 1.98 | 0.45 |
| 3:O:90:ARG:NH2 | 3:O:90:ARG:HG2 | 2.31 | 0.45 |
| 3:Q:90:ARG:HG2 | 3:Q:90:ARG:NH2 | 2.31 | 0.45 |
| 1:A:298:PHE:CD2 | 1:A:328:GLY:HA3 | 2.52 | 0.45 |
| 1:A:461:ILE:HD11 | 1:A:491:MET:HA | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:152:ILE:HG22 | 1:C:280:VAL:HB | 1.97 | 0.45 |
| 1:B:48:THR:CG2 | 1:D:45:ASN:OD1 | 2.64 | 0.45 |
| 1:F:1011:PHE:HE1 | 1:F:1018:LEU:HD13 | 1.81 | 0.45 |
| 2:I:10:PHE:HA | 2:I:14:CYS:HB2 | 1.98 | 0.45 |
| 1:A:862:TYR:HB3 | 1:A:884:TRP:N | 2.31 | 0.45 |
| 1:D:1215:THR:HG21 | 1:D:1220:LEU:HD21 | 1.98 | 0.45 |
| 1:E:1215:THR:HG21 | 1:E:1220:LEU:HD21 | 1.99 | 0.45 |
| 1:F:612:ARG:HG3 | 1:F:904:GLN:O | 2.16 | 0.45 |
| 1:G:612:ARG:HG3 | 1:G:904:GLN:O | 2.16 | 0.45 |
| 2:H:68:LEU:HB3 | 2:H:85:ILE:HD12 | 1.98 | 0.45 |
| 1:A:1150:GLU:HB2 | 1:A:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:B:461:ILE:HD11 | 1:B:491:MET:HA | 1.99 | 0.45 |
| 1:E:334:PHE:HE1 | 1:F:416:GLN:HE21 | 1.63 | 0.45 |
| 1:E:570:GLU:HB2 | 1:E:577:TYR:HB2 | 1.97 | 0.45 |
| 1:F:1150:GLU:HB2 | 1:F:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:F:472:THR:O | 1:F:473:LEU:HD12 | 2.16 | 0.45 |
| 1:G:1150:GLU:HB2 | 1:G:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:G:950:ASN:OD1 | 1:G:951:GLY:N | 2.49 | 0.45 |
| 2:J:70:ASN:HD22 | 2:J:73:LYS:HB2 | 1.81 | 0.45 |
| 2:L:10:PHE:HA | 2:L:14:CYS:HB2 | 1.98 | 0.45 |
| 1:A:152:ILE:HG22 | 1:A:280:VAL:HB | 1.97 | 0.45 |
| 1:B:1131:ARG:H | 1:B:1146:ASP:HA | 1.80 | 0.45 |
| 1:B:1150:GLU:HB2 | 1:B:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:C:1191:MET:SD | 1:C:1209:SER:OG | 2.63 | 0.45 |
| 1:C:643:LYS:HD3 | 1:C:646:THR:HG22 | 1.98 | 0.45 |
| 1:D:612:ARG:HG3 | 1:D:904:GLN:O | 2.16 | 0.45 |
| 1:F:461:ILE:HD11 | 1:F:491:MET:HA | 1.99 | 0.45 |
| 1:G:461:ILE:HD11 | 1:G:491:MET:HA | 1.99 | 0.45 |
| 1:B:298:PHE:CD2 | 1:B:328:GLY:HA3 | 2.52 | 0.45 |
| 1:B:821:ILE:HD11 | 1:B:857:VAL:HG21 | 1.99 | 0.45 |
| 1:B:612:ARG:HG3 | 1:B:904:GLN:O | 2.16 | 0.45 |
| 1:C:888:VAL:HG12 | 1:C:899:THR:HA | 1.98 | 0.45 |
| 1:E:821:ILE:HD11 | 1:E:857:VAL:HG21 | 1.99 | 0.45 |
| 1:F:888:VAL:HG12 | 1:F:899:THR:HA | 1.98 | 0.45 |
| 2:K:10:PHE:HA | 2:K:14:CYS:HB2 | 1.98 | 0.45 |
| 1:C:216:LEU:HA | 1:C:217:PRO:HD2 | 1.84 | 0.45 |
| 1:C:821:ILE:HD11 | 1:C:857:VAL:HG21 | 1.99 | 0.45 |
| 1:D:868:ASN:OD1 | 1:D:869:THR:N | 2.50 | 0.45 |
| 1:F:326:LEU:HA | 1:F:326:LEU:HD23 | 1.44 | 0.45 |
| 1:F:821:ILE:HD11 | 1:F:857:VAL:HG21 | 1.99 | 0.45 |
| 1:A:868:ASN:OD1 | 1:A:869:THR:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:868:ASN:OD1 | 1:B:869:THR:N | 2.50 | 0.45 |
| 1:E:1150:GLU:HB2 | 1:E:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:E:326:LEU:HD23 | 1:E:326:LEU:HA | 1.44 | 0.45 |
| 1:F:868:ASN:OD1 | 1:F:869:THR:N | 2.50 | 0.45 |
| 1:G:298:PHE:CD2 | 1:G:328:GLY:HA3 | 2.52 | 0.45 |
| 2:J:10:PHE:HA | 2:J:14:CYS:HB2 | 1.98 | 0.45 |
| 2:K:70:ASN:HD22 | 2:K:73:LYS:HB2 | 1.81 | 0.45 |
| 2:N:68:LEU:HB3 | 2:N:85:ILE:HD12 | 1.98 | 0.45 |
| 3:P:90:ARG:HG2 | 3:P:90:ARG:NH2 | 2.31 | 0.45 |
| 1:A:480:CYS:SG | 1:A:481:MET:N | 2.90 | 0.45 |
| 1:B:1011:PHE:HE1 | 1:B:1018:LEU:HD13 | 1.81 | 0.45 |
| 1:C:1150:GLU:HB2 | 1:C:1167:PRO:HG2 | 1.99 | 0.45 |
| 1:E:390:GLN:HB2 | 1:E:393:VAL:HG21 | 1.99 | 0.45 |
| 1:E:461:ILE:HD11 | 1:E:491:MET:HA | 1.99 | 0.45 |
| 1:F:762:SER:OG | 1:F:764:ASP:OD1 | 2.26 | 0.45 |
| 1:A:409:GLU:OE2 | 1:G:337:ARG:NH1 | 2.49 | 0.45 |
| 1:G:643:LYS:HD3 | 1:G:646:THR:HG22 | 1.98 | 0.45 |
| 1:G:868:ASN:OD1 | 1:G:869:THR:N | 2.50 | 0.45 |
| 2:N:70:ASN:HD22 | 2:N:73:LYS:HB2 | 1.81 | 0.45 |
| 1:B:600:LYS:HA | 1:B:603:ILE:HG13 | 2.00 | 0.44 |
| 1:D:821:ILE:HD11 | 1:D:857:VAL:HG21 | 1.99 | 0.44 |
| 1:E:643:LYS:HD3 | 1:E:646:THR:HG22 | 1.98 | 0.44 |
| 2:I:72:LYS:NZ | 2:I:78:THR:O | 2.51 | 0.44 |
| 3:Q:41:GLU:HA | 3:Q:44:GLN:HE21 | 1.83 | 0.44 |
| 1:A:821:ILE:HD11 | 1:A:857:VAL:HG21 | 1.99 | 0.44 |
| 1:C:868:ASN:OD1 | 1:C:869:THR:N | 2.50 | 0.44 |
| 1:D:1150:GLU:HB2 | 1:D:1167:PRO:HG2 | 1.99 | 0.44 |
| 1:D:357:SER:OG | 1:D:358:SER:N | 2.50 | 0.44 |
| 1:D:888:VAL:HG12 | 1:D:899:THR:HA | 1.98 | 0.44 |
| 1:E:480:CYS:SG | 1:E:481:MET:N | 2.90 | 0.44 |
| 1:F:230:LEU:O | 1:F:234:LYS:N | 2.41 | 0.44 |
| 1:F:643:LYS:HD3 | 1:F:646:THR:HG22 | 1.98 | 0.44 |
| 1:G:266:ASP:CG | 1:G:268:SER:HG | 2.19 | 0.44 |
| 2:L:68:LEU:HB3 | 2:L:85:ILE:HD12 | 1.98 | 0.44 |
| 1:G:1087:THR:N | 2:N:39:LYS:HZ3 | 2.15 | 0.44 |
| 3:O:45:ARG:HG2 | 3:O:45:ARG:O | 2.17 | 0.44 |
| 1:A:569:CYS:HB3 | 1:A:600:LYS:HZ3 | 1.82 | 0.44 |
| 1:B:357:SER:OG | 1:B:358:SER:N | 2.50 | 0.44 |
| 1:B:480:CYS:SG | 1:B:481:MET:N | 2.90 | 0.44 |
| 1:C:480:CYS:SG | 1:C:481:MET:N | 2.90 | 0.44 |
| 1:C:600:LYS:HA | 1:C:603:ILE:HG13 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:298:PHE:CD2 | 1:D:328:GLY:HA3 | 2.52 | 0.44 |
| 1:D:643:LYS:HD3 | 1:D:646:THR:HG22 | 1.98 | 0.44 |
| 1:E:888:VAL:HG12 | 1:E:899:THR:HA | 1.98 | 0.44 |
| 1:G:346:GLN:C | 1:G:348:LYS:N | 2.71 | 0.44 |
| 2:L:67:TYR:OH | 2:L:80:MET:SD | 2.57 | 0.44 |
| 2:M:68:LEU:HB3 | 2:M:85:ILE:HD12 | 1.98 | 0.44 |
| 2:M:72:LYS:NZ | 2:M:78:THR:O | 2.51 | 0.44 |
| 1:A:600:LYS:HA | 1:A:603:ILE:HG13 | 2.00 | 0.44 |
| 1:C:461:ILE:HD11 | 1:C:491:MET:HA | 1.99 | 0.44 |
| 1:D:342:LEU:O | 1:D:346:GLN:CG | 2.66 | 0.44 |
| 1:D:480:CYS:SG | 1:D:481:MET:N | 2.90 | 0.44 |
| 1:E:1191:MET:SD | 1:E:1209:SER:OG | 2.63 | 0.44 |
| 1:E:530:ARG:NH1 | 1:E:545:GLN:OE1 | 2.51 | 0.44 |
| 1:F:342:LEU:O | 1:F:346:GLN:CG | 2.66 | 0.44 |
| 2:J:72:LYS:NZ | 2:J:78:THR:O | 2.51 | 0.44 |
| 3:R:10:ARG:HG2 | 3:R:10:ARG:H | 1.60 | 0.44 |
| 1:A:357:SER:OG | 1:A:358:SER:N | 2.50 | 0.44 |
| 1:C:342:LEU:O | 1:C:346:GLN:CG | 2.66 | 0.44 |
| 1:D:390:GLN:HB2 | 1:D:393:VAL:HG21 | 1.99 | 0.44 |
| 1:E:357:SER:OG | 1:E:358:SER:N | 2.50 | 0.44 |
| 1:F:390:GLN:HB2 | 1:F:393:VAL:HG21 | 1.99 | 0.44 |
| 1:F:600:LYS:HA | 1:F:603:ILE:HG13 | 2.00 | 0.44 |
| 1:G:342:LEU:O | 1:G:346:GLN:CG | 2.66 | 0.44 |
| 1:G:600:LYS:HA | 1:G:603:ILE:HG13 | 2.00 | 0.44 |
| 1:G:695:TYR:HE1 | 1:G:733:LYS:HD2 | 1.83 | 0.44 |
| 1:G:821:ILE:HD11 | 1:G:857:VAL:HG21 | 1.99 | 0.44 |
| 2:I:68:LEU:HB3 | 2:I:85:ILE:HD12 | 1.98 | 0.44 |
| 2:J:3:VAL:O | 2:J:97:TYR:HB2 | 2.18 | 0.44 |
| 2:N:3:VAL:O | 2:N:97:TYR:HB2 | 2.18 | 0.44 |
| 1:B:390:GLN:HB2 | 1:B:393:VAL:HG21 | 1.99 | 0.44 |
| 1:B:550:LEU:HD23 | 1:B:607:SER:HB2 | 1.91 | 0.44 |
| 1:C:695:TYR:HE1 | 1:C:733:LYS:HD2 | 1.82 | 0.44 |
| 1:E:600:LYS:HA | 1:E:603:ILE:HG13 | 2.00 | 0.44 |
| 1:E:868:ASN:OD1 | 1:E:869:THR:N | 2.50 | 0.44 |
| 1:G:230:LEU:O | 1:G:234:LYS:N | 2.41 | 0.44 |
| 1:G:530:ARG:NH1 | 1:G:545:GLN:OE1 | 2.51 | 0.44 |
| 1:G:795:GLU:O | 1:G:795:GLU:HG3 | 2.18 | 0.44 |
| 1:A:530:ARG:NH1 | 1:A:545:GLN:OE1 | 2.51 | 0.44 |
| 1:B:695:TYR:HE1 | 1:B:733:LYS:HD2 | 1.83 | 0.44 |
| 1:C:1135:PHE:CE1 | 1:C:1142:LEU:HD13 | 2.53 | 0.44 |
| 1:C:298:PHE:CD2 | 1:C:328:GLY:HA3 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:795:GLU:O | 1:C:795:GLU:HG3 | 2.18 | 0.44 |
| 1:D:461:ILE:HD11 | 1:D:491:MET:HA | 1.99 | 0.44 |
| 1:D:600:LYS:HA | 1:D:603:ILE:HG13 | 2.00 | 0.44 |
| 1:D:685:ASN:HB3 | 1:D:688:THR:HB | 1.99 | 0.44 |
| 1:F:298:PHE:CD2 | 1:F:328:GLY:HA3 | 2.52 | 0.44 |
| 1:G:344:GLN:OE1 | 1:G:349:GLN:NE2 | 2.44 | 0.44 |
| 1:G:390:GLN:HB2 | 1:G:393:VAL:HG21 | 1.99 | 0.44 |
| 2:K:3:VAL:O | 2:K:97:TYR:HB2 | 2.18 | 0.44 |
| 2:L:3:VAL:O | 2:L:97:TYR:HB2 | 2.18 | 0.44 |
| 2:M:70:ASN:ND2 | 2:M:73:LYS:HB2 | 2.33 | 0.44 |
| 1:A:342:LEU:O | 1:A:346:GLN:CG | 2.66 | 0.44 |
| 1:A:346:GLN:C | 1:A:348:LYS:N | 2.71 | 0.44 |
| 1:A:685:ASN:HB3 | 1:A:688:THR:HB | 1.99 | 0.44 |
| 1:B:1135:PHE:CE1 | 1:B:1142:LEU:HD13 | 2.53 | 0.44 |
| 1:B:600:LYS:HZ1 | 1:B:1213:PHE:HZ | 1.65 | 0.44 |
| 1:B:346:GLN:C | 1:B:348:LYS:N | 2.71 | 0.44 |
| 1:B:391:LYS:H | 1:B:391:LYS:HG2 | 1.62 | 0.44 |
| 1:C:357:SER:OG | 1:C:358:SER:N | 2.50 | 0.44 |
| 1:D:524:HIS:N | 1:D:646:THR:OG1 | 2.51 | 0.44 |
| 2:K:72:LYS:NZ | 2:K:78:THR:O | 2.51 | 0.44 |
| 2:N:70:ASN:ND2 | 2:N:73:LYS:HB2 | 2.33 | 0.44 |
| 1:A:695:TYR:OH | 1:A:732:GLN:O | 2.31 | 0.44 |
| 1:B:685:ASN:HB3 | 1:B:688:THR:HB | 1.99 | 0.44 |
| 1:C:346:GLN:C | 1:C:348:LYS:N | 2.71 | 0.44 |
| 1:C:530:ARG:NH1 | 1:C:545:GLN:OE1 | 2.51 | 0.44 |
| 1:C:847:ASP:OD1 | 1:C:848:PHE:N | 2.51 | 0.44 |
| 1:D:530:ARG:NH1 | 1:D:545:GLN:OE1 | 2.51 | 0.44 |
| 1:D:695:TYR:HE1 | 1:D:733:LYS:HD2 | 1.83 | 0.44 |
| 1:D:847:ASP:OD1 | 1:D:848:PHE:N | 2.51 | 0.44 |
| 1:E:685:ASN:HB3 | 1:E:688:THR:HB | 2.00 | 0.44 |
| 1:G:480:CYS:SG | 1:G:481:MET:N | 2.90 | 0.44 |
| 2:H:72:LYS:NZ | 2:H:78:THR:O | 2.51 | 0.44 |
| 3:O:41:GLU:HA | 3:O:44:GLN:HE21 | 1.83 | 0.44 |
| 1:A:795:GLU:O | 1:A:795:GLU:HG3 | 2.18 | 0.43 |
| 1:B:326:LEU:HA | 1:B:326:LEU:HD23 | 1.44 | 0.43 |
| 1:B:524:HIS:N | 1:B:646:THR:OG1 | 2.51 | 0.43 |
| 1:C:390:GLN:HB2 | 1:C:393:VAL:HG21 | 1.99 | 0.43 |
| 1:E:342:LEU:O | 1:E:346:GLN:CG | 2.66 | 0.43 |
| 1:E:695:TYR:HE1 | 1:E:733:LYS:HD2 | 1.83 | 0.43 |
| 1:E:795:GLU:O | 1:E:795:GLU:HG3 | 2.18 | 0.43 |
| 1:F:524:HIS:N | 1:F:646:THR:OG1 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:795:GLU:HG3 | 1:F:795:GLU:O | 2.18 | 0.43 |
| 1:G:685:ASN:HB3 | 1:G:688:THR:HB | 1.99 | 0.43 |
| 2:L:18:HIS:CE1 | 2:L:29:GLY:HA3 | 2.53 | 0.43 |
| 2:L:72:LYS:NZ | 2:L:78:THR:O | 2.51 | 0.43 |
| 2:N:18:HIS:CE1 | 2:N:29:GLY:HA3 | 2.53 | 0.43 |
| 1:B:224:LYS:HE3 | 1:B:255:ASP:O | 2.18 | 0.43 |
| 1:B:342:LEU:O | 1:B:346:GLN:CG | 2.66 | 0.43 |
| 1:B:530:ARG:NH1 | 1:B:545:GLN:OE1 | 2.51 | 0.43 |
| 1:B:795:GLU:O | 1:B:795:GLU:HG3 | 2.18 | 0.43 |
| 1:C:334:PHE:HD2 | 1:C:337:ARG:HH11 | 1.66 | 0.43 |
| 1:E:298:PHE:CD2 | 1:E:328:GLY:HA3 | 2.52 | 0.43 |
| 1:E:891:SER:OG | 1:E:896:SER:O | 2.34 | 0.43 |
| 1:F:480:CYS:SG | 1:F:481:MET:N | 2.90 | 0.43 |
| 1:G:224:LYS:HE3 | 1:G:255:ASP:O | 2.18 | 0.43 |
| 1:G:357:SER:OG | 1:G:358:SER:N | 2.50 | 0.43 |
| 1:G:524:HIS:N | 1:G:646:THR:OG1 | 2.51 | 0.43 |
| 2:H:18:HIS:CE1 | 2:H:29:GLY:HA3 | 2.53 | 0.43 |
| 2:J:70:ASN:ND2 | 2:J:73:LYS:HB2 | 2.33 | 0.43 |
| 1:F:884:TRP:HH2 | 2:M:78:THR:C | 2.22 | 0.43 |
| 1:A:1135:PHE:CE1 | 1:A:1142:LEU:HD13 | 2.53 | 0.43 |
| 1:A:524:HIS:N | 1:A:646:THR:OG1 | 2.51 | 0.43 |
| 1:A:695:TYR:HE1 | 1:A:733:LYS:HD2 | 1.83 | 0.43 |
| 1:A:847:ASP:OD1 | 1:A:848:PHE:N | 2.51 | 0.43 |
| 1:B:428:ARG:HG2 | 1:B:433:PHE:CE1 | 2.54 | 0.43 |
| 1:E:524:HIS:N | 1:E:646:THR:OG1 | 2.51 | 0.43 |
| 1:F:357:SER:OG | 1:F:358:SER:N | 2.50 | 0.43 |
| 1:G:268:SER:O | 1:G:271:ASP:N | 2.51 | 0.43 |
| 1:G:844:GLN:HE22 | 2:N:79:LYS:HZ2 | 1.63 | 0.43 |
| 1:G:884:TRP:HH2 | 2:N:78:THR:C | 2.22 | 0.43 |
| 2:N:72:LYS:NZ | 2:N:78:THR:O | 2.51 | 0.43 |
| 3:R:41:GLU:HA | 3:R:44:GLN:HE21 | 1.83 | 0.43 |
| 1:A:386:LEU:HD23 | 1:A:386:LEU:O | 2.19 | 0.43 |
| 1:A:390:GLN:HB2 | 1:A:393:VAL:HG21 | 1.99 | 0.43 |
| 1:A:965:SER:H | 1:A:980:ASP:HA | 1.84 | 0.43 |
| 1:B:937:VAL:HB | 1:B:949:ILE:HB | 2.00 | 0.43 |
| 1:C:685:ASN:HB3 | 1:C:688:THR:HB | 2.00 | 0.43 |
| 1:C:937:VAL:HB | 1:C:949:ILE:HB | 2.00 | 0.43 |
| 1:C:965:SER:H | 1:C:980:ASP:HA | 1.84 | 0.43 |
| 1:D:582:LEU:O | 1:D:586:GLN:HG3 | 2.19 | 0.43 |
| 1:F:530:ARG:NH1 | 1:F:545:GLN:OE1 | 2.51 | 0.43 |
| 1:G:386:LEU:HD23 | 1:G:386:LEU:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:569:CYS:HB3 | 1:G:600:LYS:HZ3 | 1.83 | 0.43 |
| 2:H:70:ASN:ND2 | 2:H:73:LYS:HB2 | 2.33 | 0.43 |
| 2:M:26:HIS:O | 2:M:27:LYS:HD2 | 2.19 | 0.43 |
| 1:A:224:LYS:HE3 | 1:A:255:ASP:O | 2.18 | 0.43 |
| 1:B:334:PHE:HD2 | 1:B:337:ARG:HH11 | 1.66 | 0.43 |
| 1:B:582:LEU:O | 1:B:586:GLN:HG3 | 2.19 | 0.43 |
| 1:E:1135:PHE:CE1 | 1:E:1142:LEU:HD13 | 2.53 | 0.43 |
| 1:E:762:SER:OG | 1:E:764:ASP:OD1 | 2.26 | 0.43 |
| 1:F:965:SER:H | 1:F:980:ASP:HA | 1.84 | 0.43 |
| 1:G:1218:THR:H | 1:G:1237:ASN:ND2 | 2.17 | 0.43 |
| 2:J:18:HIS:CE1 | 2:J:29:GLY:HA3 | 2.53 | 0.43 |
| 2:N:26:HIS:O | 2:N:27:LYS:HD2 | 2.19 | 0.43 |
| 1:A:266:ASP:CG | 1:A:268:SER:H | 2.20 | 0.43 |
| 1:A:346:GLN:O | 1:A:348:LYS:N | 2.52 | 0.43 |
| 1:C:428:ARG:HG2 | 1:C:433:PHE:CE1 | 2.54 | 0.43 |
| 1:C:524:HIS:N | 1:C:646:THR:OG1 | 2.51 | 0.43 |
| 1:D:224:LYS:HE3 | 1:D:255:ASP:O | 2.18 | 0.43 |
| 1:D:386:LEU:O | 1:D:386:LEU:HD23 | 2.19 | 0.43 |
| 1:D:937:VAL:HB | 1:D:949:ILE:HB | 2.00 | 0.43 |
| 1:E:1166:ALA:HA | 1:E:1167:PRO:HD2 | 1.93 | 0.43 |
| 1:E:224:LYS:HE3 | 1:E:255:ASP:O | 2.18 | 0.43 |
| 1:E:346:GLN:C | 1:E:348:LYS:N | 2.71 | 0.43 |
| 1:E:428:ARG:HG2 | 1:E:433:PHE:CE1 | 2.54 | 0.43 |
| 1:F:346:GLN:C | 1:F:348:LYS:N | 2.71 | 0.43 |
| 1:A:884:TRP:HH2 | 2:H:78:THR:C | 2.22 | 0.43 |
| 2:I:26:HIS:O | 2:I:27:LYS:HD2 | 2.19 | 0.43 |
| 2:J:26:HIS:O | 2:J:27:LYS:HD2 | 2.19 | 0.43 |
| 1:C:884:TRP:HH2 | 2:J:78:THR:O | 2.02 | 0.43 |
| 1:E:884:TRP:HH2 | 2:L:78:THR:C | 2.22 | 0.43 |
| 2:M:18:HIS:CE1 | 2:M:29:GLY:HA3 | 2.53 | 0.43 |
| 2:N:82:PHE:HE2 | 2:N:85:ILE:HG13 | 1.84 | 0.43 |
| 1:A:379:ILE:O | 1:A:382:TYR:N | 2.52 | 0.43 |
| 1:B:346:GLN:O | 1:B:348:LYS:N | 2.52 | 0.43 |
| 1:B:386:LEU:O | 1:B:386:LEU:HD23 | 2.19 | 0.43 |
| 1:D:965:SER:H | 1:D:980:ASP:HA | 1.84 | 0.43 |
| 1:E:1100:PHE:HB3 | 1:E:1111:ILE:HD11 | 2.00 | 0.43 |
| 1:E:268:SER:O | 1:E:271:ASP:N | 2.51 | 0.43 |
| 1:F:224:LYS:HE3 | 1:F:255:ASP:O | 2.18 | 0.43 |
| 1:F:386:LEU:O | 1:F:386:LEU:HD23 | 2.19 | 0.43 |
| 1:F:685:ASN:HB3 | 1:F:688:THR:HB | 1.99 | 0.43 |
| 1:F:695:TYR:HE1 | 1:F:733:LYS:HD2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:847:ASP:OD1 | 1:F:848:PHE:N | 2.51 | 0.43 |
| 1:G:266:ASP:CG | 1:G:268:SER:H | 2.20 | 0.43 |
| 1:G:379:ILE:O | 1:G:382:TYR:N | 2.52 | 0.43 |
| 2:H:3:VAL:O | 2:H:97:TYR:HB2 | 2.18 | 0.43 |
| 2:I:18:HIS:CE1 | 2:I:29:GLY:HA3 | 2.53 | 0.43 |
| 1:A:326:LEU:HA | 1:A:326:LEU:HD23 | 1.44 | 0.43 |
| 1:C:379:ILE:O | 1:C:382:TYR:N | 2.52 | 0.43 |
| 1:D:428:ARG:HG2 | 1:D:433:PHE:CE1 | 2.54 | 0.43 |
| 1:F:582:LEU:O | 1:F:586:GLN:HG3 | 2.19 | 0.43 |
| 1:F:937:VAL:HB | 1:F:949:ILE:HB | 2.00 | 0.43 |
| 1:G:847:ASP:OD1 | 1:G:848:PHE:N | 2.51 | 0.43 |
| 2:I:70:ASN:ND2 | 2:I:73:LYS:HB2 | 2.33 | 0.43 |
| 2:I:3:VAL:O | 2:I:97:TYR:HB2 | 2.18 | 0.43 |
| 2:K:26:HIS:O | 2:K:27:LYS:HD2 | 2.19 | 0.43 |
| 2:L:41:GLY:HA2 | 2:L:48:TYR:CZ | 2.54 | 0.43 |
| 1:A:524:HIS:CB | 1:A:646:THR:HG21 | 2.36 | 0.43 |
| 1:B:1100:PHE:HB3 | 1:B:1111:ILE:HD11 | 2.00 | 0.43 |
| 1:B:379:ILE:O | 1:B:382:TYR:N | 2.52 | 0.43 |
| 1:B:767:LEU:HD21 | 1:B:801:VAL:HG11 | 2.01 | 0.43 |
| 1:C:224:LYS:HE3 | 1:C:255:ASP:O | 2.18 | 0.43 |
| 1:C:346:GLN:O | 1:C:348:LYS:N | 2.52 | 0.43 |
| 1:D:1100:PHE:HB3 | 1:D:1111:ILE:HD11 | 2.00 | 0.43 |
| 1:D:725:LEU:HD11 | 1:D:742:HIS:CD2 | 2.54 | 0.43 |
| 1:D:884:TRP:HH2 | 2:K:78:THR:C | 2.22 | 0.43 |
| 1:E:725:LEU:HD11 | 1:E:742:HIS:CD2 | 2.54 | 0.43 |
| 1:E:847:ASP:OD1 | 1:E:848:PHE:N | 2.51 | 0.43 |
| 1:E:965:SER:H | 1:E:980:ASP:HA | 1.84 | 0.43 |
| 1:F:379:ILE:O | 1:F:382:TYR:N | 2.52 | 0.43 |
| 1:G:428:ARG:HG2 | 1:G:433:PHE:CE1 | 2.54 | 0.43 |
| 2:H:41:GLY:HA2 | 2:H:48:TYR:CZ | 2.54 | 0.43 |
| 2:H:82:PHE:HE2 | 2:H:85:ILE:HG13 | 1.84 | 0.43 |
| 2:K:18:HIS:CE1 | 2:K:29:GLY:HA3 | 2.53 | 0.43 |
| 2:K:70:ASN:ND2 | 2:K:73:LYS:HB2 | 2.33 | 0.43 |
| 2:M:3:VAL:O | 2:M:97:TYR:HB2 | 2.18 | 0.43 |
| 1:B:965:SER:H | 1:B:980:ASP:HA | 1.84 | 0.43 |
| 1:C:582:LEU:O | 1:C:586:GLN:HG3 | 2.19 | 0.43 |
| 1:C:767:LEU:HD21 | 1:C:801:VAL:HG11 | 2.01 | 0.43 |
| 1:D:1135:PHE:CE1 | 1:D:1142:LEU:HD13 | 2.53 | 0.43 |
| 1:D:334:PHE:HD2 | 1:D:337:ARG:HH11 | 1.66 | 0.43 |
| 1:D:795:GLU:O | 1:D:795:GLU:HG3 | 2.18 | 0.43 |
| 1:E:1218:THR:H | 1:E:1237:ASN:ND2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:1100:PHE:HB3 | 1:F:1111:ILE:HD11 | 2.00 | 0.43 |
| 1:F:346:GLN:O | 1:F:348:LYS:N | 2.52 | 0.43 |
| 1:G:1050:PHE:CD1 | 1:G:1058:LEU:HD11 | 2.54 | 0.43 |
| 1:F:201:ASN:ND2 | 1:G:219:ASN:HD21 | 2.14 | 0.43 |
| 1:G:346:GLN:O | 1:G:348:LYS:N | 2.52 | 0.43 |
| 2:H:67:TYR:HD1 | 2:H:74:TYR:HB3 | 1.84 | 0.43 |
| 1:B:884:TRP:HH2 | 2:I:78:THR:C | 2.22 | 0.43 |
| 2:L:26:HIS:O | 2:L:27:LYS:HD2 | 2.19 | 0.43 |
| 2:L:70:ASN:ND2 | 2:L:73:LYS:HB2 | 2.33 | 0.43 |
| 2:L:82:PHE:HE2 | 2:L:85:ILE:HG13 | 1.84 | 0.43 |
| 3:P:41:GLU:HA | 3:P:44:GLN:HE21 | 1.83 | 0.43 |
| 1:C:676:SER:OG | 1:C:678:ASP:OD1 | 2.37 | 0.42 |
| 1:C:884:TRP:HH2 | 2:J:78:THR:C | 2.22 | 0.42 |
| 1:D:767:LEU:HD21 | 1:D:801:VAL:HG11 | 2.01 | 0.42 |
| 1:E:658:ASP:HB3 | 1:E:677:VAL:HB | 2.00 | 0.42 |
| 1:F:1135:PHE:CE1 | 1:F:1142:LEU:HD13 | 2.53 | 0.42 |
| 1:G:658:ASP:HB3 | 1:G:677:VAL:HB | 2.00 | 0.42 |
| 1:G:937:VAL:HB | 1:G:949:ILE:HB | 2.00 | 0.42 |
| 2:I:82:PHE:HE2 | 2:I:85:ILE:HG13 | 1.84 | 0.42 |
| 2:N:41:GLY:HA2 | 2:N:48:TYR:CZ | 2.54 | 0.42 |
| 3:P:90:ARG:HH21 | 3:P:90:ARG:HG2 | 1.84 | 0.42 |
| 1:A:1050:PHE:CD1 | 1:A:1058:LEU:HD11 | 2.54 | 0.42 |
| 1:A:658:ASP:HB3 | 1:A:677:VAL:HB | 2.00 | 0.42 |
| 1:B:266:ASP:CG | 1:B:268:SER:H | 2.20 | 0.42 |
| 1:C:1100:PHE:HB3 | 1:C:1111:ILE:HD11 | 2.00 | 0.42 |
| 1:C:550:LEU:HD23 | 1:C:607:SER:HB2 | 1.91 | 0.42 |
| 1:D:658:ASP:HB3 | 1:D:677:VAL:HB | 2.00 | 0.42 |
| 1:E:767:LEU:HD21 | 1:E:801:VAL:HG11 | 2.01 | 0.42 |
| 1:F:808:ALA:HB2 | 1:F:850:PRO:HA | 2.01 | 0.42 |
| 1:G:1135:PHE:CE1 | 1:G:1142:LEU:HD13 | 2.53 | 0.42 |
| 2:M:82:PHE:HE2 | 2:M:85:ILE:HG13 | 1.84 | 0.42 |
| 3:R:90:ARG:HH21 | 3:R:90:ARG:HG2 | 1.85 | 0.42 |
| 1:A:511:LYS:HB2 | 1:A:563:ILE:HG13 | 2.02 | 0.42 |
| 1:A:767:LEU:HD21 | 1:A:801:VAL:HG11 | 2.01 | 0.42 |
| 1:B:1218:THR:H | 1:B:1237:ASN:ND2 | 2.17 | 0.42 |
| 1:B:658:ASP:HB3 | 1:B:677:VAL:HB | 2.00 | 0.42 |
| 1:D:524:HIS:CB | 1:D:646:THR:HG21 | 2.36 | 0.42 |
| 1:F:266:ASP:CG | 1:F:268:SER:H | 2.20 | 0.42 |
| 1:G:808:ALA:HB2 | 1:G:850:PRO:HA | 2.02 | 0.42 |
| 2:J:14:CYS:SG | 5:J:500:HEC:HBB3 | 2.59 | 0.42 |
| 2:J:82:PHE:HE2 | 2:J:85:ILE:HG13 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:N:14:CYS:SG | 5:N:500:HEC:HBB3 | 2.59 | 0.42 |
| 3:O:90:ARG:HH21 | 3:O:90:ARG:HG2 | 1.85 | 0.42 |
| 1:A:1100:PHE:HB3 | 1:A:1111:ILE:HD11 | 2.00 | 0.42 |
| 1:A:1218:THR:H | 1:A:1237:ASN:ND2 | 2.17 | 0.42 |
| 1:A:428:ARG:HG2 | 1:A:433:PHE:CE1 | 2.54 | 0.42 |
| 1:A:937:VAL:HB | 1:A:949:ILE:HB | 2.00 | 0.42 |
| 1:D:346:GLN:C | 1:D:348:LYS:N | 2.71 | 0.42 |
| 1:E:379:ILE:O | 1:E:382:TYR:N | 2.52 | 0.42 |
| 1:E:937:VAL:HB | 1:E:949:ILE:HB | 2.00 | 0.42 |
| 1:F:658:ASP:HB3 | 1:F:677:VAL:HB | 2.00 | 0.42 |
| 1:F:725:LEU:HD11 | 1:F:742:HIS:CD2 | 2.54 | 0.42 |
| 1:F:767:LEU:HD21 | 1:F:801:VAL:HG11 | 2.01 | 0.42 |
| 2:J:67:TYR:HD1 | 2:J:74:TYR:HB3 | 1.84 | 0.42 |
| 2:K:14:CYS:SG | 5:K:500:HEC:HBB3 | 2.59 | 0.42 |
| 3:O:34:LEU:HA | 3:O:34:LEU:HD12 | 1.93 | 0.42 |
| 3:Q:90:ARG:HG2 | 3:Q:90:ARG:HH21 | 1.84 | 0.42 |
| 1:B:511:LYS:HB2 | 1:B:563:ILE:HG13 | 2.02 | 0.42 |
| 1:B:847:ASP:OD1 | 1:B:848:PHE:N | 2.51 | 0.42 |
| 1:B:989:GLU:HG2 | 1:B:991:VAL:H | 1.85 | 0.42 |
| 1:C:1135:PHE:HE1 | 1:C:1142:LEU:HD13 | 1.85 | 0.42 |
| 1:C:725:LEU:HD11 | 1:C:742:HIS:CD2 | 2.54 | 0.42 |
| 1:D:1218:THR:H | 1:D:1237:ASN:ND2 | 2.17 | 0.42 |
| 1:D:676:SER:OG | 1:D:678:ASP:OD1 | 2.37 | 0.42 |
| 1:E:346:GLN:O | 1:E:348:LYS:N | 2.52 | 0.42 |
| 1:E:808:ALA:HB2 | 1:E:850:PRO:HA | 2.01 | 0.42 |
| 1:G:145:GLY:HA2 | 1:G:259:GLN:HE21 | 1.85 | 0.42 |
| 2:H:26:HIS:O | 2:H:27:LYS:HD2 | 2.19 | 0.42 |
| 2:I:14:CYS:SG | 5:I:500:HEC:HBB3 | 2.59 | 0.42 |
| 2:K:41:GLY:HA2 | 2:K:48:TYR:CZ | 2.54 | 0.42 |
| 3:R:7:ARG:HA | 3:R:10:ARG:HG3 | 2.02 | 0.42 |
| 1:A:808:ALA:HB2 | 1:A:850:PRO:HA | 2.01 | 0.42 |
| 1:C:658:ASP:HB3 | 1:C:677:VAL:HB | 2.00 | 0.42 |
| 1:D:452:GLN:N | 1:D:452:GLN:OE1 | 2.53 | 0.42 |
| 1:D:14:GLU:CB | 1:E:31:SER:HG | 2.33 | 0.42 |
| 1:E:386:LEU:HD23 | 1:E:386:LEU:O | 2.19 | 0.42 |
| 1:E:582:LEU:O | 1:E:586:GLN:HG3 | 2.19 | 0.42 |
| 1:F:1050:PHE:CD1 | 1:F:1058:LEU:HD11 | 2.54 | 0.42 |
| 1:F:334:PHE:HD2 | 1:F:337:ARG:HH11 | 1.66 | 0.42 |
| 2:H:40:THR:HG23 | 2:H:57:ILE:HG13 | 2.02 | 0.42 |
| 2:K:82:PHE:HE2 | 2:K:85:ILE:HG13 | 1.84 | 0.42 |
| 2:N:67:TYR:HD1 | 2:N:74:TYR:HB3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:320:SER:HA | 1:A:321:PRO:HD3 | 1.87 | 0.42 |
| 1:B:1032:TRP:C | 1:B:1034:LEU:H | 2.23 | 0.42 |
| 1:C:1050:PHE:CD1 | 1:C:1058:LEU:HD11 | 2.54 | 0.42 |
| 1:C:386:LEU:O | 1:C:386:LEU:HD23 | 2.19 | 0.42 |
| 1:C:400:LEU:HB3 | 1:C:404:TRP:HZ3 | 1.84 | 0.42 |
| 1:G:10:LEU:CD2 | 1:G:13:ARG:NH2 | 2.83 | 0.42 |
| 1:G:320:SER:HA | 1:G:321:PRO:HD3 | 1.87 | 0.42 |
| 1:G:511:LYS:HB2 | 1:G:563:ILE:HG13 | 2.02 | 0.42 |
| 1:G:582:LEU:O | 1:G:586:GLN:HG3 | 2.19 | 0.42 |
| 2:I:94:LEU:O | 2:I:98:LEU:HG | 2.20 | 0.42 |
| 2:J:41:GLY:HA2 | 2:J:48:TYR:CZ | 2.54 | 0.42 |
| 1:D:884:TRP:HH2 | 2:K:78:THR:O | 2.02 | 0.42 |
| 2:M:41:GLY:HA2 | 2:M:48:TYR:CZ | 2.54 | 0.42 |
| 1:B:1050:PHE:CD1 | 1:B:1058:LEU:HD11 | 2.54 | 0.42 |
| 1:B:1135:PHE:HE1 | 1:B:1142:LEU:HD13 | 1.85 | 0.42 |
| 1:B:265:ARG:O | 1:B:265:ARG:HG3 | 2.20 | 0.42 |
| 1:B:320:SER:HA | 1:B:321:PRO:HD3 | 1.87 | 0.42 |
| 1:C:1218:THR:H | 1:C:1237:ASN:ND2 | 2.17 | 0.42 |
| 1:C:145:GLY:HA2 | 1:C:259:GLN:HE21 | 1.85 | 0.42 |
| 1:C:266:ASP:CG | 1:C:268:SER:H | 2.20 | 0.42 |
| 1:D:10:LEU:CD2 | 1:D:13:ARG:NH2 | 2.83 | 0.42 |
| 1:D:265:ARG:O | 1:D:265:ARG:HG3 | 2.20 | 0.42 |
| 1:D:379:ILE:O | 1:D:382:TYR:N | 2.52 | 0.42 |
| 1:F:1218:THR:H | 1:F:1237:ASN:ND2 | 2.17 | 0.42 |
| 1:G:1135:PHE:HE1 | 1:G:1142:LEU:HD13 | 1.85 | 0.42 |
| 1:G:400:LEU:HB3 | 1:G:404:TRP:HZ3 | 1.85 | 0.42 |
| 1:G:767:LEU:HD21 | 1:G:801:VAL:HG11 | 2.01 | 0.42 |
| 2:H:14:CYS:SG | 5:H:500:HEC:HBB3 | 2.59 | 0.42 |
| 2:L:14:CYS:SG | 5:L:500:HEC:HBB3 | 2.59 | 0.42 |
| 2:N:40:THR:HG23 | 2:N:57:ILE:HG13 | 2.02 | 0.42 |
| 3:O:7:ARG:HA | 3:O:10:ARG:HG3 | 2.02 | 0.42 |
| 1:A:265:ARG:O | 1:A:265:ARG:HG3 | 2.20 | 0.42 |
| 1:B:268:SER:O | 1:B:271:ASP:N | 2.51 | 0.42 |
| 1:D:346:GLN:O | 1:D:348:LYS:N | 2.52 | 0.42 |
| 1:E:1050:PHE:CD1 | 1:E:1058:LEU:HD11 | 2.54 | 0.42 |
| 1:E:452:GLN:OE1 | 1:E:452:GLN:N | 2.53 | 0.42 |
| 1:F:428:ARG:HG2 | 1:F:433:PHE:CE1 | 2.54 | 0.42 |
| 1:G:452:GLN:N | 1:G:452:GLN:OE1 | 2.53 | 0.42 |
| 2:H:94:LEU:O | 2:H:98:LEU:HG | 2.20 | 0.42 |
| 2:M:40:THR:HG23 | 2:M:57:ILE:HG13 | 2.02 | 0.42 |
| 2:M:67:TYR:HD1 | 2:M:74:TYR:HB3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1032:TRP:C | 1:A:1034:LEU:H | 2.23 | 0.42 |
| 1:A:582:LEU:O | 1:A:586:GLN:HG3 | 2.19 | 0.42 |
| 1:A:864:VAL:HB | 1:A:878:CYS:HB2 | 2.02 | 0.42 |
| 1:B:10:LEU:CD2 | 1:B:13:ARG:NH2 | 2.83 | 0.42 |
| 1:B:452:GLN:OE1 | 1:B:452:GLN:N | 2.53 | 0.42 |
| 1:C:265:ARG:O | 1:C:265:ARG:HG3 | 2.20 | 0.42 |
| 1:C:268:SER:O | 1:C:271:ASP:N | 2.51 | 0.42 |
| 1:C:452:GLN:OE1 | 1:C:452:GLN:N | 2.53 | 0.42 |
| 1:C:864:VAL:HB | 1:C:878:CYS:HB2 | 2.02 | 0.42 |
| 1:D:864:VAL:HB | 1:D:878:CYS:HB2 | 2.02 | 0.42 |
| 1:D:989:GLU:HG2 | 1:D:991:VAL:H | 1.85 | 0.42 |
| 1:E:265:ARG:O | 1:E:265:ARG:HG3 | 2.20 | 0.42 |
| 1:E:266:ASP:CG | 1:E:268:SER:H | 2.20 | 0.42 |
| 1:F:989:GLU:HG2 | 1:F:991:VAL:H | 1.85 | 0.42 |
| 1:G:334:PHE:HD2 | 1:G:337:ARG:HH11 | 1.66 | 0.42 |
| 1:G:676:SER:OG | 1:G:678:ASP:OD1 | 2.37 | 0.42 |
| 1:G:725:LEU:HD11 | 1:G:742:HIS:CD2 | 2.54 | 0.42 |
| 1:G:965:SER:H | 1:G:980:ASP:HA | 1.84 | 0.42 |
| 2:J:94:LEU:O | 2:J:98:LEU:HG | 2.20 | 0.42 |
| 2:L:67:TYR:HD1 | 2:L:74:TYR:HB3 | 1.84 | 0.42 |
| 2:M:14:CYS:SG | 5:M:500:HEC:HBB3 | 2.59 | 0.42 |
| 1:A:452:GLN:N | 1:A:452:GLN:OE1 | 2.53 | 0.41 |
| 1:A:989:GLU:HG2 | 1:A:991:VAL:H | 1.85 | 0.41 |
| 1:F:947:GLN:HG2 | 1:F:958:TYR:HD1 | 1.85 | 0.41 |
| 1:A:862:TYR:HB3 | 1:A:883:SER:C | 2.41 | 0.41 |
| 1:B:456:LEU:O | 1:B:459:LYS:HB3 | 2.20 | 0.41 |
| 1:D:1050:PHE:CD1 | 1:D:1058:LEU:HD11 | 2.54 | 0.41 |
| 1:D:266:ASP:CG | 1:D:268:SER:H | 2.20 | 0.41 |
| 1:F:369:SER:O | 1:F:373:GLU:HG2 | 2.21 | 0.41 |
| 1:F:511:LYS:HB2 | 1:F:563:ILE:HG13 | 2.01 | 0.41 |
| 1:F:864:VAL:HB | 1:F:878:CYS:HB2 | 2.02 | 0.41 |
| 2:K:67:TYR:HD1 | 2:K:74:TYR:HB3 | 1.84 | 0.41 |
| 2:K:94:LEU:O | 2:K:98:LEU:HG | 2.20 | 0.41 |
| 2:L:94:LEU:O | 2:L:98:LEU:HG | 2.20 | 0.41 |
| 1:A:1191:MET:SD | 1:A:1209:SER:OG | 2.63 | 0.41 |
| 1:A:145:GLY:HA2 | 1:A:259:GLN:HE21 | 1.85 | 0.41 |
| 1:C:269:VAL:C | 1:C:271:ASP:H | 2.24 | 0.41 |
| 1:G:1100:PHE:HB3 | 1:G:1111:ILE:HD11 | 2.00 | 0.41 |
| 1:G:282:VAL:O | 1:G:282:VAL:HG12 | 2.21 | 0.41 |
| 1:G:947:GLN:HG2 | 1:G:958:TYR:HD1 | 1.85 | 0.41 |
| 2:I:41:GLY:HA2 | 2:I:48:TYR:CZ | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:334:PHE:HD2 | 1:A:337:ARG:HH11 | 1.66 | 0.41 |
| 1:B:725:LEU:HD11 | 1:B:742:HIS:CD2 | 2.54 | 0.41 |
| 1:B:862:TYR:HB3 | 1:B:883:SER:C | 2.41 | 0.41 |
| 1:C:511:LYS:HB2 | 1:C:563:ILE:HG13 | 2.02 | 0.41 |
| 1:D:342:LEU:O | 1:D:346:GLN:HG3 | 2.21 | 0.41 |
| 1:D:456:LEU:O | 1:D:459:LYS:HB3 | 2.21 | 0.41 |
| 1:D:808:ALA:HB2 | 1:D:850:PRO:HA | 2.02 | 0.41 |
| 1:D:885:VAL:HG13 | 1:D:900:SER:O | 2.21 | 0.41 |
| 1:E:1135:PHE:HE1 | 1:E:1142:LEU:HD13 | 1.85 | 0.41 |
| 1:E:282:VAL:HG12 | 1:E:282:VAL:O | 2.20 | 0.41 |
| 1:F:265:ARG:O | 1:F:265:ARG:HG3 | 2.20 | 0.41 |
| 1:F:337:ARG:O | 1:F:340:TYR:N | 2.54 | 0.41 |
| 1:G:265:ARG:O | 1:G:265:ARG:HG3 | 2.20 | 0.41 |
| 1:G:369:SER:O | 1:G:373:GLU:HG2 | 2.20 | 0.41 |
| 2:I:40:THR:HG23 | 2:I:57:ILE:HG13 | 2.02 | 0.41 |
| 2:K:40:THR:HG23 | 2:K:57:ILE:HG13 | 2.02 | 0.41 |
| 1:A:676:SER:OG | 1:A:678:ASP:OD1 | 2.37 | 0.41 |
| 1:B:808:ALA:HB2 | 1:B:850:PRO:HA | 2.01 | 0.41 |
| 1:C:456:LEU:O | 1:C:459:LYS:HB3 | 2.21 | 0.41 |
| 1:C:808:ALA:HB2 | 1:C:850:PRO:HA | 2.01 | 0.41 |
| 1:D:268:SER:O | 1:D:271:ASP:N | 2.51 | 0.41 |
| 1:E:369:SER:O | 1:E:373:GLU:HG2 | 2.20 | 0.41 |
| 1:E:474:SER:HA | 1:E:475:PRO:HD2 | 1.91 | 0.41 |
| 1:F:452:GLN:OE1 | 1:F:452:GLN:N | 2.53 | 0.41 |
| 2:N:94:LEU:O | 2:N:98:LEU:HG | 2.20 | 0.41 |
| 1:D:30:ILE:HG21 | 3:Q:10:ARG:HB3 | 1.93 | 0.41 |
| 3:Q:7:ARG:HA | 3:Q:10:ARG:HG3 | 2.02 | 0.41 |
| 1:C:369:SER:O | 1:C:373:GLU:HG2 | 2.20 | 0.41 |
| 1:D:400:LEU:HB3 | 1:D:404:TRP:HZ3 | 1.84 | 0.41 |
| 1:D:947:GLN:HG2 | 1:D:958:TYR:HD1 | 1.85 | 0.41 |
| 1:E:337:ARG:O | 1:E:340:TYR:N | 2.54 | 0.41 |
| 1:F:268:SER:O | 1:F:271:ASP:N | 2.51 | 0.41 |
| 1:F:282:VAL:HG12 | 1:F:282:VAL:O | 2.20 | 0.41 |
| 1:F:456:LEU:O | 1:F:459:LYS:HB3 | 2.21 | 0.41 |
| 1:F:884:TRP:HH2 | 2:M:79:LYS:N | 2.18 | 0.41 |
| 1:G:337:ARG:O | 1:G:340:TYR:N | 2.54 | 0.41 |
| 1:G:989:GLU:HG2 | 1:G:991:VAL:H | 1.85 | 0.41 |
| 1:A:884:TRP:HH2 | 2:H:78:THR:O | 2.02 | 0.41 |
| 2:J:40:THR:HG23 | 2:J:57:ILE:HG13 | 2.02 | 0.41 |
| 2:L:40:THR:HG23 | 2:L:57:ILE:HG13 | 2.02 | 0.41 |
| 1:F:884:TRP:HH2 | 2:M:78:THR:O | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:94:LEU:O | 2:M:98:LEU:HG | 2.20 | 0.41 |
| 1:A:342:LEU:O | 1:A:346:GLN:HG3 | 2.21 | 0.41 |
| 1:A:947:GLN:HG2 | 1:A:958:TYR:HD1 | 1.85 | 0.41 |
| 1:B:282:VAL:HG12 | 1:B:282:VAL:O | 2.21 | 0.41 |
| 1:C:700:GLU:HB2 | 1:C:720:SER:HB2 | 2.03 | 0.41 |
| 1:D:216:LEU:HA | 1:D:217:PRO:HD2 | 1.84 | 0.41 |
| 1:D:282:VAL:O | 1:D:282:VAL:HG12 | 2.20 | 0.41 |
| 1:G:342:LEU:O | 1:G:346:GLN:HG3 | 2.21 | 0.41 |
| 1:G:862:TYR:HB3 | 1:G:883:SER:C | 2.41 | 0.41 |
| 1:A:1135:PHE:HE1 | 1:A:1142:LEU:HD13 | 1.85 | 0.41 |
| 1:A:725:LEU:HD11 | 1:A:742:HIS:CD2 | 2.54 | 0.41 |
| 1:B:145:GLY:HA2 | 1:B:259:GLN:HE21 | 1.85 | 0.41 |
| 1:B:569:CYS:CB | 1:B:600:LYS:HZ3 | 2.33 | 0.41 |
| 1:B:885:VAL:HG13 | 1:B:900:SER:O | 2.21 | 0.41 |
| 1:C:153:HIS:HA | 1:C:264:THR:O | 2.21 | 0.41 |
| 1:C:584:ALA:CA | 1:C:594:TYR:CE2 | 2.98 | 0.41 |
| 1:C:762:SER:OG | 1:C:764:ASP:OD1 | 2.26 | 0.41 |
| 1:D:196:LEU:O | 1:D:199:LEU:HB2 | 2.21 | 0.41 |
| 1:E:1032:TRP:C | 1:E:1034:LEU:H | 2.23 | 0.41 |
| 1:E:334:PHE:HD2 | 1:E:337:ARG:HH11 | 1.66 | 0.41 |
| 1:E:864:VAL:HB | 1:E:878:CYS:HB2 | 2.02 | 0.41 |
| 1:F:322:LEU:HD23 | 1:F:364:LEU:HD13 | 2.03 | 0.41 |
| 1:F:676:SER:OG | 1:F:678:ASP:OD1 | 2.37 | 0.41 |
| 1:F:885:VAL:HG13 | 1:F:900:SER:O | 2.21 | 0.41 |
| 1:G:864:VAL:HB | 1:G:878:CYS:HB2 | 2.02 | 0.41 |
| 2:I:30:PRO:HB3 | 2:I:46:PHE:CD2 | 2.56 | 0.41 |
| 2:K:30:PRO:HB3 | 2:K:46:PHE:CD2 | 2.56 | 0.41 |
| 2:M:55:LYS:HG2 | 2:M:75:ILE:HG12 | 2.03 | 0.41 |
| 1:A:400:LEU:HB3 | 1:A:404:TRP:HZ3 | 1.84 | 0.41 |
| 1:B:369:SER:O | 1:B:373:GLU:HG2 | 2.21 | 0.41 |
| 1:B:400:LEU:HB3 | 1:B:404:TRP:HZ3 | 1.84 | 0.41 |
| 1:B:700:GLU:HB2 | 1:B:720:SER:HB2 | 2.03 | 0.41 |
| 1:C:196:LEU:O | 1:C:199:LEU:HB2 | 2.21 | 0.41 |
| 1:C:282:VAL:O | 1:C:282:VAL:HG12 | 2.21 | 0.41 |
| 1:C:342:LEU:O | 1:C:346:GLN:HG3 | 2.21 | 0.41 |
| 1:C:862:TYR:HB3 | 1:C:883:SER:C | 2.41 | 0.41 |
| 1:D:1032:TRP:C | 1:D:1034:LEU:H | 2.23 | 0.41 |
| 1:D:369:SER:O | 1:D:373:GLU:HG2 | 2.21 | 0.41 |
| 1:E:530:ARG:HD2 | 1:E:545:GLN:NE2 | 2.36 | 0.41 |
| 1:E:884:TRP:HH2 | 2:L:78:THR:O | 2.02 | 0.41 |
| 1:F:1141:LEU:HG | 1:F:1155:ASN:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:228:ARG:HD3 | 1:G:256:SER:HB3 | 2.03 | 0.41 |
| 1:G:326:LEU:HA | 1:G:326:LEU:HD23 | 1.44 | 0.41 |
| 2:I:67:TYR:HD1 | 2:I:74:TYR:HB3 | 1.84 | 0.41 |
| 2:L:55:LYS:HG2 | 2:L:75:ILE:HG12 | 2.03 | 0.41 |
| 1:B:864:VAL:HB | 1:B:878:CYS:HB2 | 2.02 | 0.41 |
| 1:D:530:ARG:HD2 | 1:D:545:GLN:NE2 | 2.36 | 0.41 |
| 1:E:10:LEU:CD2 | 1:E:13:ARG:NH2 | 2.83 | 0.41 |
| 1:E:565:GLN:OE1 | 1:E:1212:THR:HB | 2.21 | 0.41 |
| 1:E:322:LEU:HD23 | 1:E:364:LEU:HD13 | 2.03 | 0.41 |
| 1:E:456:LEU:O | 1:E:459:LYS:HB3 | 2.21 | 0.41 |
| 1:E:511:LYS:HB2 | 1:E:563:ILE:HG13 | 2.02 | 0.41 |
| 1:F:565:GLN:OE1 | 1:F:1212:THR:HB | 2.21 | 0.41 |
| 1:F:862:TYR:HB3 | 1:F:883:SER:C | 2.41 | 0.41 |
| 1:G:565:GLN:OE1 | 1:G:1212:THR:HB | 2.21 | 0.41 |
| 1:G:456:LEU:O | 1:G:459:LYS:HB3 | 2.21 | 0.41 |
| 2:L:30:PRO:HB3 | 2:L:46:PHE:CD2 | 2.56 | 0.41 |
| 5:M:500:HEC:HMC1 | 5:M:500:HEC:CBC | 2.51 | 0.41 |
| 1:A:153:HIS:HA | 1:A:264:THR:O | 2.21 | 0.41 |
| 1:B:337:ARG:O | 1:B:340:TYR:N | 2.54 | 0.41 |
| 1:B:342:LEU:O | 1:B:346:GLN:HG3 | 2.21 | 0.41 |
| 1:B:676:SER:OG | 1:B:678:ASP:OD1 | 2.37 | 0.41 |
| 1:C:569:CYS:HB3 | 1:C:600:LYS:HZ3 | 1.85 | 0.41 |
| 1:D:474:SER:HA | 1:D:475:PRO:HD2 | 1.91 | 0.41 |
| 1:D:511:LYS:HB2 | 1:D:563:ILE:HG13 | 2.02 | 0.41 |
| 1:D:700:GLU:HB2 | 1:D:720:SER:HB2 | 2.03 | 0.41 |
| 1:E:342:LEU:O | 1:E:346:GLN:HG3 | 2.21 | 0.41 |
| 1:E:676:SER:OG | 1:E:678:ASP:OD1 | 2.37 | 0.41 |
| 1:E:947:GLN:HG2 | 1:E:958:TYR:HD1 | 1.85 | 0.41 |
| 1:F:1032:TRP:C | 1:F:1034:LEU:H | 2.23 | 0.41 |
| 1:F:153:HIS:HA | 1:F:264:THR:O | 2.21 | 0.41 |
| 1:F:400:LEU:HB3 | 1:F:404:TRP:HZ3 | 1.85 | 0.41 |
| 2:J:30:PRO:HB3 | 2:J:46:PHE:CD2 | 2.56 | 0.41 |
| 5:N:500:HEC:CBC | 5:N:500:HEC:HMC1 | 2.51 | 0.41 |
| 1:A:1155:ASN:HB3 | 1:A:1162:LEU:HB2 | 2.04 | 0.40 |
| 1:B:269:VAL:C | 1:B:271:ASP:H | 2.24 | 0.40 |
| 1:B:351:LYS:NZ | 1:B:365:ASP:OD2 | 2.54 | 0.40 |
| 1:C:1141:LEU:HG | 1:C:1155:ASN:HA | 2.03 | 0.40 |
| 1:C:322:LEU:HD23 | 1:C:364:LEU:HD13 | 2.03 | 0.40 |
| 1:C:326:LEU:HD23 | 1:C:326:LEU:HA | 1.44 | 0.40 |
| 1:C:885:VAL:HG13 | 1:C:900:SER:O | 2.21 | 0.40 |
| 1:D:1141:LEU:HG | 1:D:1155:ASN:HA | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1166:ALA:HA | 1:D:1167:PRO:HD2 | 1.93 | 0.40 |
| 1:D:37:ILE:HG12 | 3:Q:10:ARG:HD2 | 2.03 | 0.40 |
| 1:D:862:TYR:HB3 | 1:D:883:SER:C | 2.41 | 0.40 |
| 1:E:153:HIS:HA | 1:E:264:THR:O | 2.21 | 0.40 |
| 1:E:885:VAL:HG13 | 1:E:900:SER:O | 2.21 | 0.40 |
| 1:F:1155:ASN:HB3 | 1:F:1162:LEU:HB2 | 2.04 | 0.40 |
| 1:F:631:ALA:H | 1:F:665:PHE:HZ | 1.69 | 0.40 |
| 1:G:1141:LEU:HG | 1:G:1155:ASN:HA | 2.03 | 0.40 |
| 1:G:1155:ASN:HB3 | 1:G:1162:LEU:HB2 | 2.04 | 0.40 |
| 1:G:322:LEU:HD23 | 1:G:364:LEU:HD13 | 2.03 | 0.40 |
| 2:N:55:LYS:HG2 | 2:N:75:ILE:HG12 | 2.03 | 0.40 |
| 3:R:14:LEU:HA | 3:R:14:LEU:HD13 | 1.97 | 0.40 |
| 1:A:228:ARG:HD3 | 1:A:256:SER:HB3 | 2.03 | 0.40 |
| 1:A:282:VAL:HG12 | 1:A:282:VAL:O | 2.21 | 0.40 |
| 1:A:289:GLU:OE2 | 1:A:303:LYS:NZ | 2.43 | 0.40 |
| 1:D:1135:PHE:HE1 | 1:D:1142:LEU:HD13 | 1.85 | 0.40 |
| 1:D:565:GLN:OE1 | 1:D:1212:THR:HB | 2.21 | 0.40 |
| 1:D:153:HIS:HA | 1:D:264:THR:O | 2.21 | 0.40 |
| 1:E:1155:ASN:HB3 | 1:E:1162:LEU:HB2 | 2.04 | 0.40 |
| 1:E:196:LEU:O | 1:E:199:LEU:HB2 | 2.21 | 0.40 |
| 1:E:862:TYR:HB3 | 1:E:883:SER:C | 2.41 | 0.40 |
| 1:F:530:ARG:HD2 | 1:F:545:GLN:NE2 | 2.36 | 0.40 |
| 1:F:584:ALA:CA | 1:F:594:TYR:CE2 | 2.98 | 0.40 |
| 1:G:196:LEU:O | 1:G:199:LEU:HB2 | 2.21 | 0.40 |
| 2:H:30:PRO:HB3 | 2:H:46:PHE:CD2 | 2.56 | 0.40 |
| 5:H:500:HEC:HMC1 | 5:H:500:HEC:CBC | 2.51 | 0.40 |
| 5:I:500:HEC:CBC | 5:I:500:HEC:HMC1 | 2.51 | 0.40 |
| 5:J:500:HEC:CBC | 5:J:500:HEC:HMC1 | 2.51 | 0.40 |
| 3:P:34:LEU:HD12 | 3:P:34:LEU:HA | 1.93 | 0.40 |
| 1:A:885:VAL:HG13 | 1:A:900:SER:O | 2.21 | 0.40 |
| 1:B:884:TRP:HH2 | 2:I:79:LYS:N | 2.18 | 0.40 |
| 1:B:947:GLN:HG2 | 1:B:958:TYR:HD1 | 1.85 | 0.40 |
| 1:C:1032:TRP:C | 1:C:1034:LEU:H | 2.23 | 0.40 |
| 1:C:947:GLN:HG2 | 1:C:958:TYR:HD1 | 1.85 | 0.40 |
| 1:E:351:LYS:NZ | 1:E:365:ASP:OD2 | 2.54 | 0.40 |
| 1:E:7:ASN:CG | 1:F:236:PRO:CG | 2.81 | 0.40 |
| 1:E:989:GLU:HG2 | 1:E:991:VAL:H | 1.85 | 0.40 |
| 1:G:153:HIS:HA | 1:G:264:THR:O | 2.21 | 0.40 |
| 1:G:631:ALA:H | 1:G:665:PHE:HZ | 1.69 | 0.40 |
| 2:K:55:LYS:HG2 | 2:K:75:ILE:HG12 | 2.03 | 0.40 |
| 5:L:500:HEC:CBC | 5:L:500:HEC:HMC1 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:14:LEU:HD13 | 3:Q:14:LEU:HA | 1.98 | 0.40 |
| 1:A:1141:LEU:HG | 1:A:1155:ASN:HA | 2.03 | 0.40 |
| 1:A:196:LEU:O | 1:A:199:LEU:HB2 | 2.21 | 0.40 |
| 1:B:1146:ASP:HB2 | 1:B:1150:GLU:HG2 | 2.04 | 0.40 |
| 1:B:228:ARG:HD3 | 1:B:256:SER:HB3 | 2.03 | 0.40 |
| 1:B:266:ASP:CG | 1:B:268:SER:HG | 2.23 | 0.40 |
| 1:C:337:ARG:O | 1:C:340:TYR:N | 2.54 | 0.40 |
| 1:C:351:LYS:NZ | 1:C:365:ASP:OD2 | 2.54 | 0.40 |
| 1:C:884:TRP:HH2 | 2:J:79:LYS:N | 2.18 | 0.40 |
| 1:C:989:GLU:HG2 | 1:C:991:VAL:H | 1.85 | 0.40 |
| 1:D:597:TRP:CD2 | 1:D:600:LYS:HE3 | 2.57 | 0.40 |
| 1:E:631:ALA:H | 1:E:665:PHE:HZ | 1.69 | 0.40 |
| 1:F:289:GLU:OE2 | 1:F:303:LYS:NZ | 2.43 | 0.40 |
| 2:H:55:LYS:HG2 | 2:H:75:ILE:HG12 | 2.03 | 0.40 |
| 2:H:39:LYS:HD2 | 2:H:56:GLY:O | 2.22 | 0.40 |
| 2:I:71:PRO:CD | 2:I:84:GLY:HA2 | 2.52 | 0.40 |
| 2:J:55:LYS:HG2 | 2:J:75:ILE:HG12 | 2.03 | 0.40 |
| 2:M:39:LYS:HD2 | 2:M:56:GLY:O | 2.22 | 0.40 |
| 1:A:217:PRO:HG3 | 1:A:226:ARG:NH1 | 2.36 | 0.40 |
| 1:A:369:SER:O | 1:A:373:GLU:HG2 | 2.21 | 0.40 |
| 1:A:597:TRP:CD2 | 1:A:600:LYS:HE3 | 2.57 | 0.40 |
| 1:B:322:LEU:HD23 | 1:B:364:LEU:HD13 | 2.02 | 0.40 |
| 1:D:145:GLY:HA2 | 1:D:259:GLN:HE21 | 1.85 | 0.40 |
| 1:E:400:LEU:HB3 | 1:E:404:TRP:HZ3 | 1.84 | 0.40 |
| 2:I:55:LYS:HG2 | 2:I:75:ILE:HG12 | 2.03 | 0.40 |
| 5:K:500:HEC:CBC | 5:K:500:HEC:HMC1 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 EM 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 | 1135/1248 (91%) | 1045 (92%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | B | 1228/1248 (98%) | 1138 (93%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | C | 1135/1248 (91%) | 1045 (92%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | D | 1228/1248 (98%) | 1138 (93%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | E | 1228/1248 (98%) | 1138 (93%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | F | 1135/1248 (91%) | 1045 (92%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 1 | G | 1228/1248 (98%) | 1138 (93%) | 84 (7%) | 6 (0%) | 34 | 76 |
| 2 | H | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | I | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | J | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | K | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | L | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | M | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | N | 102/104 (98%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 3 | O | 93/95 (98%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | P | 93/95 (98%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | Q | 93/95 (98%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | R | 93/95 (98%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| All | All | 9403/9844 (96%) | 8741 (93%) | 620 (7%) | 42 (0%) | 43 | 79 |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1073 | ILE |
| 1 | B | 1073 | ILE |
| 1 | C | 1073 | ILE |
| 1 | D | 1073 | ILE |
| 1 | E | 1073 | ILE |
| 1 | F | 1073 | ILE |
| 1 | G | 1073 | ILE |
| 1 | A | 591 | GLY |
| 1 | B | 591 | GLY |
| 1 | C | 591 | GLY |
| 1 | D | 591 | GLY |
| 1 | E | 591 | GLY |
| 1 | F | 591 | GLY |
| 1 | G | 591 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 347 | ASN |
| 1 | B | 347 | ASN |
| 1 | C | 347 | ASN |
| 1 | D | 347 | ASN |
| 1 | E | 347 | ASN |
| 1 | F | 347 | ASN |
| 1 | G | 347 | ASN |
| 1 | A | 266 | ASP |
| 1 | B | 266 | ASP |
| 1 | C | 266 | ASP |
| 1 | D | 266 | ASP |
| 1 | E | 266 | ASP |
| 1 | F | 266 | ASP |
| 1 | G | 266 | ASP |
| 1 | A | 613 | PRO |
| 1 | B | 613 | PRO |
| 1 | C | 613 | PRO |
| 1 | D | 613 | PRO |
| 1 | E | 613 | PRO |
| 1 | F | 613 | PRO |
| 1 | G | 613 | PRO |
| 1 | A | 1205 | VAL |
| 1 | B | 1205 | VAL |
| 1 | C | 1205 | VAL |
| 1 | D | 1205 | VAL |
| 1 | E | 1205 | VAL |
| 1 | F | 1205 | VAL |
| 1 | G | 1205 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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 | 1022/1119 (91%) | 1019 (100%) | 3 (0%) | 94 | 96 |
| 1 | B | 1106/1119 (99%) | 1101 (100%) | 5 (0%) | 92 | 96 |
| 1 | C | 1022/1119 (91%) | 1019 (100%) | 3 (0%) | 94 | 96 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1 | D | 1106/1119 (99%) | 1101 (100%) | 5 (0%) | 92 | 96 |
| 1 | E | 1106/1119 (99%) | 1101 (100%) | 5 (0%) | 92 | 96 |
| 1 | F | 1022/1119 (91%) | 1019 (100%) | 3 (0%) | 94 | 96 |
| 1 | G | 1106/1119 (99%) | 1101 (100%) | 5 (0%) | 92 | 96 |
| 2 | H | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | I | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | J | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | K | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | L | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | M | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 2 | N | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 3 | O | 84/84 (100%) | 77 (92%) | 7 (8%) | 14 | 52 |
| 3 | P | 84/84 (100%) | 77 (92%) | 7 (8%) | 14 | 52 |
| 3 | Q | 84/84 (100%) | 77 (92%) | 7 (8%) | 14 | 52 |
| 3 | R | 84/84 (100%) | 77 (92%) | 7 (8%) | 14 | 52 |
| All | All | 8414/8757 (96%) | 8357 (99%) | 57 (1%) | 89 | 94 |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 391 | LYS |
| 1 | A | 392 | ASP |
| 1 | A | 884 | TRP |
| 1 | B | 58 | LYS |
| 1 | B | 81 | LYS |
| 1 | B | 391 | LYS |
| 1 | B | 392 | ASP |
| 1 | B | 884 | TRP |
| 1 | C | 391 | LYS |
| 1 | C | 392 | ASP |
| 1 | C | 884 | TRP |
| 1 | D | 58 | LYS |
| 1 | D | 81 | LYS |
| 1 | D | 391 | LYS |
| 1 | D | 392 | ASP |
| 1 | D | 884 | TRP |
| 1 | E | 58 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 81 | LYS |
| 1 | E | 391 | LYS |
| 1 | E | 392 | ASP |
| 1 | E | 884 | TRP |
| 1 | F | 391 | LYS |
| 1 | F | 392 | ASP |
| 1 | F | 884 | TRP |
| 1 | G | 58 | LYS |
| 1 | G | 81 | LYS |
| 1 | G | 391 | LYS |
| 1 | G | 392 | ASP |
| 1 | G | 884 | TRP |
| 3 | O | 10 | ARG |
| 3 | O | 14 | LEU |
| 3 | O | 20 | LEU |
| 3 | O | 34 | LEU |
| 3 | O | 87 | SER |
| 3 | O | 92 | ASN |
| 3 | O | 93 | ARG |
| 3 | P | 10 | ARG |
| 3 | P | 14 | LEU |
| 3 | P | 20 | LEU |
| 3 | P | 34 | LEU |
| 3 | P | 87 | SER |
| 3 | P | 92 | ASN |
| 3 | P | 93 | ARG |
| 3 | Q | 10 | ARG |
| 3 | Q | 14 | LEU |
| 3 | Q | 20 | LEU |
| 3 | Q | 34 | LEU |
| 3 | Q | 87 | SER |
| 3 | Q | 92 | ASN |
| 3 | Q | 93 | ARG |
| 3 | R | 10 | ARG |
| 3 | R | 14 | LEU |
| 3 | R | 20 | LEU |
| 3 | R | 34 | LEU |
| 3 | R | 87 | SER |
| 3 | R | 92 | ASN |
| 3 | R | 93 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 121 | GLN |
| 1 | A | 201 | ASN |
| 1 | A | 214 | GLN |
| 1 | A | 602 | ASN |
| 1 | A | 703 | ASN |
| 1 | A | 712 | HIS |
| 1 | A | 713 | HIS |
| 1 | A | 782 | ASN |
| 1 | A | 819 | ASN |
| 1 | A | 844 | GLN |
| 1 | A | 924 | GLN |
| 1 | A | 992 | ASN |
| 1 | A | 1076 | ASN |
| 1 | A | 1126 | HIS |
| 1 | B | 11 | GLN |
| 1 | B | 45 | ASN |
| 1 | B | 51 | GLN |
| 1 | B | 201 | ASN |
| 1 | B | 214 | GLN |
| 1 | B | 602 | ASN |
| 1 | B | 703 | ASN |
| 1 | B | 712 | HIS |
| 1 | B | 713 | HIS |
| 1 | B | 782 | ASN |
| 1 | B | 819 | ASN |
| 1 | B | 844 | GLN |
| 1 | B | 924 | GLN |
| 1 | B | 992 | ASN |
| 1 | B | 1076 | ASN |
| 1 | B | 1126 | HIS |
| 1 | C | 121 | GLN |
| 1 | C | 201 | ASN |
| 1 | C | 214 | GLN |
| 1 | C | 416 | GLN |
| 1 | C | 602 | ASN |
| 1 | C | 703 | ASN |
| 1 | C | 712 | HIS |
| 1 | C | 713 | HIS |
| 1 | C | 782 | ASN |
| 1 | C | 819 | ASN |
| 1 | C | 844 | GLN |
| 1 | C | 924 | GLN |
| 1 | C | 992 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1076 | ASN |
| 1 | C | 1126 | HIS |
| 1 | D | 11 | GLN |
| 1 | D | 51 | GLN |
| 1 | D | 201 | ASN |
| 1 | D | 214 | GLN |
| 1 | D | 416 | GLN |
| 1 | D | 602 | ASN |
| 1 | D | 703 | ASN |
| 1 | D | 712 | HIS |
| 1 | D | 713 | HIS |
| 1 | D | 782 | ASN |
| 1 | D | 819 | ASN |
| 1 | D | 844 | GLN |
| 1 | D | 924 | GLN |
| 1 | D | 992 | ASN |
| 1 | D | 1076 | ASN |
| 1 | D | 1126 | HIS |
| 1 | E | 11 | GLN |
| 1 | E | 45 | ASN |
| 1 | E | 51 | GLN |
| 1 | E | 201 | ASN |
| 1 | E | 214 | GLN |
| 1 | E | 602 | ASN |
| 1 | E | 703 | ASN |
| 1 | E | 712 | HIS |
| 1 | E | 713 | HIS |
| 1 | E | 782 | ASN |
| 1 | E | 819 | ASN |
| 1 | E | 844 | GLN |
| 1 | E | 924 | GLN |
| 1 | E | 992 | ASN |
| 1 | E | 1076 | ASN |
| 1 | E | 1126 | HIS |
| 1 | F | 201 | ASN |
| 1 | F | 214 | GLN |
| 1 | F | 416 | GLN |
| 1 | F | 602 | ASN |
| 1 | F | 703 | ASN |
| 1 | F | 712 | HIS |
| 1 | F | 713 | HIS |
| 1 | F | 782 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | F | 819 | ASN |
| 1 | F | 844 | GLN |
| 1 | F | 924 | GLN |
| 1 | F | 992 | ASN |
| 1 | F | 1076 | ASN |
| 1 | F | 1126 | HIS |
| 1 | G | 11 | GLN |
| 1 | G | 45 | ASN |
| 1 | G | 51 | GLN |
| 1 | G | 121 | GLN |
| 1 | G | 201 | ASN |
| 1 | G | 214 | GLN |
| 1 | G | 416 | GLN |
| 1 | G | 602 | ASN |
| 1 | G | 703 | ASN |
| 1 | G | 712 | HIS |
| 1 | G | 713 | HIS |
| 1 | G | 782 | ASN |
| 1 | G | 819 | ASN |
| 1 | G | 844 | GLN |
| 1 | G | 924 | GLN |
| 1 | G | 992 | ASN |
| 1 | G | 1076 | ASN |
| 1 | G | 1126 | HIS |
| 2 | H | 70 | ASN |
| 2 | I | 70 | ASN |
| 2 | K | 70 | ASN |
| 2 | M | 70 | ASN |
| 2 | N | 70 | ASN |
| 3 | O | 44 | GLN |
| 3 | O | 92 | ASN |
| 3 | P | 44 | GLN |
| 3 | P | 92 | ASN |
| 3 | Q | 44 | GLN |
| 3 | Q | 92 | ASN |
| 3 | R | 38 | HIS |
| 3 | R | 44 | GLN |
| 3 | R | 92 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 4 | DTP | A | 1301 | - | 25,32,32 | 3.23 | 7 (28%) | 26,50,50 | 2.80 | 3 (11%) |
| 4 | DTP | B | 1301 | - | 25,32,32 | 3.22 | 7 (28%) | 26,50,50 | 2.80 | 3 (11%) |
| 4 | DTP | C | 1301 | - | 25,32,32 | 3.23 | 7 (28%) | 26,50,50 | 2.80 | 3 (11%) |
| 4 | DTP | D | 1301 | - | 25,32,32 | 3.24 | 7 (28%) | 26,50,50 | 2.81 | 3 (11%) |
| 4 | DTP | E | 1301 | - | 25,32,32 | 3.23 | 7 (28%) | 26,50,50 | 2.81 | 3 (11%) |
| 4 | DTP | F | 1301 | - | 25,32,32 | 3.23 | 7 (28%) | 26,50,50 | 2.79 | 3 (11%) |
| 4 | DTP | G | 1301 | - | 25,32,32 | 3.23 | 7 (28%) | 26,50,50 | 2.81 | 3 (11%) |
| 5 | HEC | H | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.84 | 4 (21%) |
| 5 | HEC | I | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.83 | 4 (21%) |
| 5 | HEC | J | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.83 | 4 (21%) |
| 5 | HEC | K | 500 | - | 24,50,50 | 2.46 | 6 (25%) | 19,82,82 | 1.84 | 4 (21%) |
| 5 | HEC | L | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.84 | 4 (21%) |
| 5 | HEC | M | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.84 | 4 (21%) |
| 5 | HEC | N | 500 | - | 24,50,50 | 2.45 | 6 (25%) | 19,82,82 | 1.84 | 4 (21%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 4 | DTP | A | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | B | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | C | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | D | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | E | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | F | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 4 | DTP | G | 1301 | - | - | 0/18/34/34 | 0/3/3/3 |
| 5 | HEC | H | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | I | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | J | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | K | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | L | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | M | 500 | - | - | 0/6/54/54 | 0/0/8/8 |
| 5 | HEC | N | 500 | - | - | 0/6/54/54 | 0/0/8/8 |

All (91) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 4 | D | 1301 | DTP | C2'-C3' | -11.56 | 1.21 | 1.52 |
| 4 | G | 1301 | DTP | C2'-C3' | -11.55 | 1.21 | 1.52 |
| 4 | F | 1301 | DTP | C2'-C3' | -11.55 | 1.21 | 1.52 |
| 4 | A | 1301 | DTP | C2'-C3' | -11.54 | 1.21 | 1.52 |
| 4 | E | 1301 | DTP | C2'-C3' | -11.54 | 1.21 | 1.52 |
| 4 | C | 1301 | DTP | C2'-C3' | -11.54 | 1.21 | 1.52 |
| 4 | B | 1301 | DTP | C2'-C3' | -11.51 | 1.21 | 1.52 |
| 4 | G | 1301 | DTP | O4'-C4' | -8.06 | 1.26 | 1.45 |
| 4 | D | 1301 | DTP | O4'-C4' | -8.05 | 1.26 | 1.45 |
| 4 | F | 1301 | DTP | O4'-C4' | -8.04 | 1.26 | 1.45 |
| 4 | A | 1301 | DTP | O4'-C4' | -8.04 | 1.26 | 1.45 |
| 4 | E | 1301 | DTP | O4'-C4' | -8.04 | 1.26 | 1.45 |
| 4 | C | 1301 | DTP | O4'-C4' | -8.04 | 1.26 | 1.45 |
| 4 | B | 1301 | DTP | O4'-C4' | -8.02 | 1.26 | 1.45 |
| 5 | K | 500 | HEC | C3B-C2B | -5.59 | 1.35 | 1.40 |
| 5 | N | 500 | HEC | C3B-C2B | -5.55 | 1.35 | 1.40 |
| 5 | J | 500 | HEC | C3B-C2B | -5.55 | 1.35 | 1.40 |
| 5 | L | 500 | HEC | C3B-C2B | -5.55 | 1.35 | 1.40 |
| 5 | I | 500 | HEC | C3B-C2B | -5.54 | 1.35 | 1.40 |
| 5 | M | 500 | HEC | C3B-C2B | -5.54 | 1.35 | 1.40 |
| 5 | H | 500 | HEC | C3B-C2B | -5.52 | 1.35 | 1.40 |
| 5 | J | 500 | HEC | C3C-C2C | -5.21 | 1.35 | 1.40 |
| 5 | I | 500 | HEC | C3C-C2C | -5.20 | 1.35 | 1.40 |
| 5 | K | 500 | HEC | C3C-C2C | -5.20 | 1.35 | 1.40 |
| 5 | H | 500 | HEC | C3C-C2C | -5.20 | 1.35 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | L | 500 | HEC | C3C-C2C | -5.18 | 1.35 | 1.40 |
| 5 | N | 500 | HEC | C3C-C2C | -5.18 | 1.35 | 1.40 |
| 5 | M | 500 | HEC | C3C-C2C | -5.17 | 1.35 | 1.40 |
| 5 | N | 500 | HEC | CBB-CAB | -3.87 | 1.34 | 1.49 |
| 5 | H | 500 | HEC | CBB-CAB | -3.86 | 1.34 | 1.49 |
| 5 | M | 500 | HEC | CBB-CAB | -3.86 | 1.34 | 1.49 |
| 5 | L | 500 | HEC | CBB-CAB | -3.86 | 1.34 | 1.49 |
| 5 | J | 500 | HEC | CBB-CAB | -3.86 | 1.34 | 1.49 |
| 5 | K | 500 | HEC | CBB-CAB | -3.85 | 1.34 | 1.49 |
| 5 | I | 500 | HEC | CBB-CAB | -3.85 | 1.34 | 1.49 |
| 5 | H | 500 | HEC | CBC-CAC | -3.80 | 1.34 | 1.49 |
| 5 | J | 500 | HEC | CBC-CAC | -3.80 | 1.34 | 1.49 |
| 5 | N | 500 | HEC | CBC-CAC | -3.80 | 1.34 | 1.49 |
| 5 | L | 500 | HEC | CBC-CAC | -3.79 | 1.34 | 1.49 |
| 5 | K | 500 | HEC | CBC-CAC | -3.79 | 1.34 | 1.49 |
| 5 | I | 500 | HEC | CBC-CAC | -3.79 | 1.34 | 1.49 |
| 5 | M | 500 | HEC | CBC-CAC | -3.78 | 1.34 | 1.49 |
| 4 | C | 1301 | DTP | C5-C4 | -2.82 | 1.34 | 1.40 |
| 4 | A | 1301 | DTP | C5-C4 | -2.80 | 1.34 | 1.40 |
| 4 | F | 1301 | DTP | C5-C4 | -2.80 | 1.34 | 1.40 |
| 4 | B | 1301 | DTP | C5-C4 | -2.80 | 1.34 | 1.40 |
| 4 | D | 1301 | DTP | C5-C4 | -2.79 | 1.34 | 1.40 |
| 4 | E | 1301 | DTP | C5-C4 | -2.79 | 1.34 | 1.40 |
| 4 | G | 1301 | DTP | C5-C4 | -2.79 | 1.34 | 1.40 |
| 5 | H | 500 | HEC | CAA-C2A | 2.02 | 1.54 | 1.52 |
| 5 | I | 500 | HEC | CAA-C2A | 2.06 | 1.54 | 1.52 |
| 5 | K | 500 | HEC | CAA-C2A | 2.07 | 1.54 | 1.52 |
| 5 | L | 500 | HEC | CAA-C2A | 2.08 | 1.54 | 1.52 |
| 5 | N | 500 | HEC | CAA-C2A | 2.10 | 1.55 | 1.52 |
| 5 | J | 500 | HEC | CAA-C2A | 2.11 | 1.55 | 1.52 |
| 5 | M | 500 | HEC | CAA-C2A | 2.13 | 1.55 | 1.52 |
| 4 | F | 1301 | DTP | C2-N3 | 2.19 | 1.36 | 1.32 |
| 4 | B | 1301 | DTP | C2-N3 | 2.22 | 1.36 | 1.32 |
| 4 | A | 1301 | DTP | C2-N3 | 2.22 | 1.36 | 1.32 |
| 4 | C | 1301 | DTP | C2-N3 | 2.23 | 1.36 | 1.32 |
| 4 | E | 1301 | DTP | C2-N3 | 2.24 | 1.36 | 1.32 |
| 4 | D | 1301 | DTP | C2-N3 | 2.24 | 1.36 | 1.32 |
| 4 | G | 1301 | DTP | C2-N3 | 2.27 | 1.36 | 1.32 |
| 4 | E | 1301 | DTP | O3'-C3' | 2.55 | 1.49 | 1.43 |
| 4 | D | 1301 | DTP | O3'-C3' | 2.56 | 1.49 | 1.43 |
| 4 | B | 1301 | DTP | O3'-C3' | 2.56 | 1.49 | 1.43 |
| 4 | A | 1301 | DTP | O3'-C3' | 2.57 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4 | C | 1301 | DTP | O3'-C3' | 2.58 | 1.49 | 1.43 |
| 4 | F | 1301 | DTP | O3'-C3' | 2.59 | 1.49 | 1.43 |
| 4 | G | 1301 | DTP | O3'-C3' | 2.62 | 1.49 | 1.43 |
| 4 | B | 1301 | DTP | O4'-C1' | 3.20 | 1.49 | 1.42 |
| 4 | F | 1301 | DTP | O4'-C1' | 3.20 | 1.49 | 1.42 |
| 4 | C | 1301 | DTP | O4'-C1' | 3.20 | 1.49 | 1.42 |
| 4 | G | 1301 | DTP | O4'-C1' | 3.21 | 1.49 | 1.42 |
| 4 | A | 1301 | DTP | O4'-C1' | 3.22 | 1.49 | 1.42 |
| 4 | D | 1301 | DTP | O4'-C1' | 3.23 | 1.49 | 1.42 |
| 4 | E | 1301 | DTP | O4'-C1' | 3.25 | 1.49 | 1.42 |
| 4 | F | 1301 | DTP | C3'-C4' | 3.88 | 1.64 | 1.53 |
| 4 | A | 1301 | DTP | C3'-C4' | 3.89 | 1.64 | 1.53 |
| 4 | B | 1301 | DTP | C3'-C4' | 3.89 | 1.64 | 1.53 |
| 4 | C | 1301 | DTP | C3'-C4' | 3.89 | 1.64 | 1.53 |
| 4 | G | 1301 | DTP | C3'-C4' | 3.89 | 1.64 | 1.53 |
| 4 | E | 1301 | DTP | C3'-C4' | 3.91 | 1.64 | 1.53 |
| 4 | D | 1301 | DTP | C3'-C4' | 3.92 | 1.64 | 1.53 |
| 5 | N | 500 | HEC | C3D-C2D | 5.43 | 1.53 | 1.37 |
| 5 | M | 500 | HEC | C3D-C2D | 5.45 | 1.53 | 1.37 |
| 5 | L | 500 | HEC | C3D-C2D | 5.46 | 1.53 | 1.37 |
| 5 | J | 500 | HEC | C3D-C2D | 5.46 | 1.53 | 1.37 |
| 5 | H | 500 | HEC | C3D-C2D | 5.47 | 1.53 | 1.37 |
| 5 | I | 500 | HEC | C3D-C2D | 5.47 | 1.53 | 1.37 |
| 5 | K | 500 | HEC | C3D-C2D | 5.48 | 1.53 | 1.37 |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 4 | D | 1301 | DTP | N3-C2-N1 | -11.29 | 120.00 | 128.87 |
| 4 | G | 1301 | DTP | N3-C2-N1 | -11.29 | 120.01 | 128.87 |
| 4 | E | 1301 | DTP | N3-C2-N1 | -11.28 | 120.01 | 128.87 |
| 4 | C | 1301 | DTP | N3-C2-N1 | -11.24 | 120.04 | 128.87 |
| 4 | A | 1301 | DTP | N3-C2-N1 | -11.24 | 120.04 | 128.87 |
| 4 | B | 1301 | DTP | N3-C2-N1 | -11.21 | 120.07 | 128.87 |
| 4 | F | 1301 | DTP | N3-C2-N1 | -11.16 | 120.10 | 128.87 |
| 4 | D | 1301 | DTP | N6-C6-N1 | -7.32 | 106.23 | 118.52 |
| 4 | G | 1301 | DTP | N6-C6-N1 | -7.32 | 106.24 | 118.52 |
| 4 | E | 1301 | DTP | N6-C6-N1 | -7.32 | 106.24 | 118.52 |
| 4 | F | 1301 | DTP | N6-C6-N1 | -7.32 | 106.24 | 118.52 |
| 4 | B | 1301 | DTP | N6-C6-N1 | -7.31 | 106.25 | 118.52 |
| 4 | A | 1301 | DTP | N6-C6-N1 | -7.31 | 106.25 | 118.52 |
| 4 | C | 1301 | DTP | N6-C6-N1 | -7.29 | 106.28 | 118.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | K | 500 | HEC | CMB-C2B-C1B | -3.49 | 122.38 | 128.31 |
| 5 | I | 500 | HEC | CMB-C2B-C1B | -3.46 | 122.42 | 128.31 |
| 5 | N | 500 | HEC | CMB-C2B-C1B | -3.46 | 122.43 | 128.31 |
| 5 | J | 500 | HEC | CMB-C2B-C1B | -3.46 | 122.43 | 128.31 |
| 5 | M | 500 | HEC | CMB-C2B-C1B | -3.46 | 122.43 | 128.31 |
| 5 | L | 500 | HEC | CMB-C2B-C1B | -3.46 | 122.43 | 128.31 |
| 5 | H | 500 | HEC | CMB-C2B-C1B | -3.45 | 122.44 | 128.31 |
| 4 | D | 1301 | DTP | C1'-N9-C4 | -2.99 | 122.70 | 127.07 |
| 4 | B | 1301 | DTP | C1'-N9-C4 | -2.98 | 122.72 | 127.07 |
| 4 | E | 1301 | DTP | C1'-N9-C4 | -2.98 | 122.72 | 127.07 |
| 5 | N | 500 | HEC | CMC-C2C-C1C | -2.97 | 123.26 | 128.31 |
| 4 | A | 1301 | DTP | C1'-N9-C4 | -2.96 | 122.74 | 127.07 |
| 5 | J | 500 | HEC | CMC-C2C-C1C | -2.96 | 123.28 | 128.31 |
| 5 | M | 500 | HEC | CMC-C2C-C1C | -2.96 | 123.28 | 128.31 |
| 4 | G | 1301 | DTP | C1'-N9-C4 | -2.96 | 122.75 | 127.07 |
| 5 | I | 500 | HEC | CMC-C2C-C1C | -2.96 | 123.28 | 128.31 |
| 5 | L | 500 | HEC | CMC-C2C-C1C | -2.95 | 123.29 | 128.31 |
| 5 | H | 500 | HEC | CMC-C2C-C1C | -2.95 | 123.29 | 128.31 |
| 4 | F | 1301 | DTP | C1'-N9-C4 | -2.95 | 122.76 | 127.07 |
| 4 | C | 1301 | DTP | C1'-N9-C4 | -2.95 | 122.77 | 127.07 |
| 5 | K | 500 | HEC | CMC-C2C-C1C | -2.94 | 123.31 | 128.31 |
| 5 | I | 500 | HEC | CMC-C2C-C3C | 2.96 | 129.10 | 125.67 |
| 5 | K | 500 | HEC | CMC-C2C-C3C | 2.96 | 129.10 | 125.67 |
| 5 | L | 500 | HEC | CMC-C2C-C3C | 2.99 | 129.13 | 125.67 |
| 5 | J | 500 | HEC | CMC-C2C-C3C | 2.99 | 129.13 | 125.67 |
| 5 | H | 500 | HEC | CMC-C2C-C3C | 2.99 | 129.14 | 125.67 |
| 5 | M | 500 | HEC | CMC-C2C-C3C | 3.01 | 129.16 | 125.67 |
| 5 | N | 500 | HEC | CMC-C2C-C3C | 3.03 | 129.18 | 125.67 |
| 5 | J | 500 | HEC | CMB-C2B-C3B | 3.35 | 129.55 | 125.67 |
| 5 | I | 500 | HEC | CMB-C2B-C3B | 3.38 | 129.58 | 125.67 |
| 5 | N | 500 | HEC | CMB-C2B-C3B | 3.38 | 129.59 | 125.67 |
| 5 | L | 500 | HEC | CMB-C2B-C3B | 3.38 | 129.59 | 125.67 |
| 5 | M | 500 | HEC | CMB-C2B-C3B | 3.40 | 129.62 | 125.67 |
| 5 | H | 500 | HEC | CMB-C2B-C3B | 3.41 | 129.62 | 125.67 |
| 5 | K | 500 | HEC | CMB-C2B-C3B | 3.43 | 129.64 | 125.67 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 49 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | A | 1301 | DTP | 3 | 0 |
| 4 | B | 1301 | DTP | 3 | 0 |
| 4 | C | 1301 | DTP | 3 | 0 |
| 4 | D | 1301 | DTP | 3 | 0 |
| 4 | E | 1301 | DTP | 3 | 0 |
| 4 | F | 1301 | DTP | 3 | 0 |
| 4 | G | 1301 | DTP | 3 | 0 |
| 5 | H | 500 | HEC | 4 | 0 |
| 5 | I | 500 | HEC | 4 | 0 |
| 5 | J | 500 | HEC | 4 | 0 |
| 5 | K | 500 | HEC | 4 | 0 |
| 5 | L | 500 | HEC | 4 | 0 |
| 5 | M | 500 | HEC | 4 | 0 |
| 5 | N | 500 | HEC | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.