# Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 02:19 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5IJO |
| EMDB ID | : | EMD-8085 |
| Title | : | Alternative composite structure of the inner ring of the human nuclear pore complex (16 copies of Nup188, 16 copies of Nup205) |
| Authors | : | Kosinski, J.; Mosalaganti, S.; von Appen, A.; Beck, M. |
| Deposited on | : | 2016-03-02 |
| Resolution | : | 21.40 Å(reported) |

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

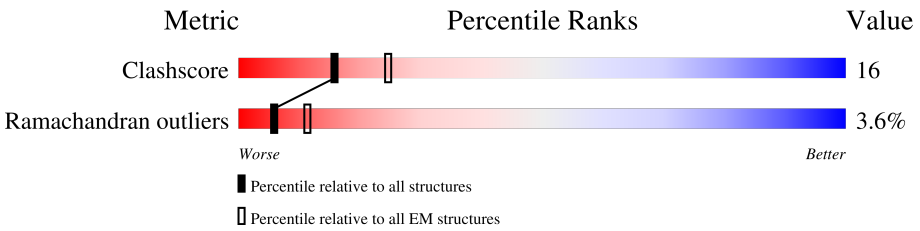
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 21.40 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1391 | • 43% • 53% |
| 1 | B | 1391 | 5% 43% • 53% |
| 1 | E | 1391 | 10% 73% • • 22% |
| 1 | K | 1391 | 35% 73% 5% • 22% |
| 1 | Q | 1391 | 9% 73% • 22% |
| 1 | W | 1391 | 17% 73% 5% 22% |
| 2 | C | 819 | 12% 64% 11% • 22% |
| 2 | I | 819 | 14% 66% 10% • 22% |
| 2 | O | 819 | 9% 65% 10% • 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | U | 819 | 16% 66% 10% 22% |
| 3 | D | 2012 | 5% 45% 49% |
| 3 | P | 2012 | 5% 46% 49% |
| 4 | F | 507 | 13% 35% 16% 9% 5% 34% |
| 4 | L | 507 | 13% 35% 16% 9% 5% 34% |
| 4 | R | 507 | 15% 35% 16% 9% 5% 34% |
| 4 | X | 507 | 10% 36% 16% 9% 5% 34% |
| 5 | G | 599 | 17% 7% 71% |
| 5 | M | 599 | 17% 7% 71% |
| 5 | S | 599 | 17% 7% 71% |
| 5 | Y | 599 | 17% 7% 71% |
| 6 | H | 522 | 6% 18% 11% 68% |
| 6 | N | 522 | 18% 11% 68% |
| 6 | T | 522 | 8% 18% 11% 68% |
| 6 | Z | 522 | 5% 18% 11% 68% |
| 7 | J | 1749 | 9% 63% 7% 28% |
| 7 | V | 1749 | 7% 64% 7% 28% |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 76526 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 Nuclear pore complex protein Nup155.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 1 | A | 650 | 3214 | 1914 | 650 | 650 | 0 | 0 |
| 1 | B | 650 | 3214 | 1914 | 650 | 650 | 0 | 0 |
| 1 | E | 1083 | 5366 | 3200 | 1083 | 1083 | 0 | 0 |
| 1 | K | 1083 | 5366 | 3200 | 1083 | 1083 | 0 | 0 |
| 1 | Q | 1083 | 5366 | 3200 | 1083 | 1083 | 0 | 0 |
| 1 | W | 1083 | 5366 | 3200 | 1083 | 1083 | 0 | 0 |

- Molecule 2 is a protein called Nuclear pore complex protein Nup93.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 2 | C | 636 | 3152 | 1880 | 636 | 636 | 0 | 0 |
| 2 | I | 636 | 3152 | 1880 | 636 | 636 | 0 | 0 |
| 2 | O | 636 | 3152 | 1880 | 636 | 636 | 0 | 0 |
| 2 | U | 636 | 3152 | 1880 | 636 | 636 | 0 | 0 |

- Molecule 3 is a protein called Nuclear pore complex protein Nup205.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | D | 1028 | 5094 | 3038 | 1028 | 1028 | 0 | 0 |
| 3 | P | 1028 | 5094 | 3038 | 1028 | 1028 | 0 | 0 |

- Molecule 4 is a protein called Nucleoporin p54.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 4 | F | 335 | 1658 | 988 | 335 | 335 | 0 | 0 |
| 4 | L | 335 | 1658 | 988 | 335 | 335 | 0 | 0 |
| 4 | R | 335 | 1658 | 988 | 335 | 335 | 0 | 0 |
| 4 | X | 335 | 1658 | 988 | 335 | 335 | 0 | 0 |

- Molecule 5 is a protein called Nucleoporin p58/p45.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | G | 171 | 853 | 511 | 171 | 171 | 0 | 0 |
| 5 | M | 171 | 853 | 511 | 171 | 171 | 0 | 0 |
| 5 | S | 171 | 853 | 511 | 171 | 171 | 0 | 0 |
| 5 | Y | 171 | 853 | 511 | 171 | 171 | 0 | 0 |

- Molecule 6 is a protein called Nuclear pore glycoprotein p62.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 6 | H | 169 | 842 | 504 | 169 | 169 | 0 | 0 |
| 6 | N | 169 | 842 | 504 | 169 | 169 | 0 | 0 |
| 6 | T | 169 | 842 | 504 | 169 | 169 | 0 | 0 |
| 6 | Z | 169 | 842 | 504 | 169 | 169 | 0 | 0 |

- Molecule 7 is a protein called Nucleoporin NUP188 homolog.

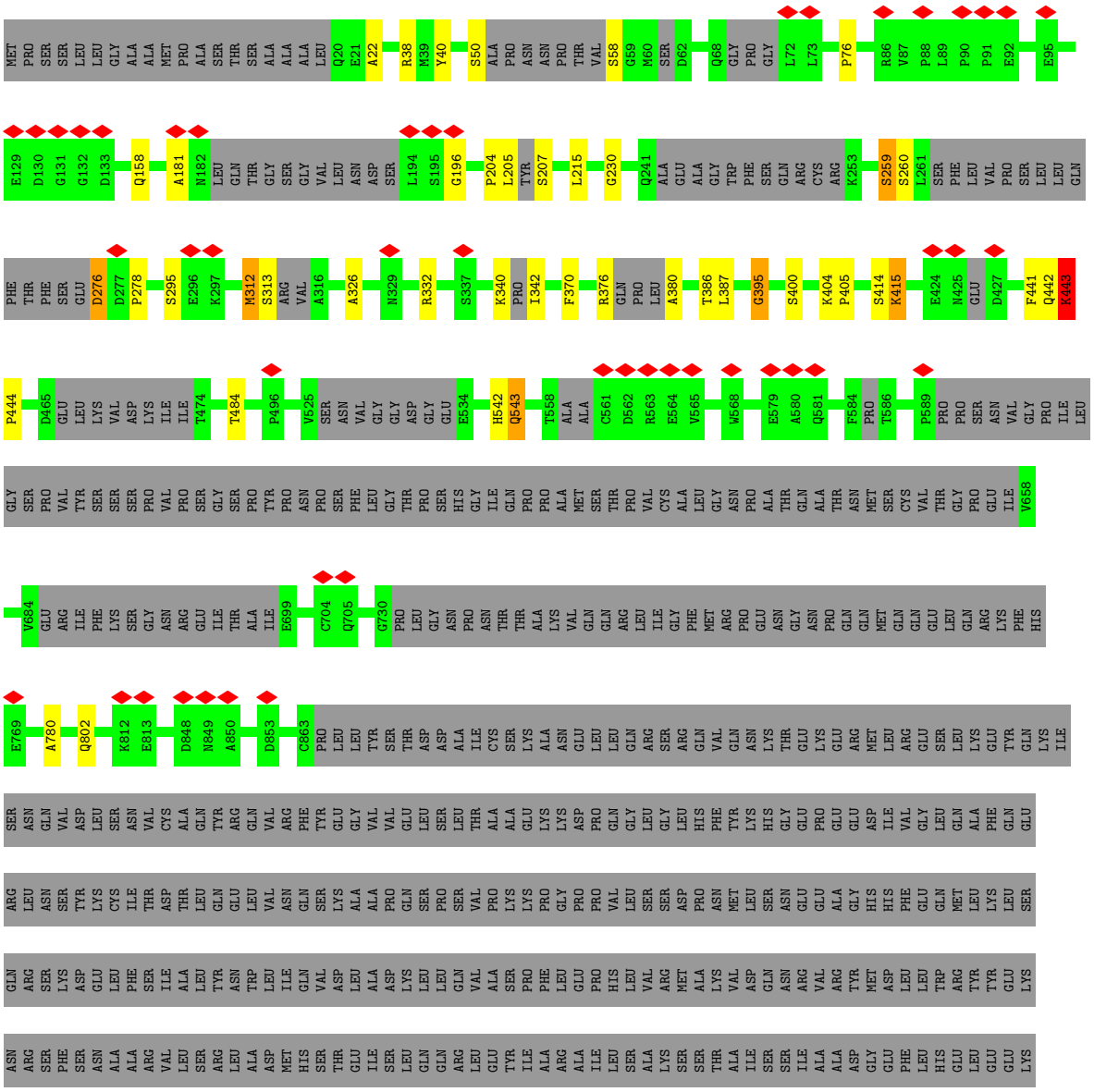
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 7 | J | 1256 | 6213 | 3701 | 1256 | 1256 | 0 | 0 |
| 7 | V | 1256 | 6213 | 3701 | 1256 | 1256 | 0 | 0 |

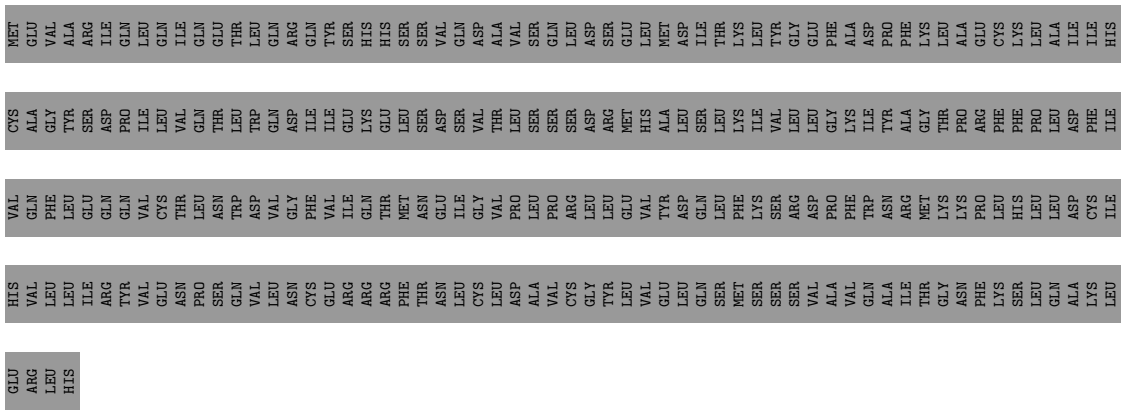
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Nuclear pore complex protein Nup155

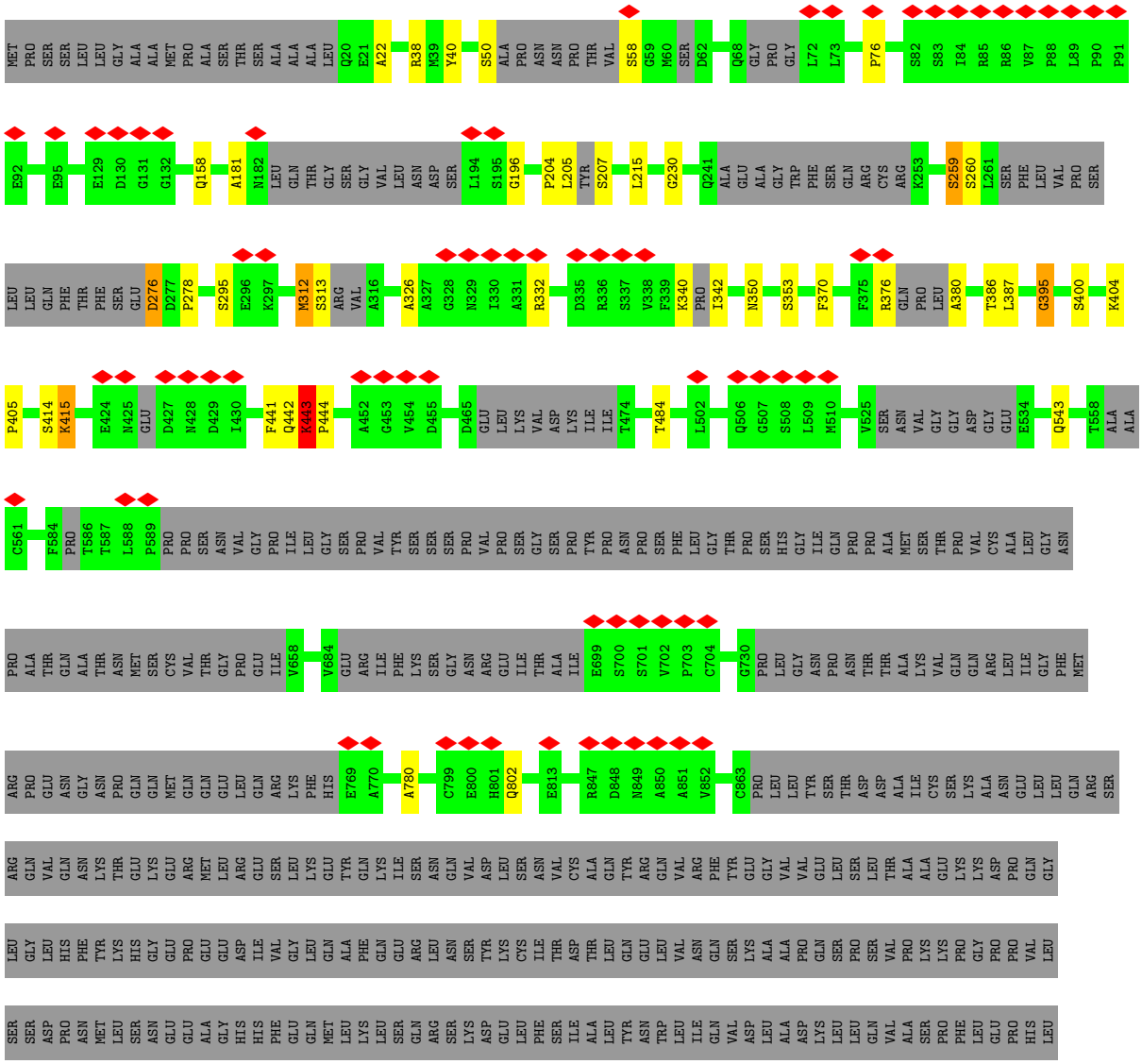
Chain A:

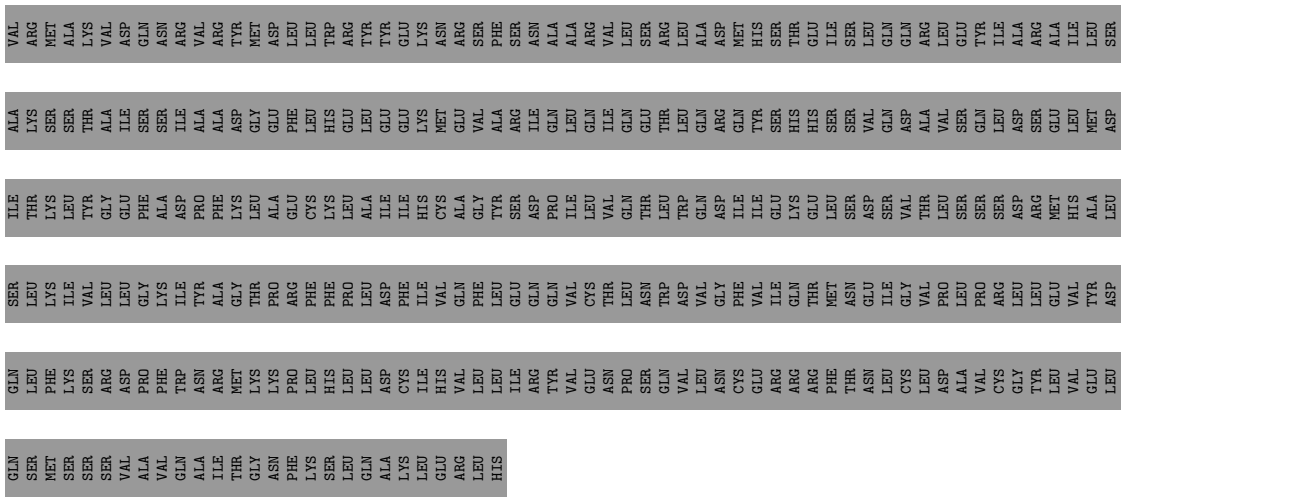




- Molecule 1: Nuclear pore complex protein Nup155

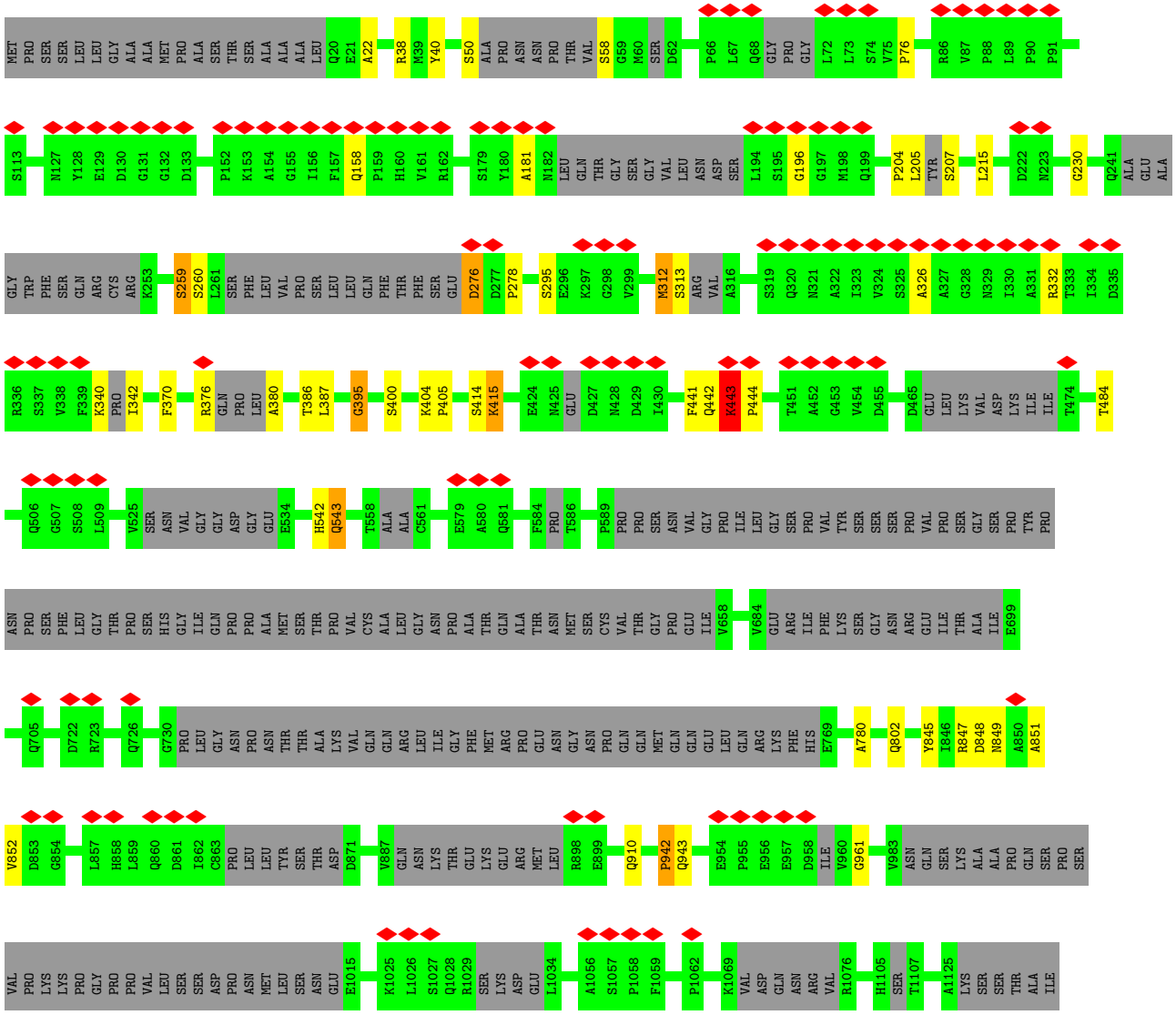
Chain B: 5% 43% • 53%

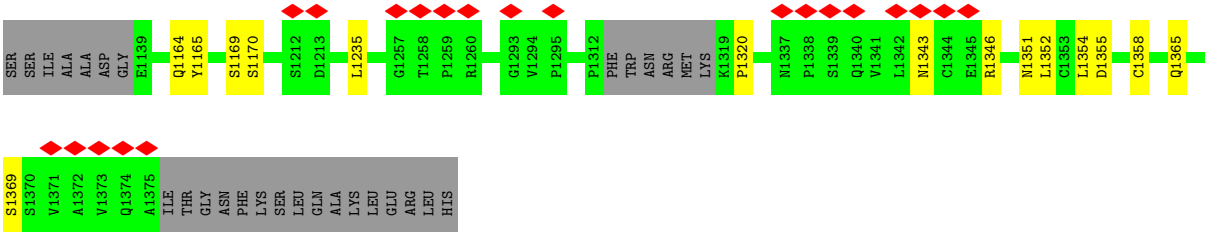




- Molecule 1: Nuclear pore complex protein Nup155

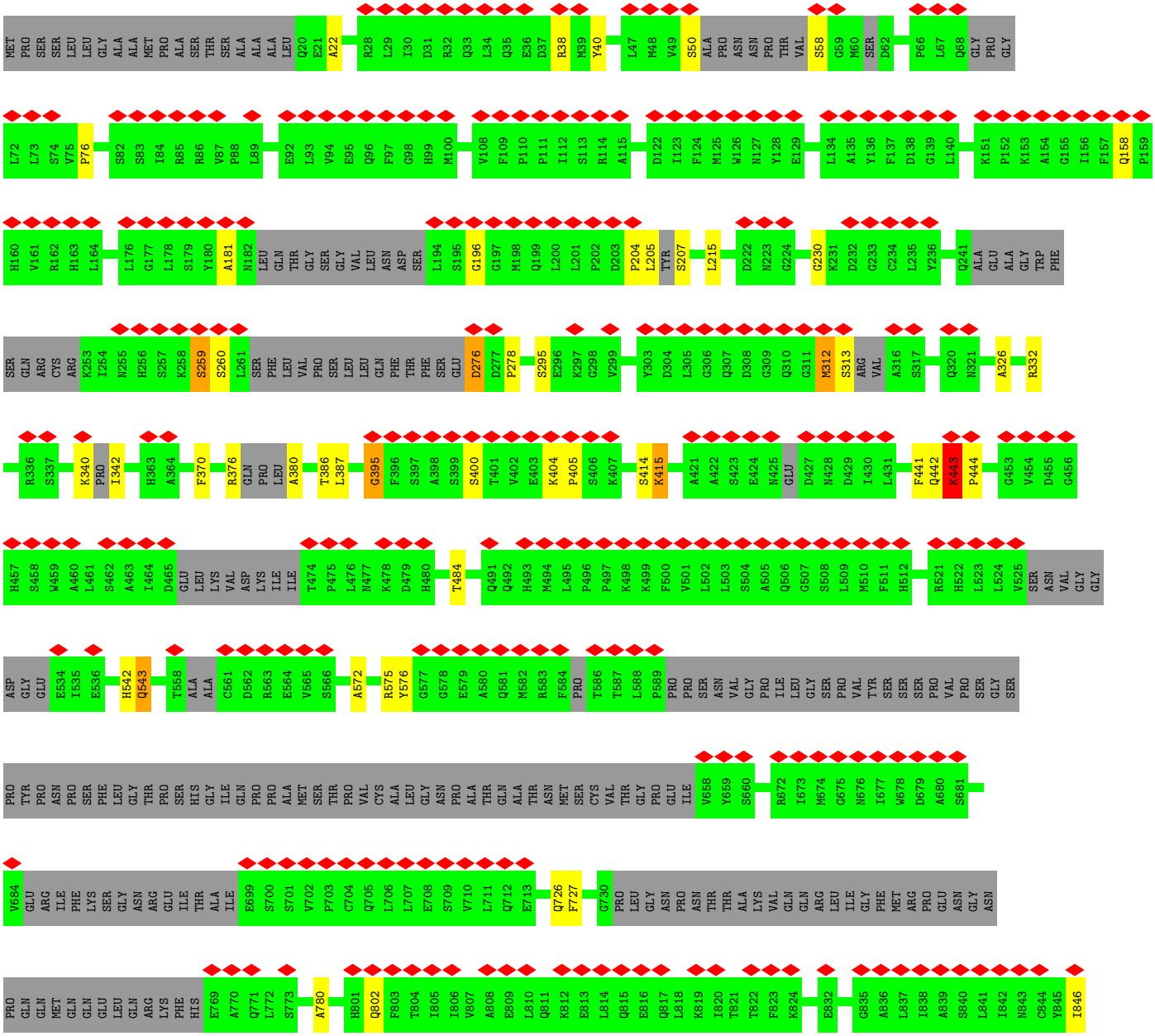
Chain E:

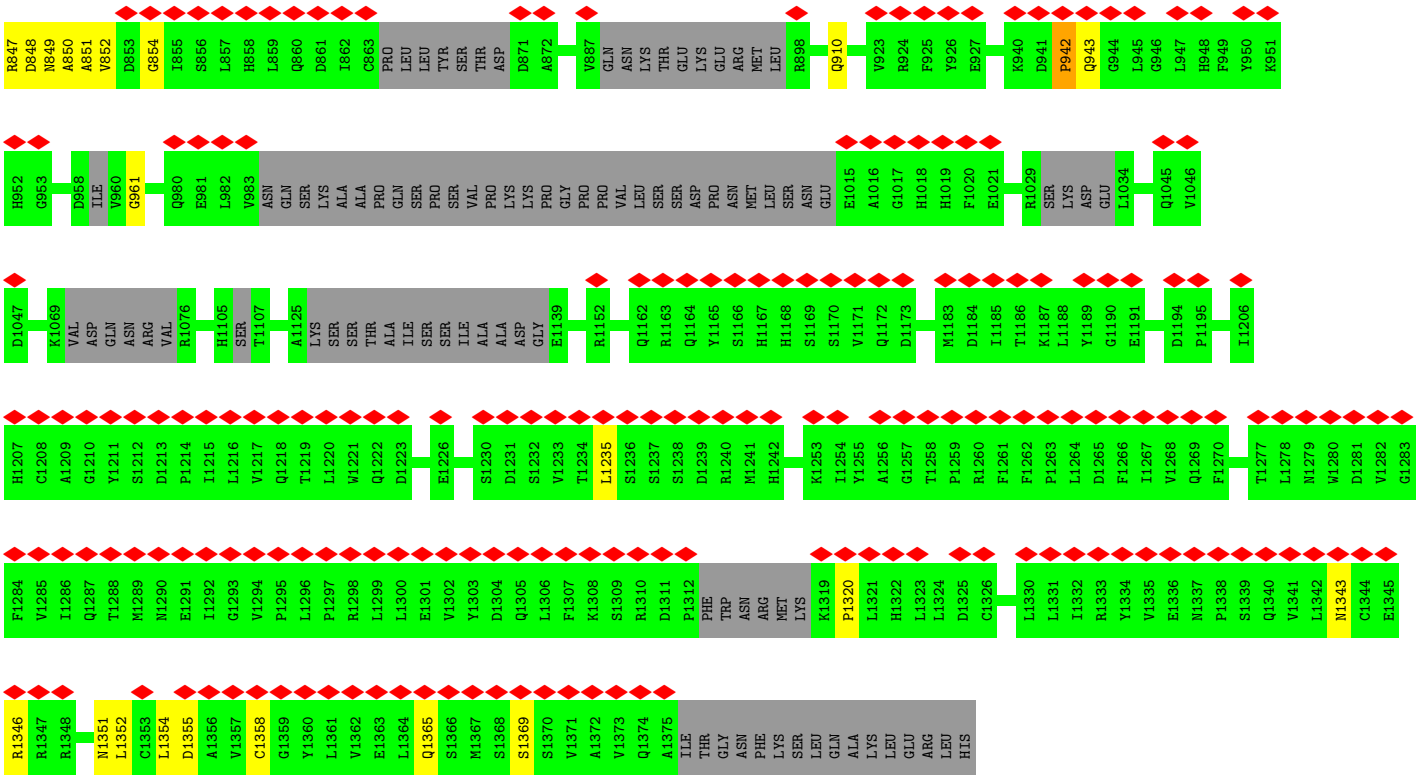





- Molecule 1: Nuclear pore complex protein Nup155

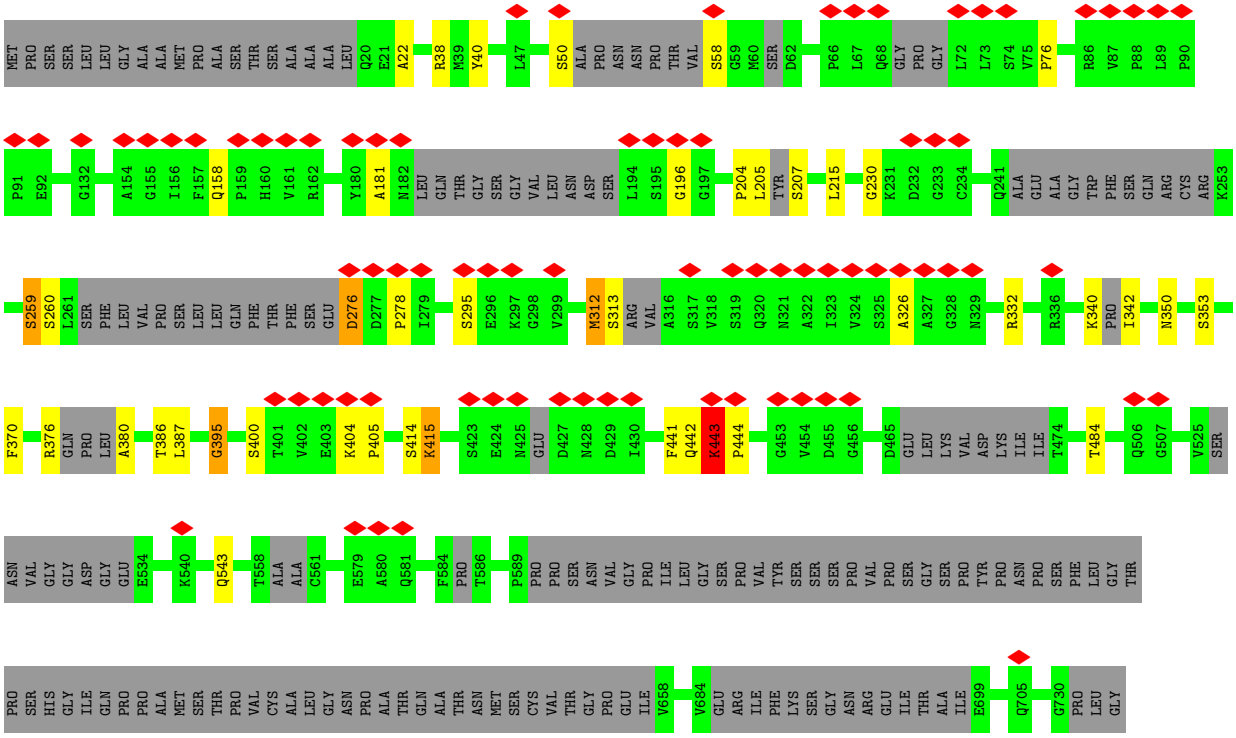
Chain K:

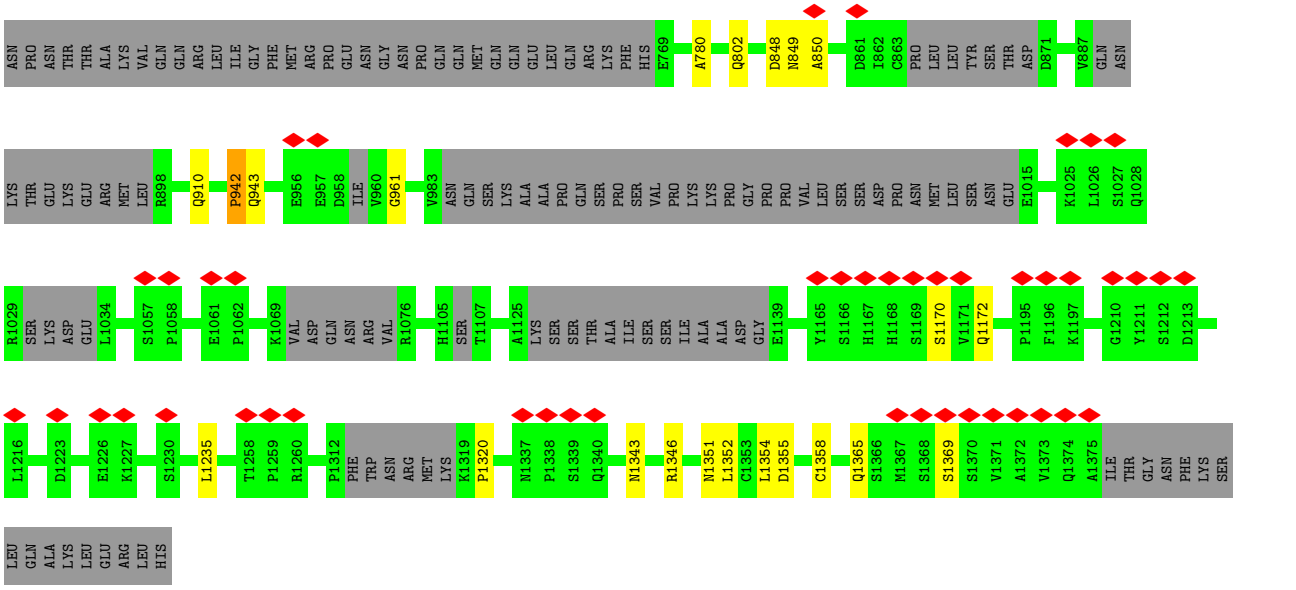




- Molecule 1: Nuclear pore complex protein Nup155

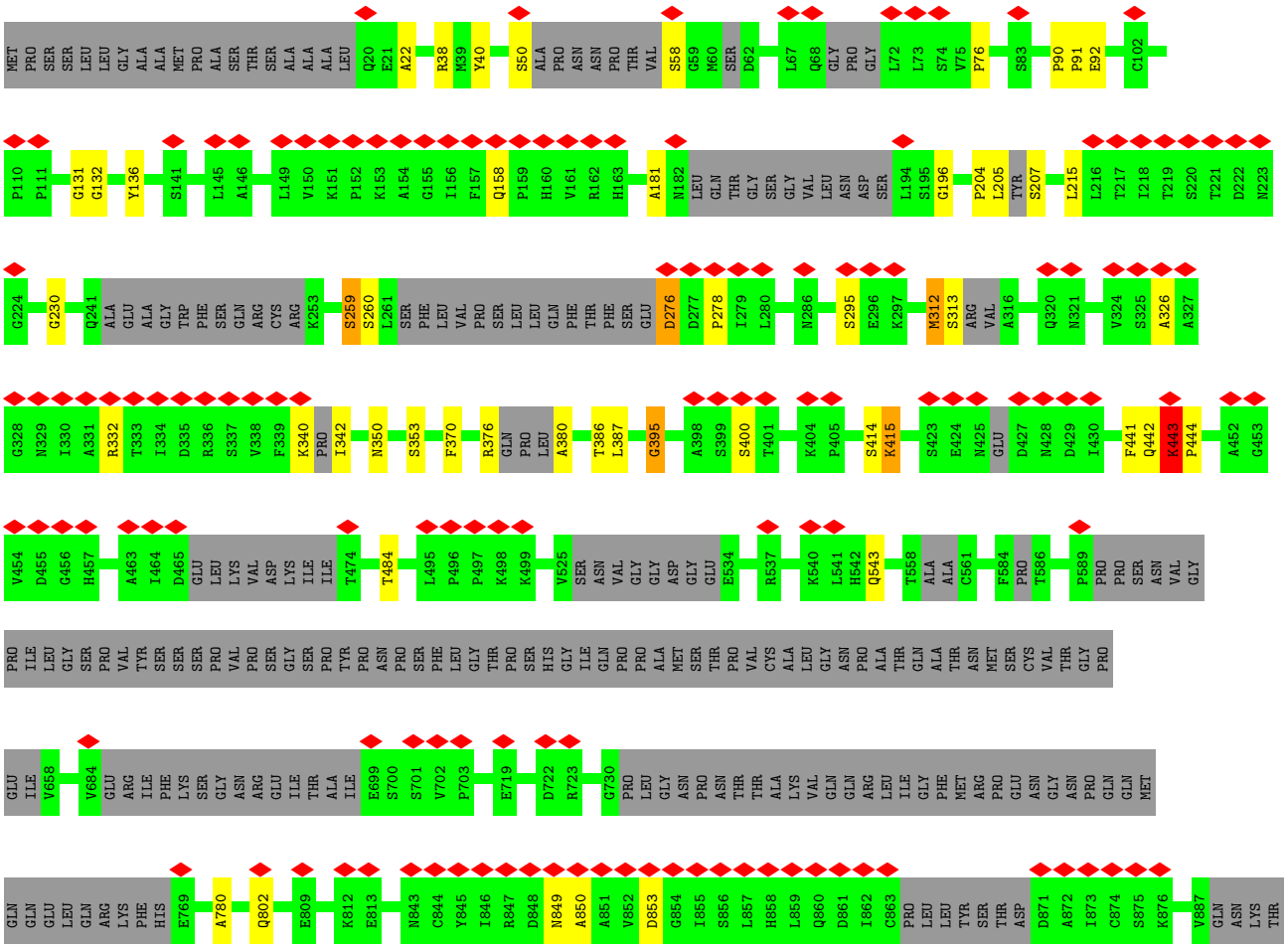
Chain Q:

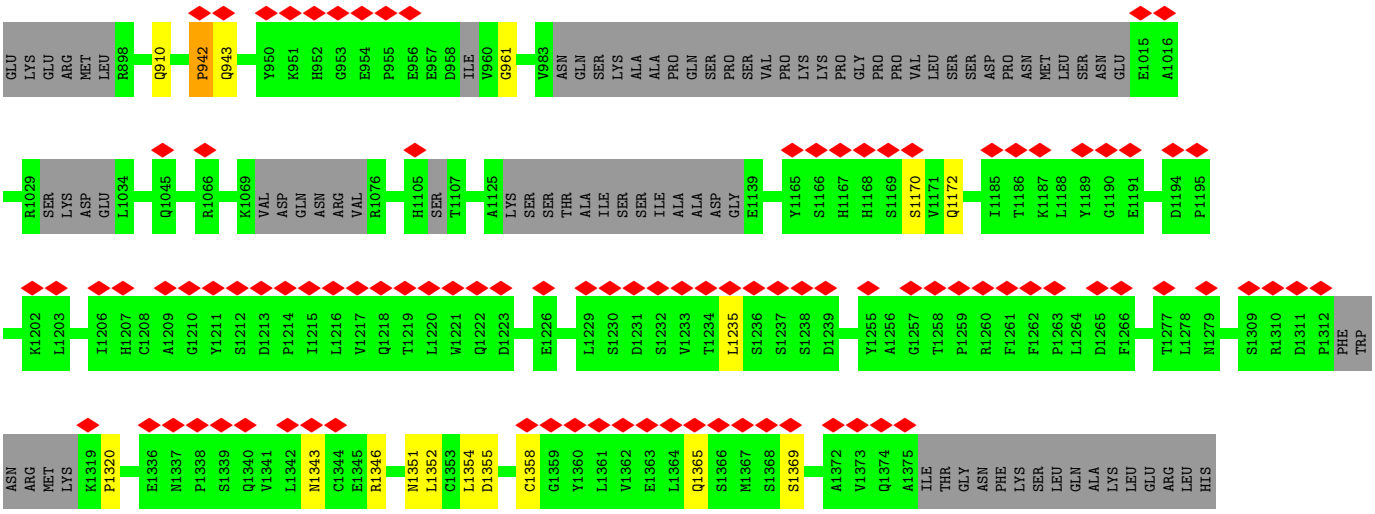





- Molecule 1: Nuclear pore complex protein Nup155

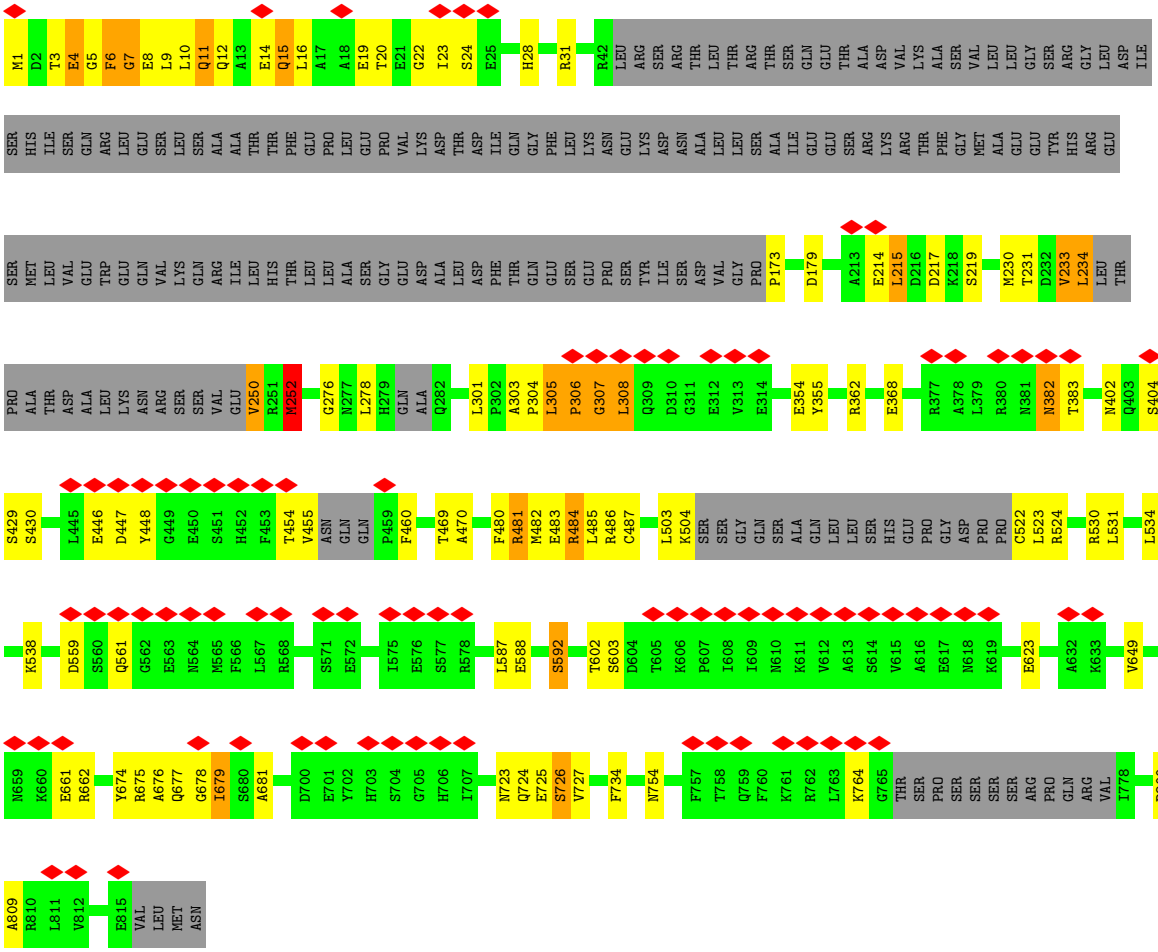
Chain W:





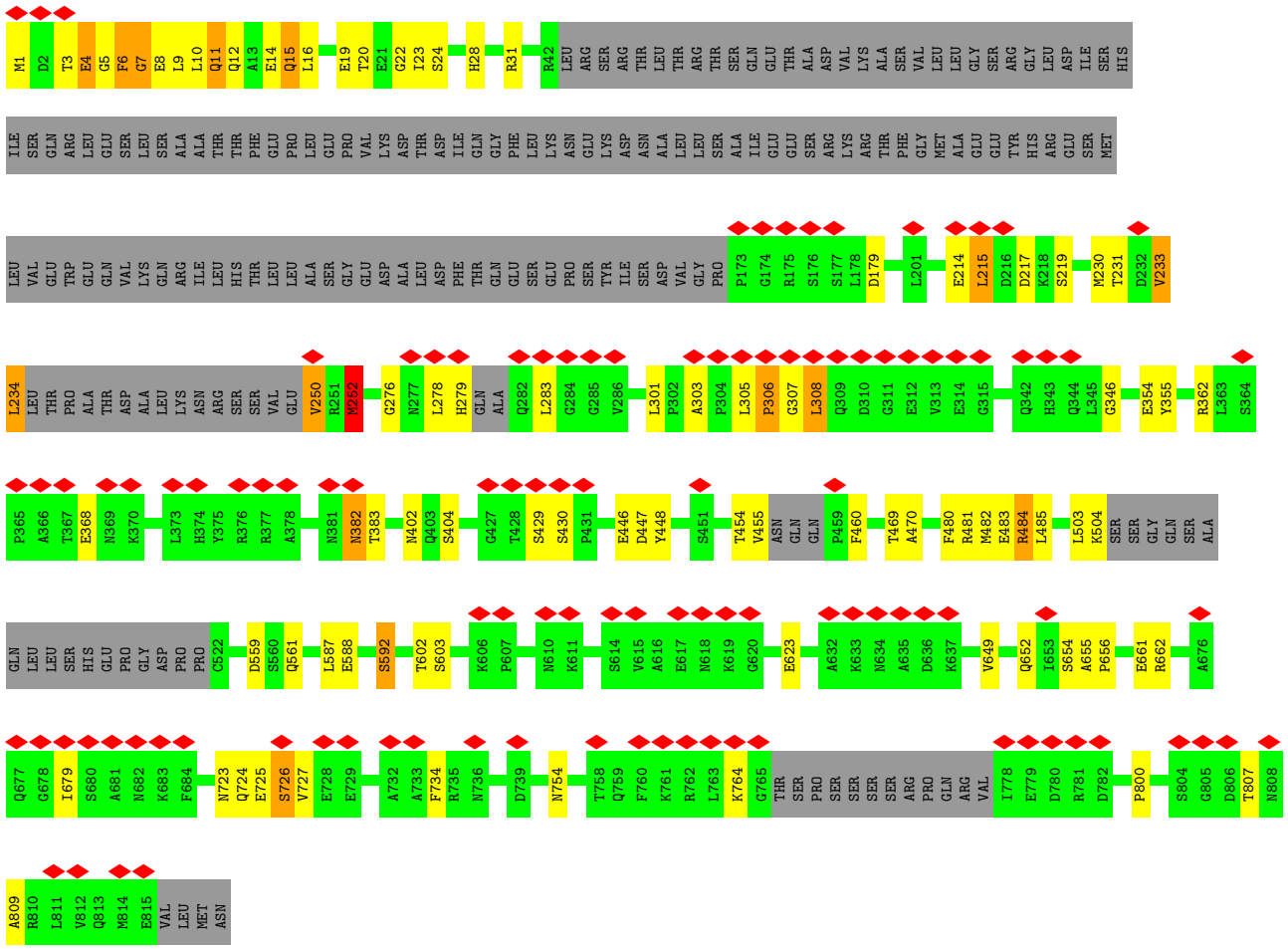

- Molecule 2: Nuclear pore complex protein Nup93

Chain C:



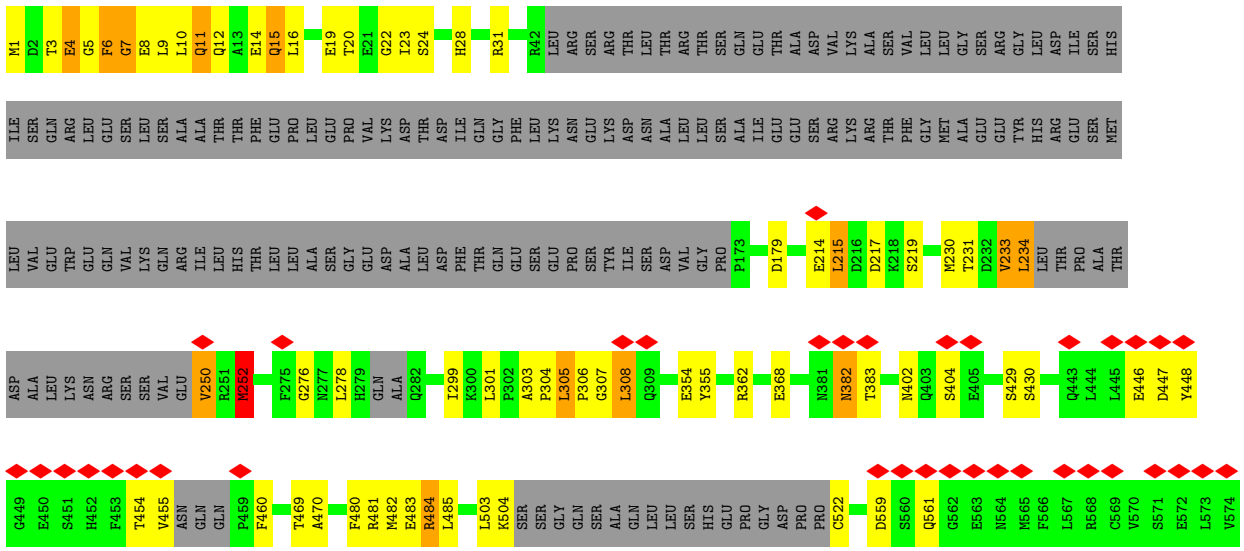

- Molecule 2: Nuclear pore complex protein Nup93

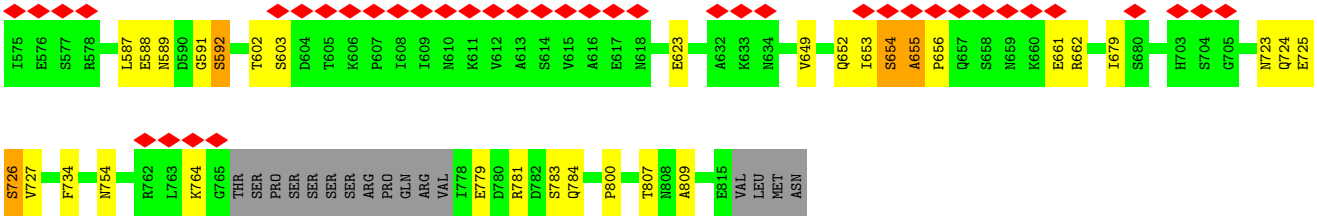
Chain I:



• Molecule 2: Nuclear pore complex protein Nup93

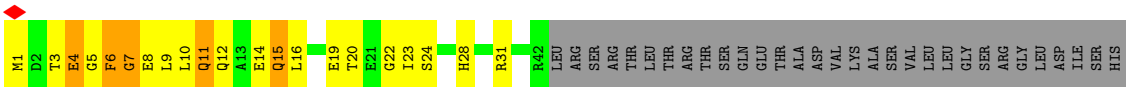
Chain O:

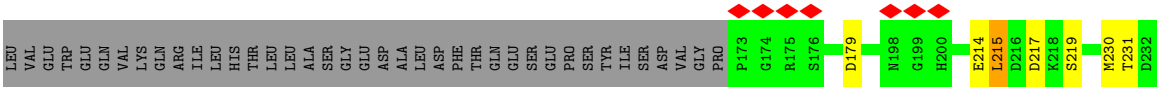


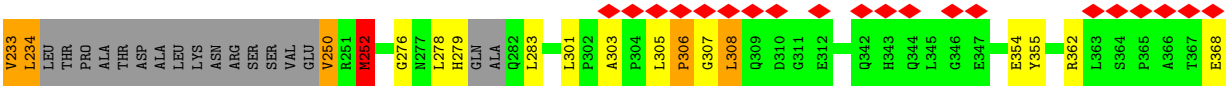


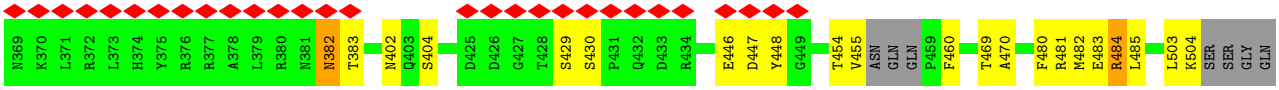

- Molecule 2: Nuclear pore complex protein Nup93

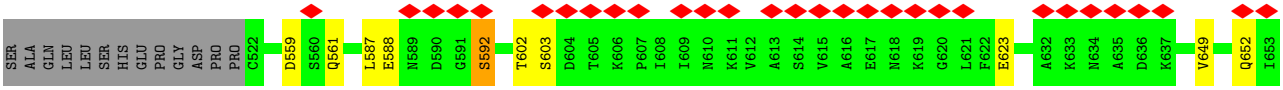
Chain U:

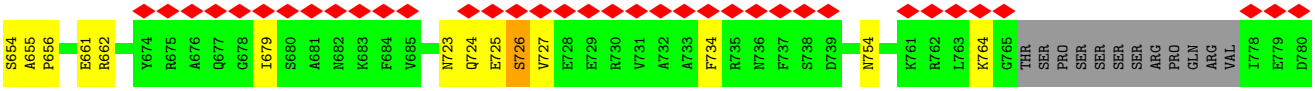


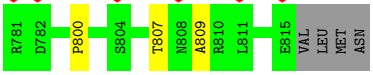


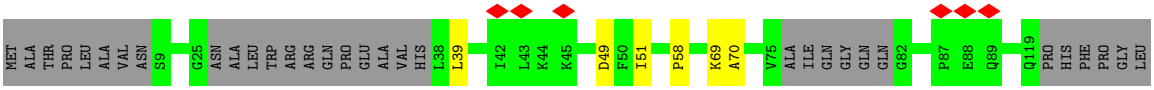



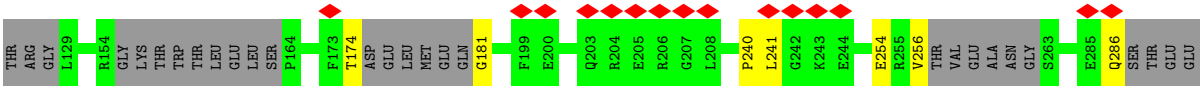



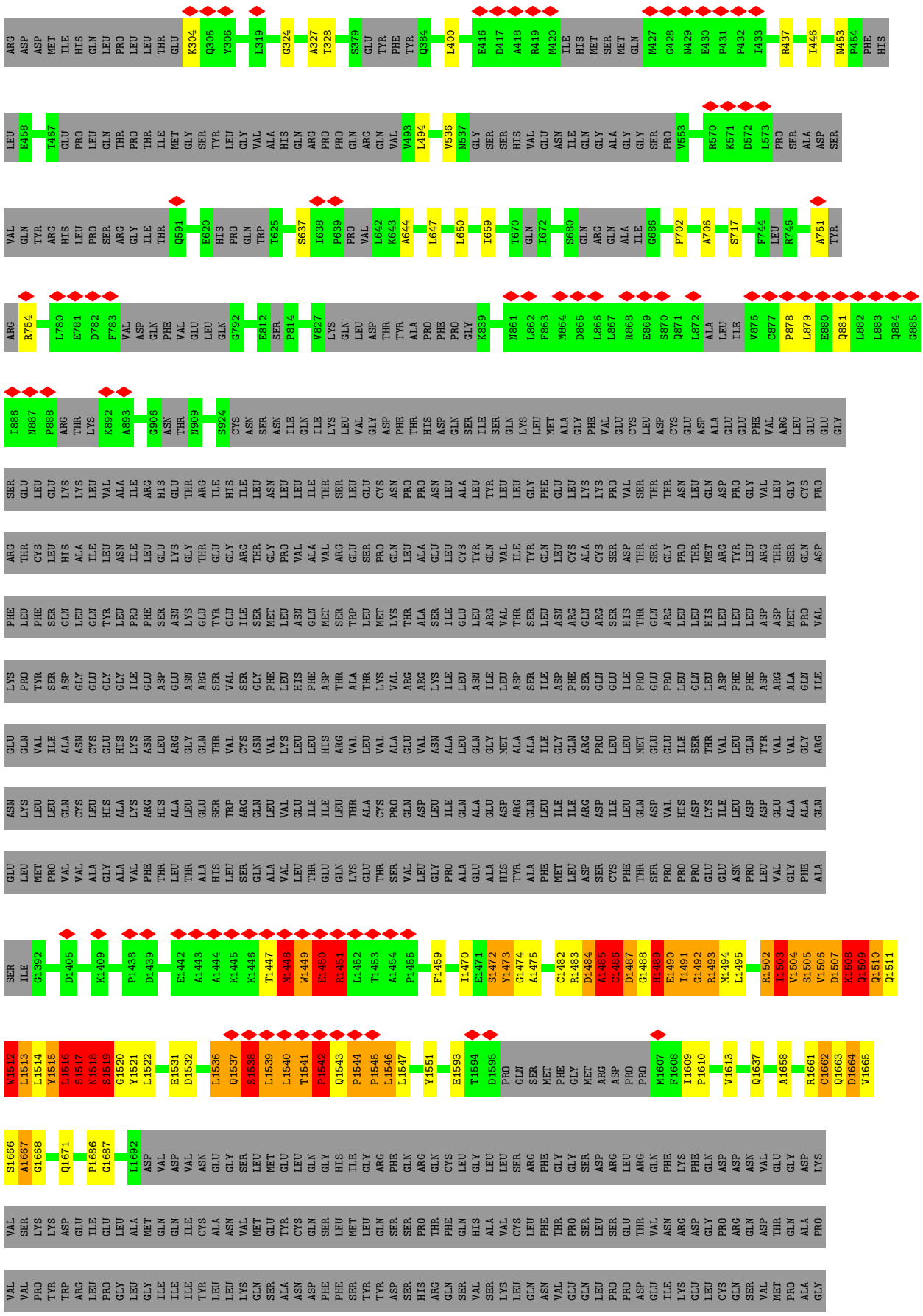



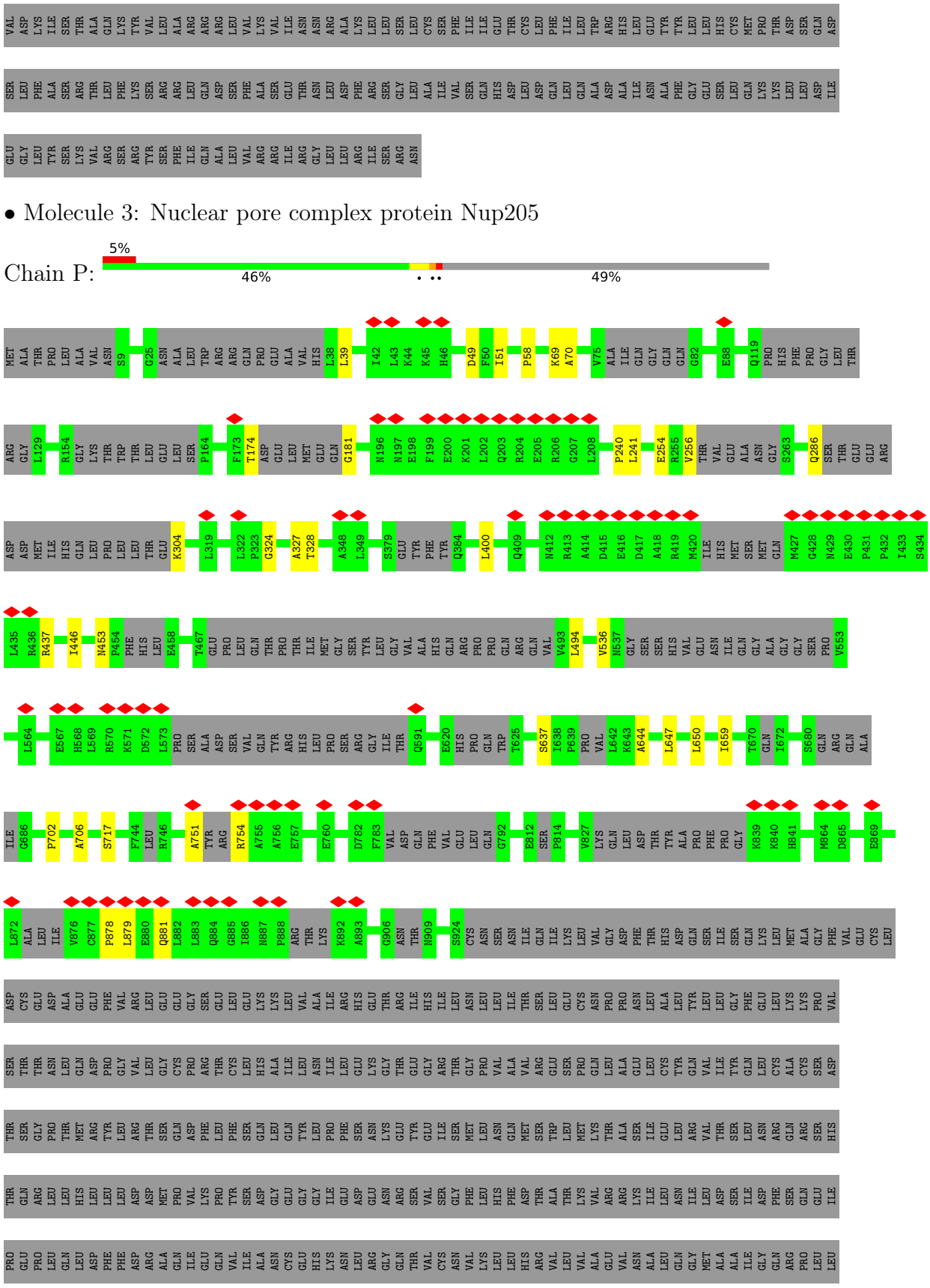

- Molecule 3: Nuclear pore complex protein Nup205

Chain D:



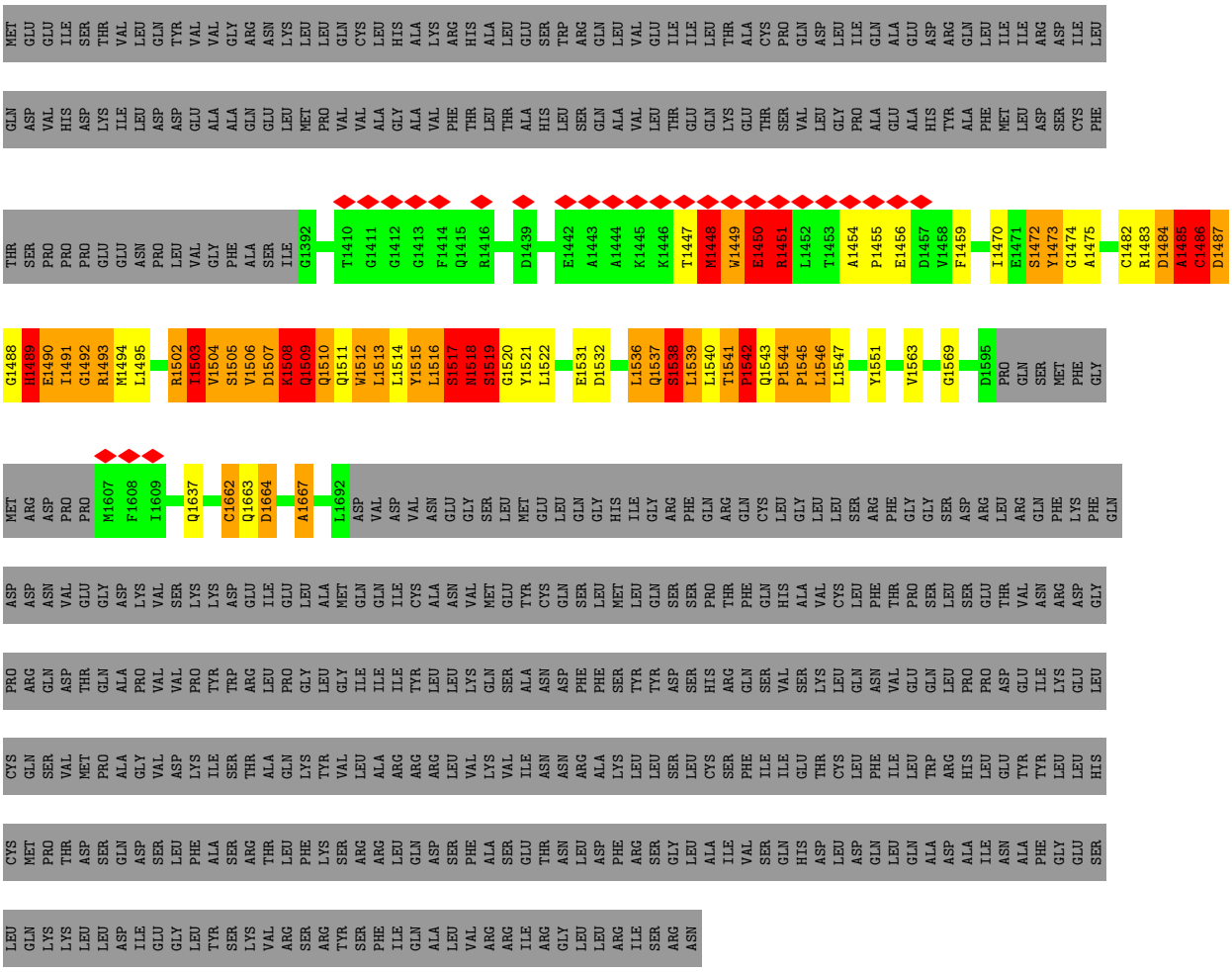




ARG ASP ASP MET ILE HIS GLN LEU PRO LEU LEU THR GLU K304 Q305 Y306 L319 G324 A327 T328 S379 GLU TYR PHE TYR Q384 L400 E416 D417 A418 R419 M420 ILE HIS MET SER MET GLN M427 G428 N429 E430 P431 P432 I433 R437 I446 N453 P454 PHE HIS
LEU E458 T467 GLU PRO LEU GLN THR PRO THR ILE MET GLY SER TYR LEU GLY VAL ALA HIS GLN ARG PRO PRO GLN ARG GLN VAL V493 L494 V536 N537 GLY SER SER HIS VAL GLU ASN ILE GLN GLY ALA GLY GLY SER PRO V553 R570 K571 D572 L573 PRO SER ALA ASP SER
VAL GLN TYR ARG HIS LEU PRO SER ARG GLY ILE THR Q591 E620 HIS PRO GLN TRP T625 S637 I638 P639 PRO VAL L642 K643 A644 L647 L650 I659 T670 GLN I672 S680 GLN ARG GLN ALA ILE G686 P702 A706 S717 F744 LEU R746 A751 TYR
ARG R754 L780 E781 D782 F783 VAL ASP GLN PHE VAL GLU LEU GLN G792 E812 SER P814 V827 LYS GLN LEU ASP THR TYR ALA PRO PHE PRO GLY K839 N861 L862 F863 M864 D865 L866 L867 R868 E869 S870 Q871 L872 ALA LEU ILE V876 C877 P878 L879 E880 Q881 L882 L883 Q884 G885
I886 N887 P888 ARG THR LYS K892 A893 G906 ASN THR N909 S924 CYS ASN SER ASN ILE GLN ILE LYS LEU VAL GLY ASP PHE THR HIS ASP GLN SER ILE SER GLN LYS LEU MET ALA GLY PHE VAL GLU CYS LEU ASP CYS GLU ASP ALA GLU GLU PHE VAL ARG LEU GLU GLU GLY
SER GLU LEU GLU LYS LYS LEU VAL ALA ILE ARG HIS GLU THR ARG ILE HIS ILE LEU ASN LEU LEU LEU THR SER LEU GLU CYS ASN PRO PRO ASN LEU ALA LEU TYR LEU LEU GLY PHE GLU LEU LYS LYS PRO VAL SER THR THR ASN LEU GLN ASP PRO GLY VAL LEU GLY CYS PRO
ARG THR CYS LEU HIS ALA ILE LEU ASN ILE LEU GLU LYS GLY THR GLU GLY ARG THR GLY PRO VAL ALA VAL ARG GLU SER PRO GLN LEU ALA GLU LEU CYS TYR GLN VAL ILE TYR GLN LEU CYS ALA CYS SER ASP THR SER GLY PRO THR MET ARG TYR LEU ARG THR SER GLN ASP
PHE LEU PHE SER GLN LEU GLN TYR LEU PRO PHE SER ASN LYS GLU TYR GLU ILE SER MET LEU ASN GLN MET SER TRP LEU MET LYS THR ALA SER ILE GLU LEU ARG VAL THR SER LEU ASN ARG GLN ARG SER HIS THR GLN ARG LEU LEU HIS LEU LEU LEU LEU ASP ASP MET PRO VAL
LYS PRO TYR SER ASP GLY GLU GLY GLY ILE GLU ASP GLU ASN ARG SER VAL SER GLY PHE LEU HIS PHE ASP THR ALA THR LYS VAL ARG ARG LYS ILE LEU ASN ILE LEU ASP SER ILE ASP PHE SER GLN GLU ILE PRO GLU PRO LEU GLN ILE PHE ASP ARG ALA GLN ILE
GLU GLN VAL ILE ALA ASN CYS GLU HIS LYS ASN LEU ARG GLY GLN THR VAL CYS ASN VAL LYS LEU LEU LEU HIS ARG VAL LEU VAL ALA GLU VAL ASN ASN ALA LEU GLN GLY MET ALA ALA ILE GLY GLN ARG PRO LEU LEU MET GLU GLU ILE SER THR VAL LEU GLN TYR VAL VAL GLY ARG
ASN LYS LEU LEU GLN CYS LEU HIS ALA LYS ARG HIS ALA LEU GLU SER TRP ARG GLN LEU VAL GLU ILE ILE LEU THR ALA CYS PRO GLN ASP LEU ILE ALA GLU ALA GLN LEU ILE ILE ARG ASP ILE LEU GLN ASP VAL HIS ASP LYS ILE VAL ALA ALA GLN
GLU LEU MET PRO VAL VAL ALA GLY ALA VAL PHE THR LEU THR ALA HIS LEU SER GLN ALA VAL LEU THR GLU GLN LYS GLU THR SER VAL LEU GLY PRO ALA GLU ALA HIS TYR ALA PHE MET LEU ASP SER CYS PHE THR SER PRO PRO PRO GLU GLU PRO LEU LEU GLN LEU VAL LEU GLN TYR VAL VAL GLY ALA
SER ILE G1392 D1405 K1409 P1438 D1439 E1442 A1443 A1444 K1445 K1446 T1447 M1448 W1449 E1450 R1451 L1452 T1453 A1454 P1455 F1459 I1470 E1471 S1472 Y1473 G1474 A1475 C1482 R1483 D1484 A1485 C1486 D1487 G1488 H1489 E1490 I1491 G1492 R1493 M1494 L1495 R1502 I1503 V1504 S1505 V1506 D1507 K1508 Q1509 Q1510 Q1511
W1512 L1513 L1514 Y1515 L1516 S1517 N1518 S1519 G1520 Y1521 L1522 E1531 D1532 L1536 Q1537 S1538 L1539 L1540 T1541 P1542 Q1543 P1544 P1545 L1546 L1547 Y1551 E1593 T1594 D1595 PRO GLN SER MET PHE GLY MET ARG ASP PRO PRO M1607 F1608 I1609 P1610 V1613 Q1637 A1658 R1661 C1662 Q1663 D1664 V1665
S1666 A1667 G1668 Q1671 P1686 G1687 L1692 ASP VAL ASP VAL ASN GLU GLY SER LEU MET GLU LEU GLN GLY HIS ILE GLY ARG PHE GLN ARG GLN CYS LEU GLY LEU LEU SER ARG PHE GLY GLY SER ASP ARG LEU ARG GLN PHE LYS PHE GLN ASP ASP ASN VAL GLU GLY ASP LYS
VAL SER LYS LYS ASP GLU ILE GLU LEU ALA MET GLN GLN ILE CYS ALA ASN VAL MET GLU TYR CYS GLN SER LEU MET GLU LEU GLN SER SER PRO THR PHE GLN HIS ALA VAL CYS LEU PHE THR PRO GLY GLY PRO SER LEU SER GLU THR VAL GLN ARG ASP THR GLN ALA PRO
VAL VAL PRO TYR TRP ARG LEU PRO GLY LEU GLY ILE ILE ILE TYR LEU LEU LYS GLN SER ALA ASN ASP PHE PHE SER TYR TYR ASP SER HIS ARG GLN SER VAL SER LYS LEU GLN ASN VAL GLU GLN LEU PRO PRO ASP GLU ILE LYS GLU LEU CYS GLN SER VAL MET PRO ALA GLY



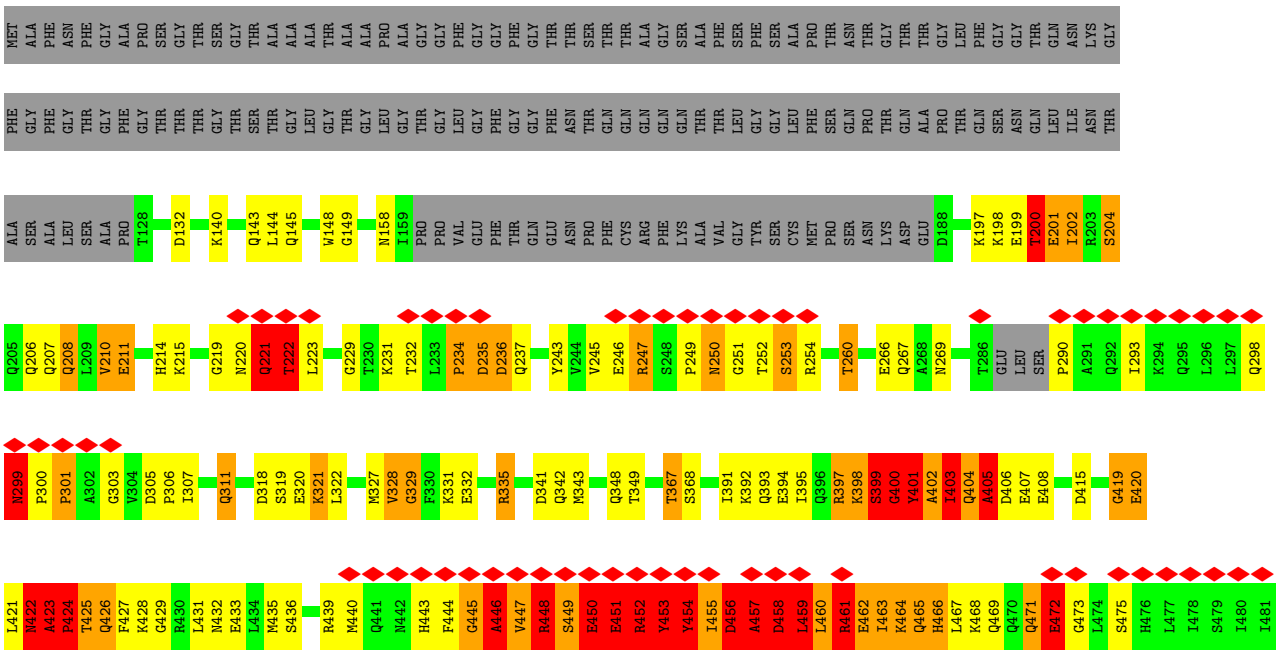
• Molecule 3: Nuclear pore complex protein Nup205

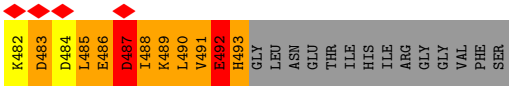
Chain P: 5% 46% 49%



- Molecule 4: Nucleoporin p54

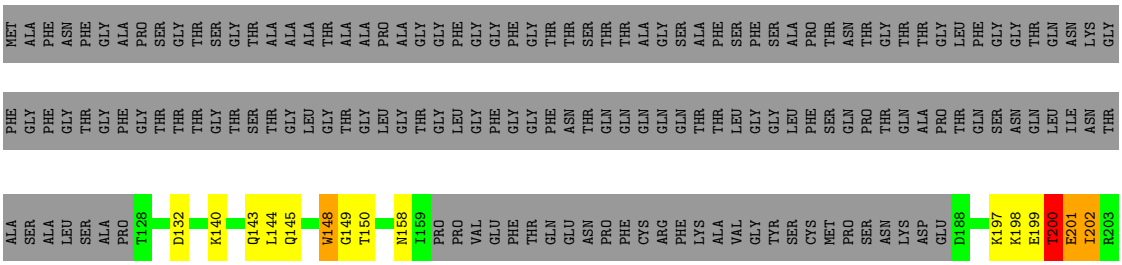
Chain F:

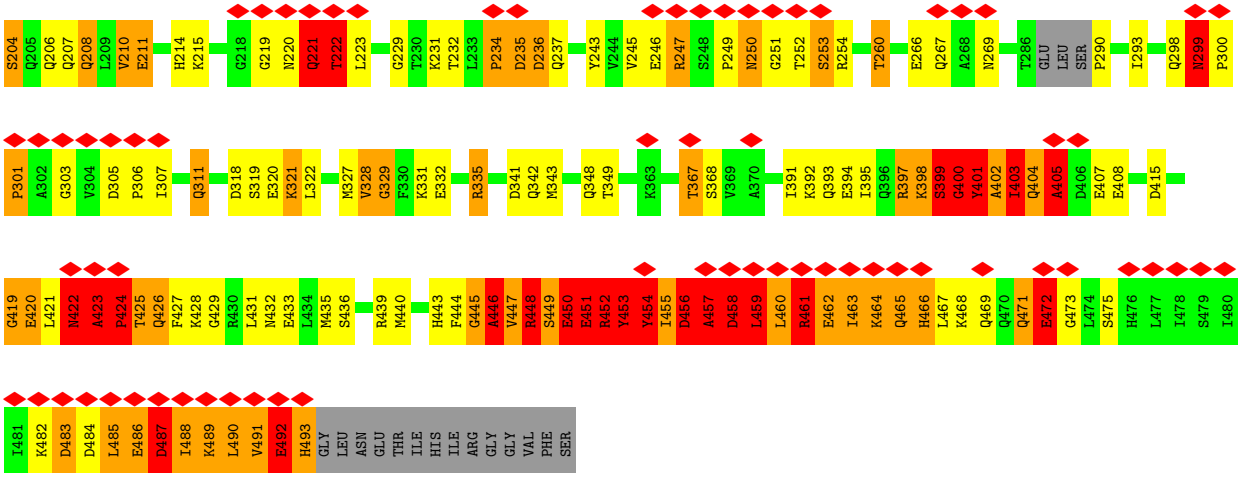





• Molecule 4: Nucleoporin p54

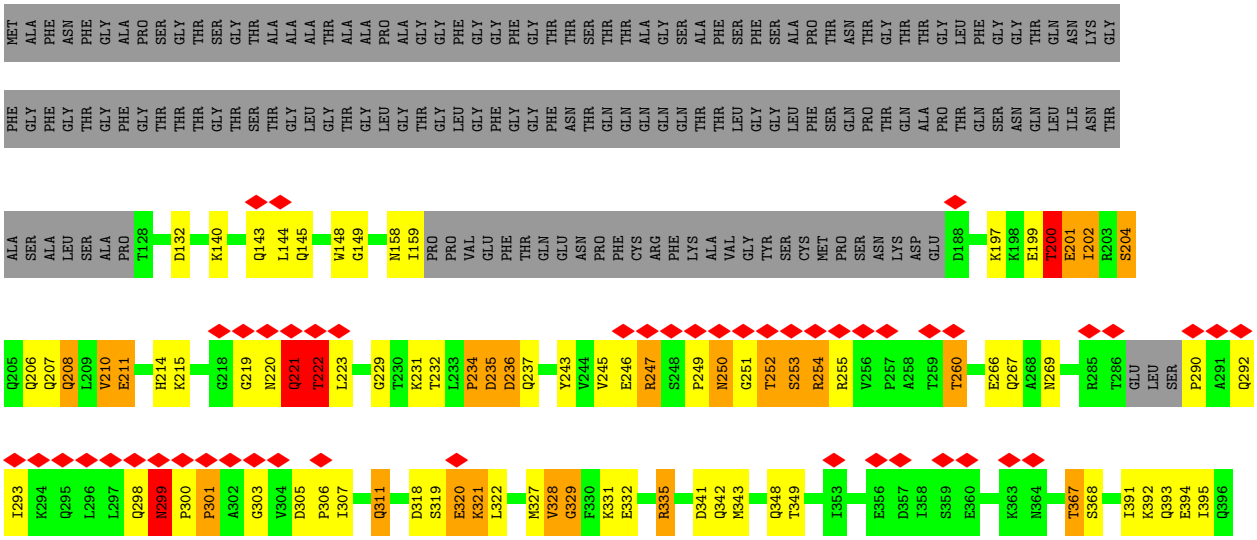
Chain L:

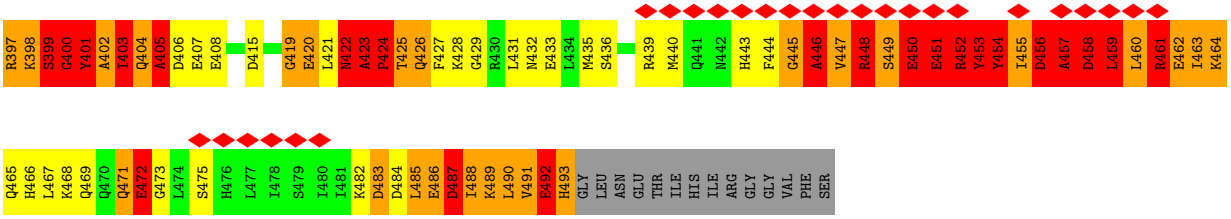



• Molecule 4: Nucleoporin p54

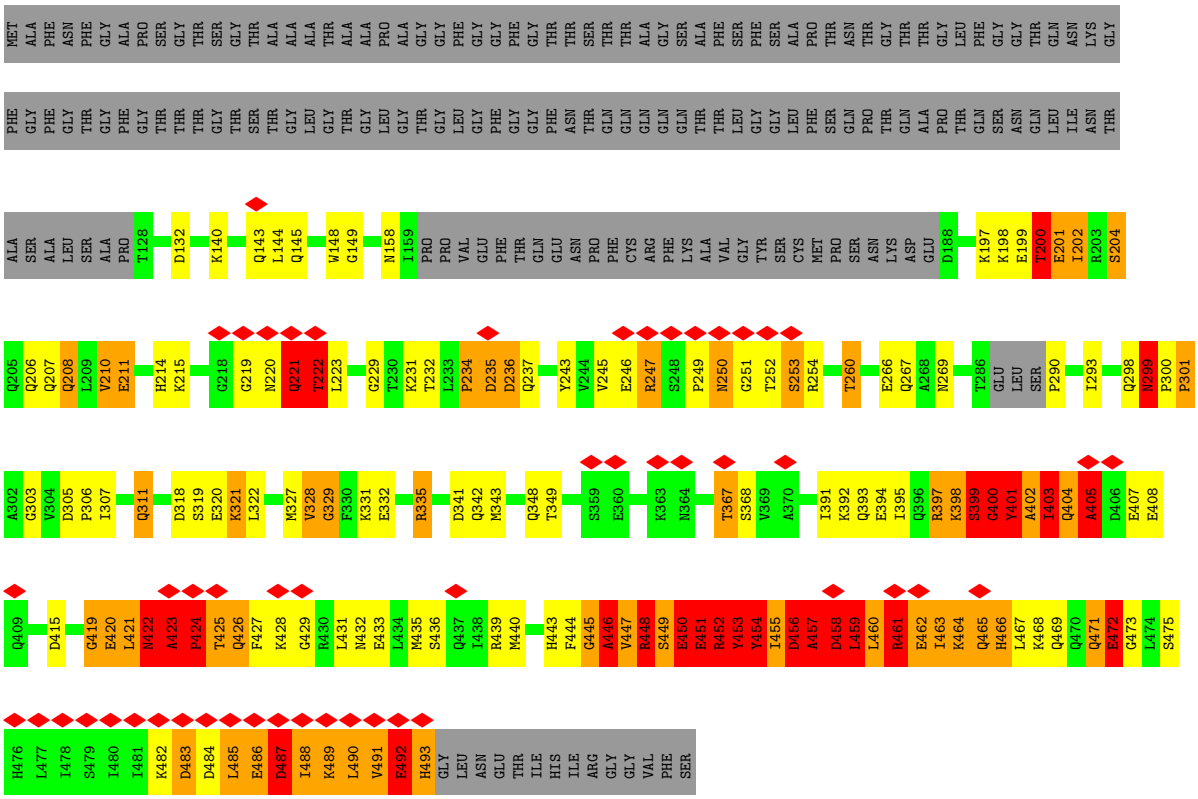
Chain R:





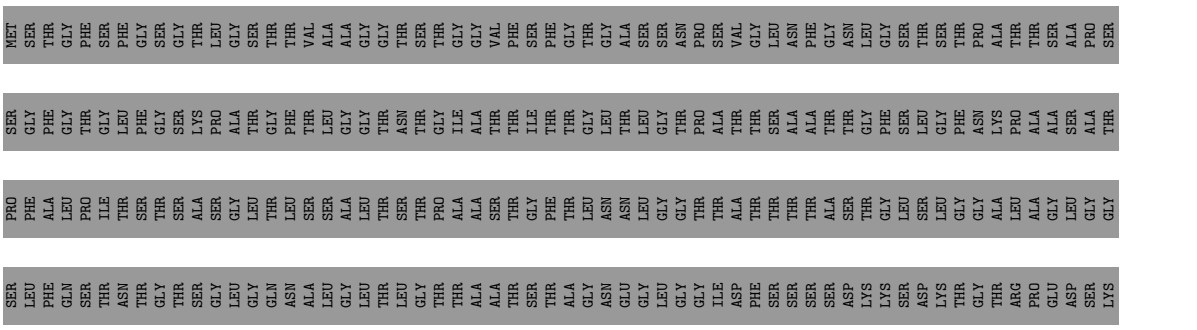

- Molecule 4: Nucleoporin p54

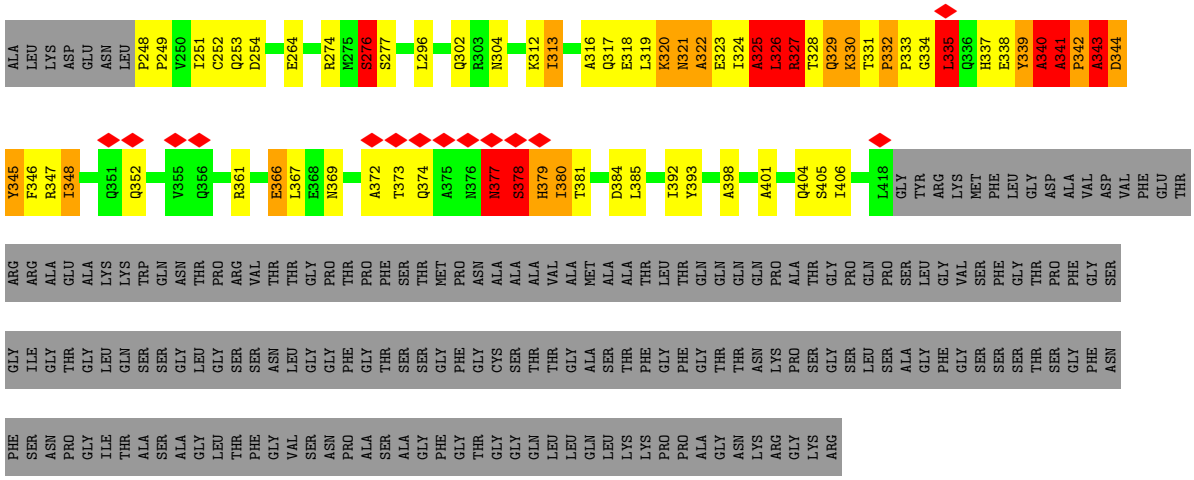
Chain X:




- Molecule 5: Nucleoporin p58/p45

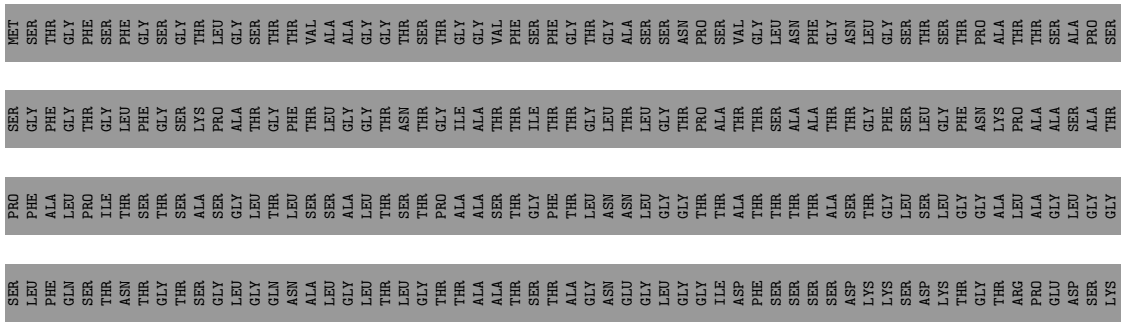
Chain G:

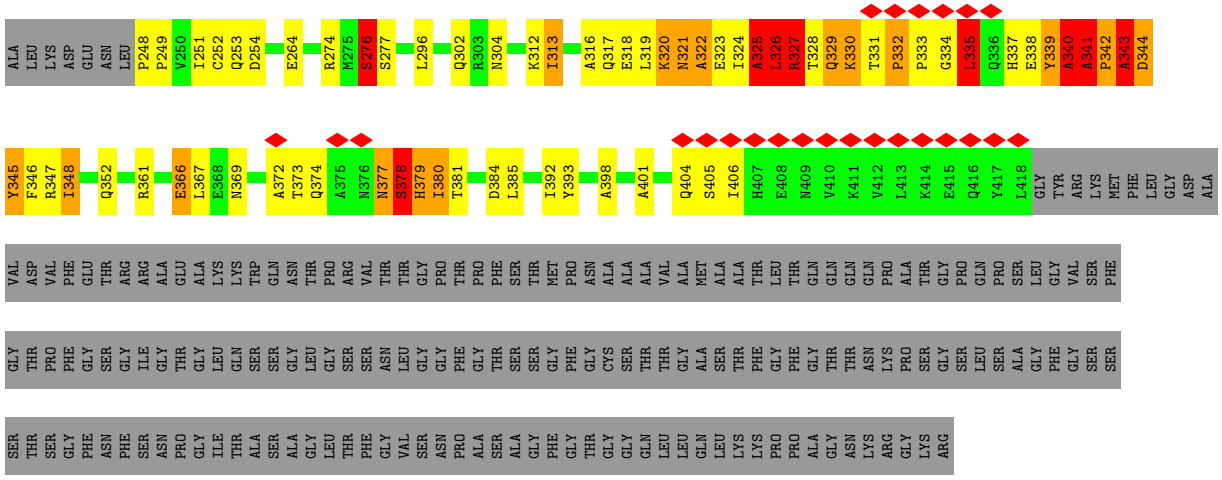




• Molecule 5: Nucleoporin p58/p45

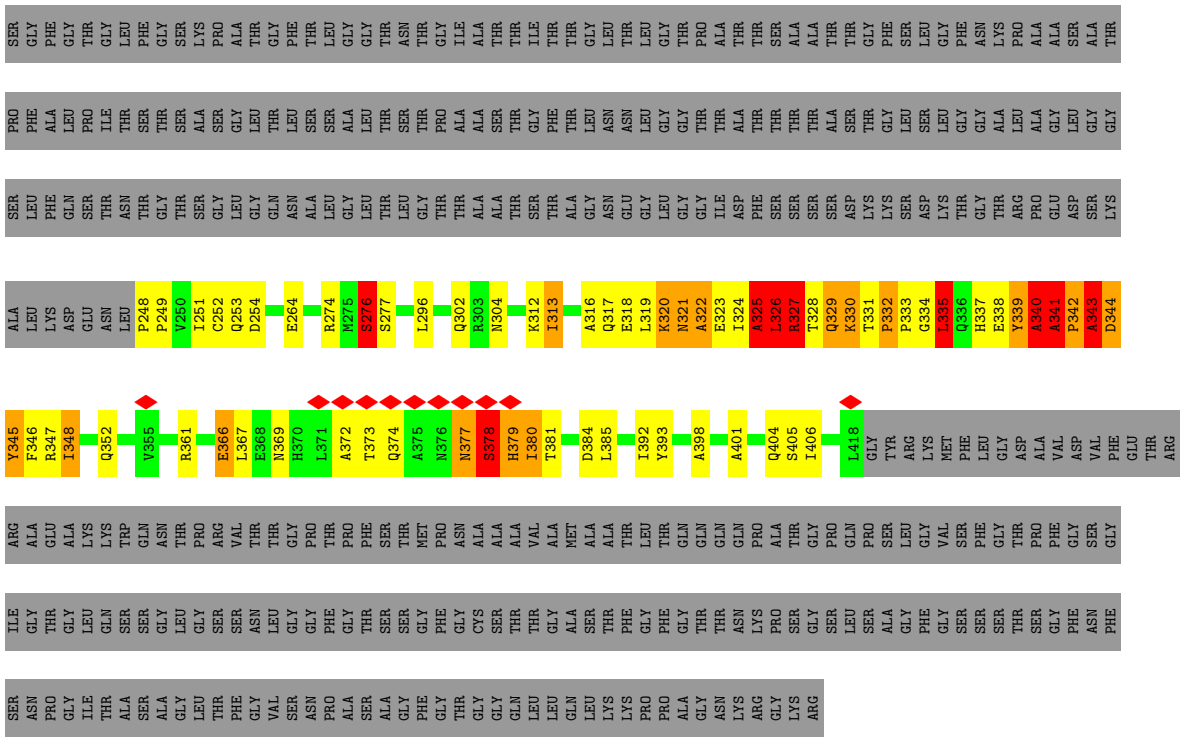
Chain M:





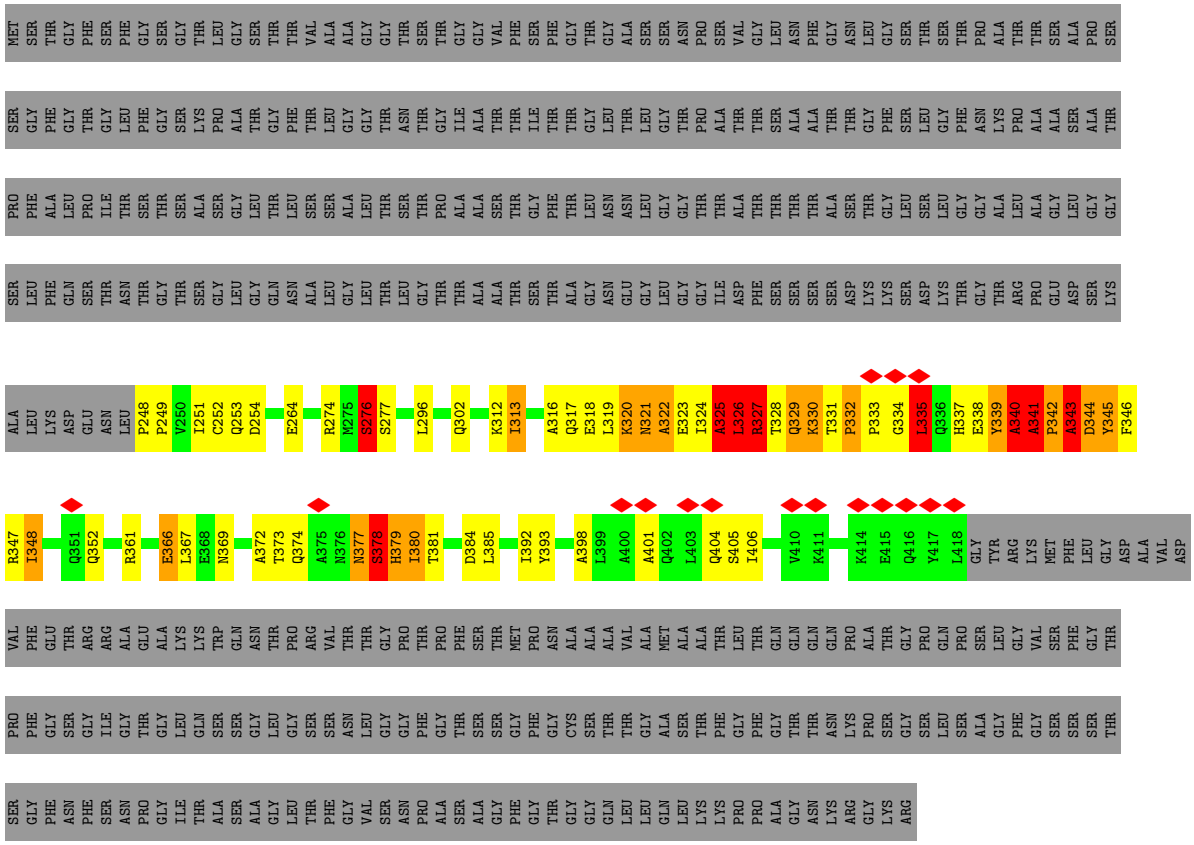
• Molecule 5: Nucleoporin p58/p45

Chain S:



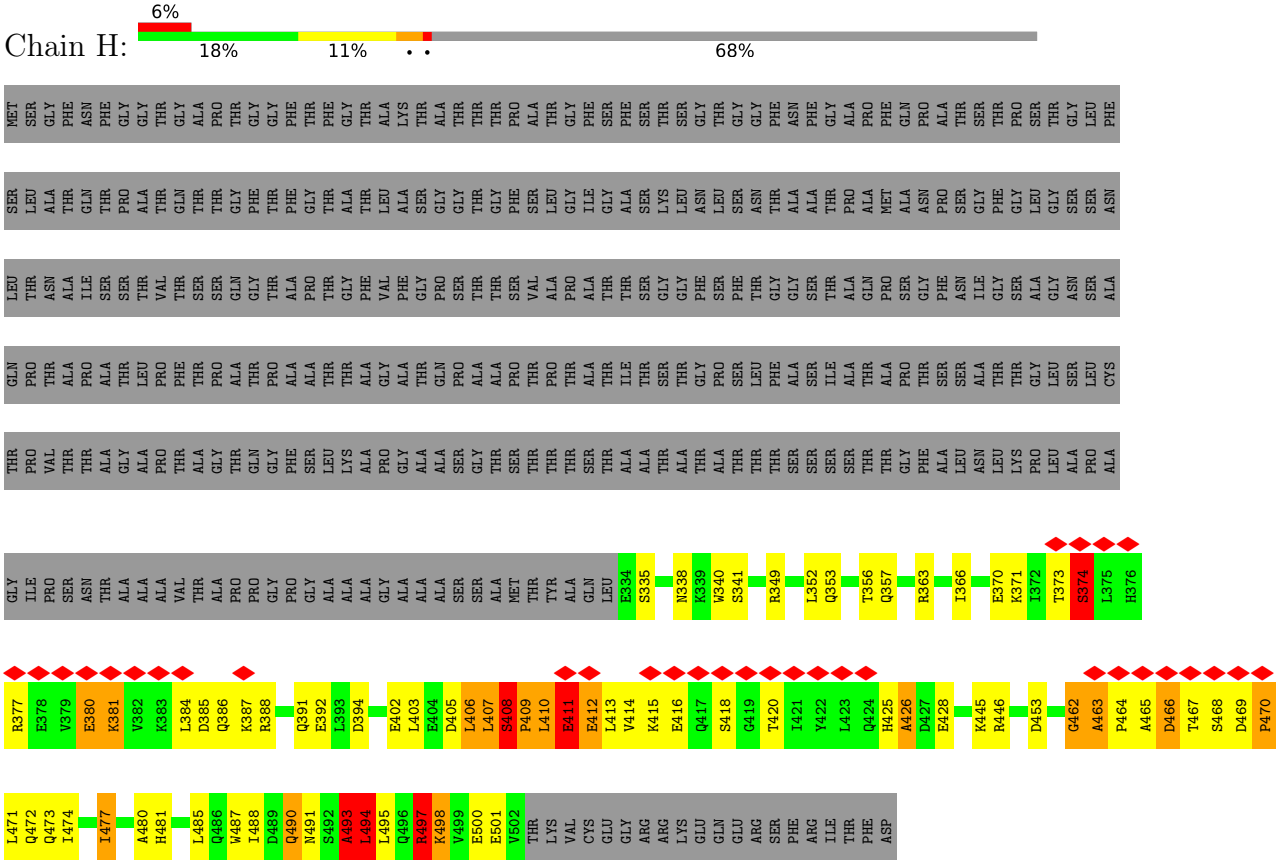
- Molecule 5: Nucleoporin p58/p45

Chain Y:



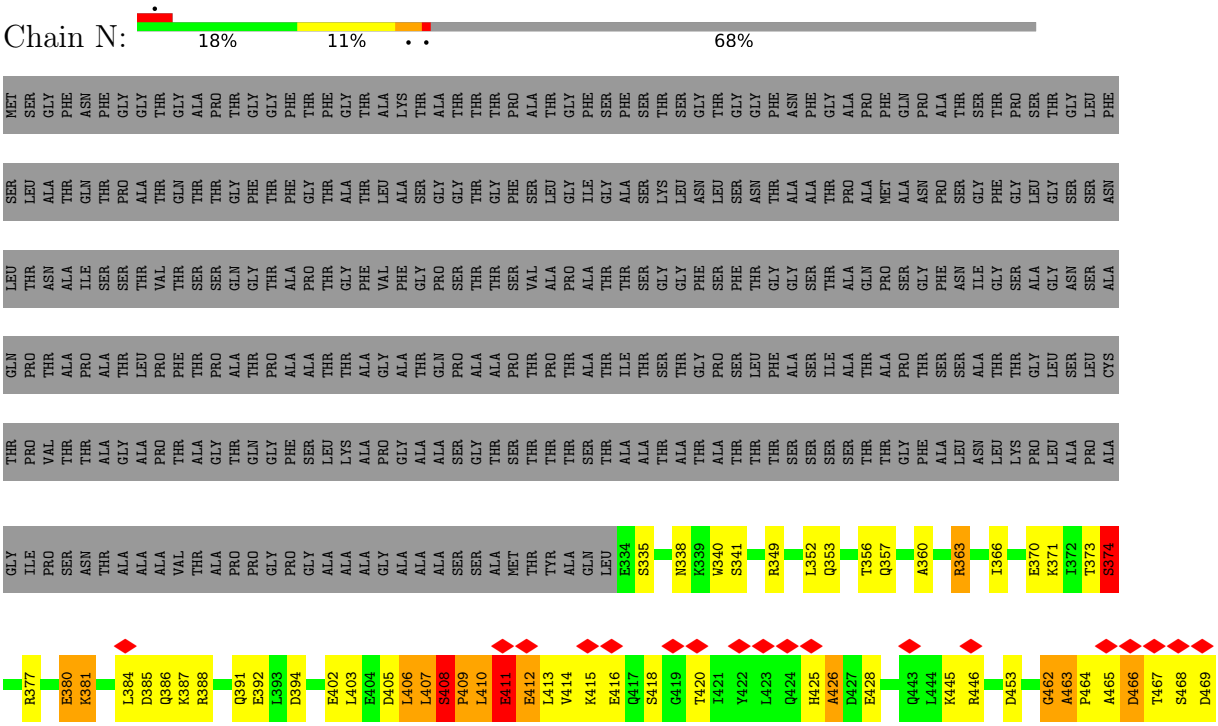
- Molecule 6: Nuclear pore glycoprotein p62

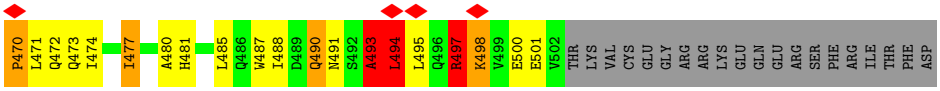
Chain H:



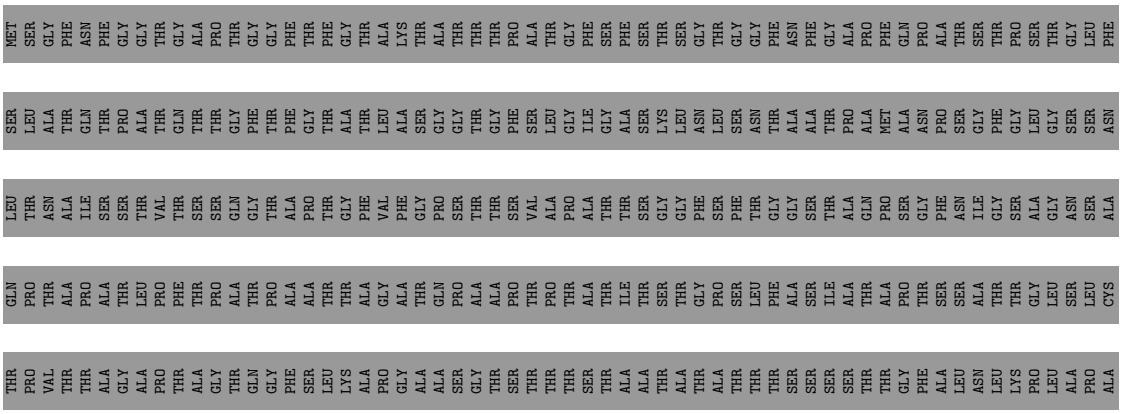

- Molecule 6: Nuclear pore glycoprotein p62

Chain N:

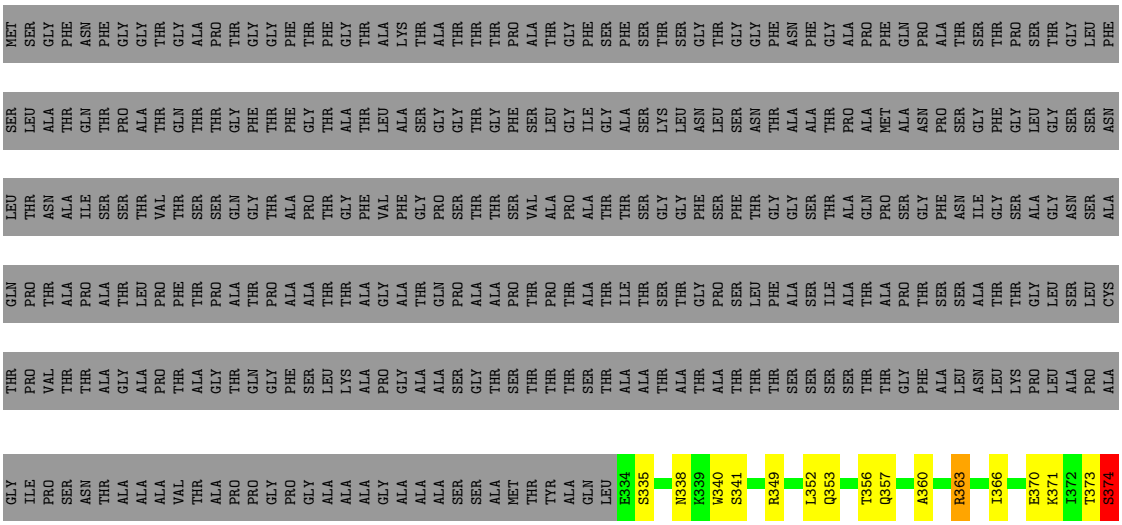


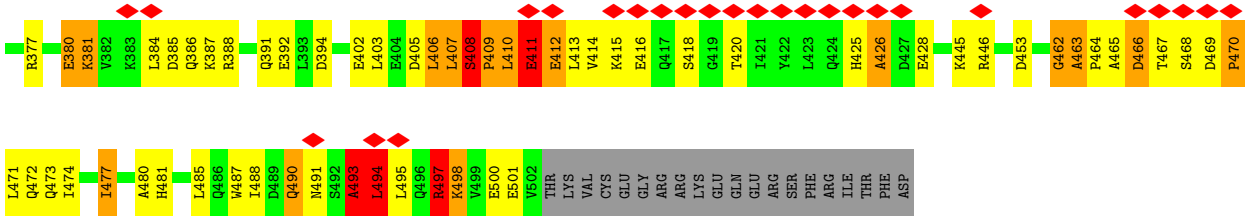



- Molecule 6: Nuclear pore glycoprotein p62



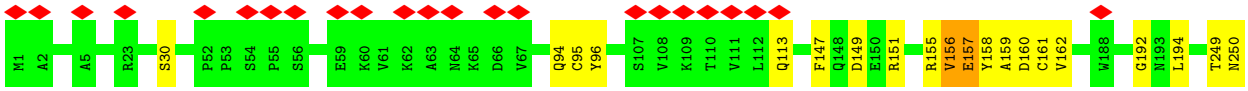

- Molecule 6: Nuclear pore glycoprotein p62

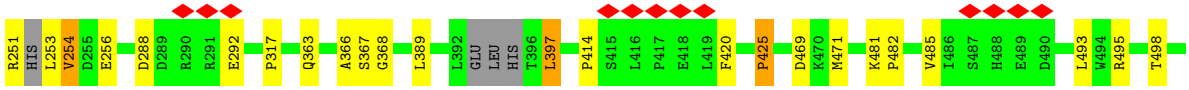


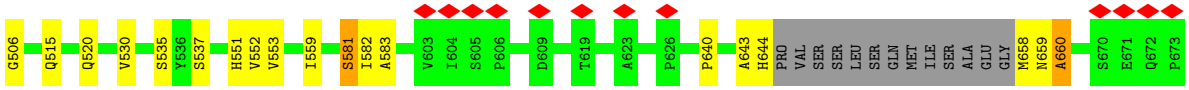


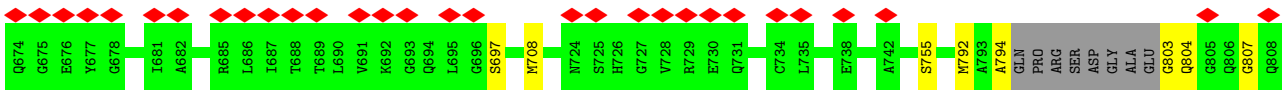

• Molecule 7: Nucleoporin NUP188 homolog

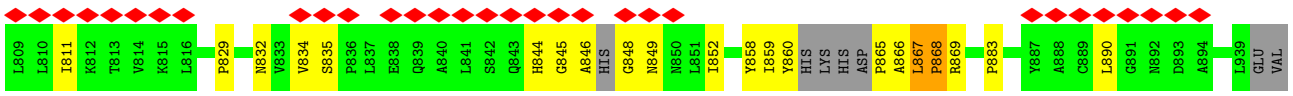
Chain J:

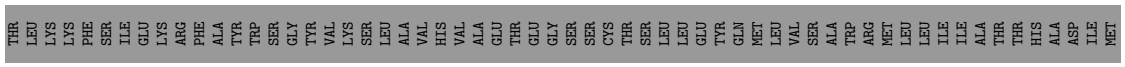


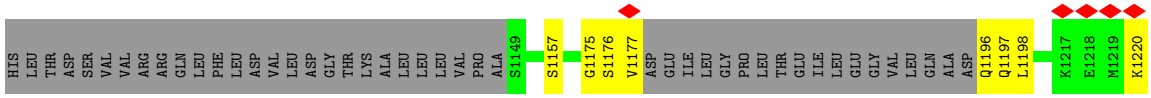



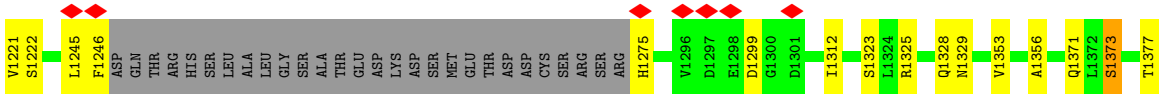



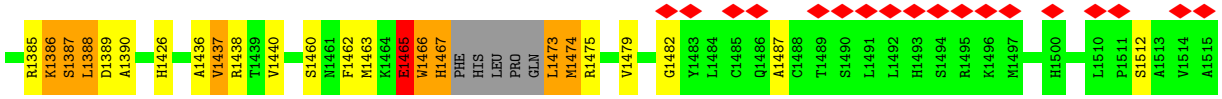



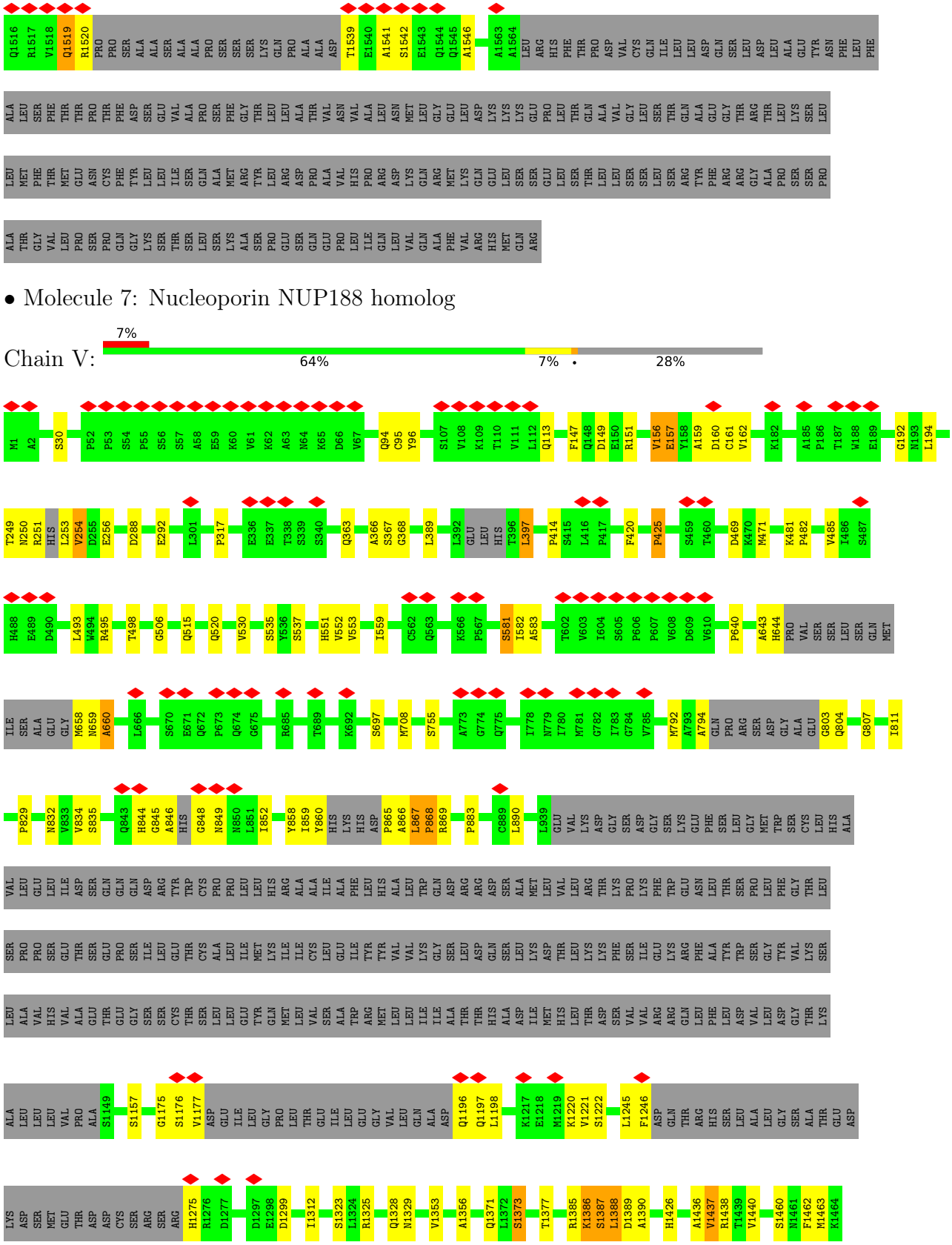





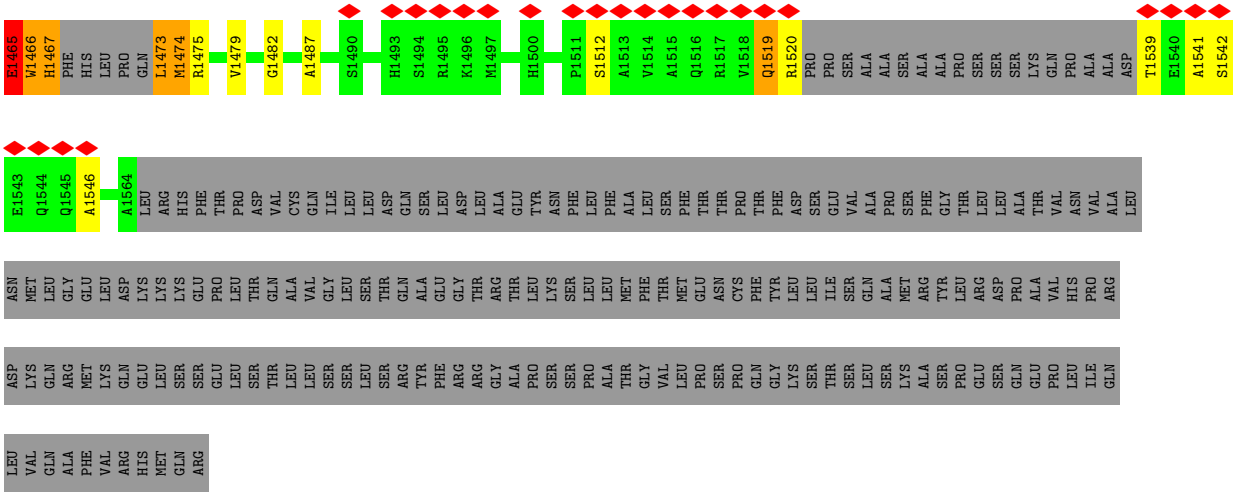





• Molecule 7: Nucleoporin NUP188 homolog

Chain V: 7% 64% 7% 28%


E1465 W1466 H1467 PHE HIS LEU PRO GLN L1473 M1474 R1475 V1479 G1482 A1487 S1490 H1493 S1494 R1495 K1496 M1497 H1500 P1511 S1512 A1513 V1514 A1515 Q1516 R1517 V1518 Q1519 R1520 PRO PRO SER ALA ALA SER ALA ALA PRO SER SER SER LYS GLN PRO ALA ALA ASP T1539 E1540 A1541 S1542
E1543 Q1544 Q1545 A1546 A1564 LEU ARG HIS PHE THR PRO ASP VAL CYS GLN ILE LEU LEU ASP GLN SER LEU ASP LEU ALA GLU TYR ASN PHE LEU PHE ALA LEU SER PHE THR THR PRO THR PHE ASP SER GLU VAL ALA PRO SER PHE GLY THR LEU LEU ALA THR VAL ASN VAL ALA LEU
ASN MET LEU GLY GLU LEU ASP LYS LYS LYS GLU PRO LEU THR GLN ALA VAL GLY LEU SER THR GLN ALA GLU GLY THR ARG THR LEU LYS SER LEU LEU MET PHE THR MET GLU ASN CYS PHE TYR LEU LEU ILE SER GLN ALA MET ARG TYR LEU ARG ASP PRO ALA LEU PRO SER PHE SER LEU SER LYS ALA SER PRO GLU SER GLN GLU PRO LEU ILE GLN
ASP LYS GLN ARG MET LYS GLN GLU LEU SER SER GLU LEU SER THR LEU LEU SER SER LEU SER ARG TYR PHE ARG ARG GLY ALA PRO SER SER PRO ALA THR GLY VAL LEU PRO SER PRO GLN GLY LYS SER THR SER LEU SER LYS ALA SER PRO GLU SER GLN GLU PRO LEU ILE GLN
LEU VAL GLN ALA PHE VAL ARG HIS MET GLN ARG

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of subtomograms used | 8400 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 3 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 315.784 | Depositor |
| Minimum map value | 0.000 | Depositor |
| Average map value | 1.328 | Depositor |
| Map value standard deviation | 10.659 | Depositor |
| Recommended contour level | 36.6 | Depositor |
| Map size (Å) | 964.8, 964.8, 964.8 | wwPDB |
| Map dimensions | 144, 144, 144 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 6.7, 6.7, 6.7 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | A | 0.94 | 0/3195 | 1.25 | 10/4421 (0.2%) |
| 1 | B | 0.94 | 0/3195 | 1.25 | 10/4421 (0.2%) |
| 1 | E | 0.93 | 0/5338 | 1.17 | 10/7399 (0.1%) |
| 1 | K | 0.93 | 0/5338 | 1.18 | 10/7399 (0.1%) |
| 1 | Q | 0.93 | 0/5338 | 1.17 | 10/7399 (0.1%) |
| 1 | W | 0.93 | 0/5338 | 1.17 | 10/7399 (0.1%) |
| 2 | C | 1.13 | 13/3143 (0.4%) | 1.44 | 45/4369 (1.0%) |
| 2 | I | 1.13 | 13/3143 (0.4%) | 1.44 | 45/4369 (1.0%) |
| 2 | O | 1.13 | 13/3143 (0.4%) | 1.44 | 45/4369 (1.0%) |
| 2 | U | 1.13 | 13/3143 (0.4%) | 1.44 | 45/4369 (1.0%) |
| 3 | D | 1.22 | 38/5066 (0.8%) | 1.74 | 122/7020 (1.7%) |
| 3 | P | 1.22 | 38/5066 (0.8%) | 1.74 | 121/7020 (1.7%) |
| 4 | F | 4.14 | 197/1655 (11.9%) | 4.03 | 272/2302 (11.8%) |
| 4 | L | 4.14 | 197/1655 (11.9%) | 4.03 | 272/2302 (11.8%) |
| 4 | R | 4.14 | 197/1655 (11.9%) | 4.03 | 272/2302 (11.8%) |
| 4 | X | 4.14 | 199/1655 (12.0%) | 4.03 | 273/2302 (11.9%) |
| 5 | G | 3.95 | 84/852 (9.9%) | 3.81 | 121/1190 (10.2%) |
| 5 | M | 3.95 | 84/852 (9.9%) | 3.81 | 121/1190 (10.2%) |
| 5 | S | 3.95 | 84/852 (9.9%) | 3.81 | 121/1190 (10.2%) |
| 5 | Y | 3.95 | 85/852 (10.0%) | 3.81 | 120/1190 (10.1%) |
| 6 | H | 3.44 | 83/841 (9.9%) | 3.10 | 110/1174 (9.4%) |
| 6 | N | 3.44 | 83/841 (9.9%) | 3.10 | 110/1174 (9.4%) |
| 6 | T | 3.44 | 83/841 (9.9%) | 3.09 | 109/1174 (9.3%) |
| 6 | Z | 3.44 | 83/841 (9.9%) | 3.10 | 110/1174 (9.4%) |
| 7 | J | 0.92 | 0/6201 | 1.20 | 27/8622 (0.3%) |
| 7 | V | 0.92 | 0/6201 | 1.20 | 27/8622 (0.3%) |
| All | All | 1.89 | 1587/76240 (2.1%) | 2.00 | 2548/105862 (2.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | K | 0 | 1 |
| 1 | Q | 0 | 1 |
| 1 | W | 0 | 1 |
| 2 | C | 1 | 4 |
| 2 | I | 1 | 4 |
| 2 | O | 1 | 4 |
| 2 | U | 1 | 4 |
| 3 | D | 0 | 21 |
| 3 | P | 0 | 20 |
| 4 | F | 10 | 40 |
| 4 | L | 10 | 40 |
| 4 | R | 10 | 40 |
| 4 | X | 10 | 40 |
| 5 | G | 9 | 10 |
| 5 | M | 9 | 10 |
| 5 | S | 9 | 10 |
| 5 | Y | 9 | 10 |
| 6 | H | 5 | 5 |
| 6 | N | 5 | 5 |
| 6 | T | 5 | 4 |
| 6 | Z | 5 | 5 |
| 7 | J | 0 | 3 |
| 7 | V | 0 | 3 |
| All | All | 100 | 288 |

All (1587) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | S | 380 | ILE | N-CA | 38.58 | 2.23 | 1.46 |
| 5 | M | 380 | ILE | N-CA | 38.56 | 2.23 | 1.46 |
| 5 | G | 380 | ILE | N-CA | 38.55 | 2.23 | 1.46 |
| 5 | Y | 380 | ILE | N-CA | 38.48 | 2.23 | 1.46 |
| 5 | M | 379 | HIS | CA-C | 37.09 | 2.49 | 1.52 |
| 5 | S | 379 | HIS | CA-C | 37.09 | 2.49 | 1.52 |
| 5 | G | 379 | HIS | CA-C | 37.07 | 2.49 | 1.52 |
| 5 | Y | 379 | HIS | CA-C | 37.05 | 2.49 | 1.52 |
| 4 | F | 453 | TYR | CA-C | 36.23 | 2.47 | 1.52 |
| 4 | X | 453 | TYR | CA-C | 36.23 | 2.47 | 1.52 |
| 4 | R | 453 | TYR | CA-C | 36.18 | 2.47 | 1.52 |
| 4 | L | 453 | TYR | CA-C | 36.17 | 2.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 493 | HIS | CA-CB | 32.64 | 2.25 | 1.53 |
| 4 | X | 493 | HIS | CA-CB | 32.63 | 2.25 | 1.53 |
| 4 | F | 493 | HIS | CA-CB | 32.60 | 2.25 | 1.53 |
| 4 | L | 493 | HIS | CA-CB | 32.59 | 2.25 | 1.53 |
| 4 | L | 493 | HIS | CA-C | -31.42 | 0.71 | 1.52 |
| 4 | X | 493 | HIS | CA-C | -31.39 | 0.71 | 1.52 |
| 4 | F | 493 | HIS | CA-C | -31.38 | 0.71 | 1.52 |
| 4 | R | 493 | HIS | CA-C | -31.34 | 0.71 | 1.52 |
| 6 | N | 374 | SER | CA-CB | 29.08 | 1.96 | 1.52 |
| 6 | Z | 374 | SER | CA-CB | 29.04 | 1.96 | 1.52 |
| 6 | H | 374 | SER | CA-CB | 29.02 | 1.96 | 1.52 |
| 6 | T | 374 | SER | CA-CB | 29.00 | 1.96 | 1.52 |
| 5 | M | 379 | HIS | C-N | 28.26 | 1.99 | 1.34 |
| 5 | Y | 379 | HIS | C-N | 28.25 | 1.99 | 1.34 |
| 5 | S | 379 | HIS | C-N | 28.21 | 1.99 | 1.34 |
| 5 | G | 379 | HIS | C-N | 28.21 | 1.99 | 1.34 |
| 6 | T | 411 | GLU | CA-C | 28.19 | 2.26 | 1.52 |
| 6 | N | 411 | GLU | CA-C | 28.18 | 2.26 | 1.52 |
| 6 | H | 411 | GLU | CA-C | 28.16 | 2.26 | 1.52 |
| 6 | Z | 411 | GLU | CA-C | 28.16 | 2.26 | 1.52 |
| 4 | L | 222 | THR | N-CA | 26.75 | 1.99 | 1.46 |
| 4 | R | 222 | THR | N-CA | 26.74 | 1.99 | 1.46 |
| 4 | X | 222 | THR | N-CA | 26.73 | 1.99 | 1.46 |
| 4 | F | 222 | THR | N-CA | 26.66 | 1.99 | 1.46 |
| 4 | L | 450 | GLU | CA-C | 24.57 | 2.16 | 1.52 |
| 4 | F | 450 | GLU | CA-C | 24.57 | 2.16 | 1.52 |
| 4 | X | 450 | GLU | CA-C | 24.57 | 2.16 | 1.52 |
| 4 | R | 450 | GLU | CA-C | 24.54 | 2.16 | 1.52 |
| 4 | X | 400 | GLY | N-CA | 24.30 | 1.82 | 1.46 |
| 4 | F | 400 | GLY | N-CA | 24.30 | 1.82 | 1.46 |
| 4 | L | 400 | GLY | N-CA | 24.28 | 1.82 | 1.46 |
| 4 | R | 400 | GLY | N-CA | 24.27 | 1.82 | 1.46 |
| 5 | G | 341 | ALA | N-CA | 23.84 | 1.94 | 1.46 |
| 5 | Y | 341 | ALA | N-CA | 23.83 | 1.94 | 1.46 |
| 5 | S | 341 | ALA | N-CA | 23.80 | 1.94 | 1.46 |
| 5 | M | 341 | ALA | N-CA | 23.77 | 1.93 | 1.46 |
| 4 | R | 487 | ASP | CA-C | 23.16 | 2.13 | 1.52 |
| 4 | F | 487 | ASP | CA-C | 23.15 | 2.13 | 1.52 |
| 4 | L | 487 | ASP | CA-C | 23.12 | 2.13 | 1.52 |
| 4 | X | 487 | ASP | CA-C | 23.11 | 2.13 | 1.52 |
| 4 | L | 401 | TYR | N-CA | 21.90 | 1.90 | 1.46 |
| 4 | X | 401 | TYR | N-CA | 21.89 | 1.90 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 401 | TYR | N-CA | 21.88 | 1.90 | 1.46 |
| 4 | F | 401 | TYR | N-CA | 21.86 | 1.90 | 1.46 |
| 4 | R | 450 | GLU | C-O | 21.44 | 1.64 | 1.23 |
| 4 | X | 450 | GLU | C-O | 21.42 | 1.64 | 1.23 |
| 4 | F | 450 | GLU | C-O | 21.41 | 1.64 | 1.23 |
| 4 | L | 450 | GLU | C-O | 21.39 | 1.64 | 1.23 |
| 6 | N | 462 | GLY | CA-C | 21.17 | 1.85 | 1.51 |
| 6 | T | 462 | GLY | CA-C | 21.14 | 1.85 | 1.51 |
| 4 | R | 458 | ASP | C-N | 21.12 | 1.82 | 1.34 |
| 6 | H | 462 | GLY | CA-C | 21.12 | 1.85 | 1.51 |
| 6 | Z | 462 | GLY | CA-C | 21.11 | 1.85 | 1.51 |
| 4 | X | 458 | ASP | C-N | 21.08 | 1.82 | 1.34 |
| 4 | L | 458 | ASP | C-N | 21.06 | 1.82 | 1.34 |
| 4 | F | 458 | ASP | C-N | 21.05 | 1.82 | 1.34 |
| 4 | R | 453 | TYR | CA-CB | 19.94 | 1.97 | 1.53 |
| 5 | Y | 341 | ALA | CA-CB | -19.92 | 1.10 | 1.52 |
| 5 | S | 341 | ALA | CA-CB | -19.90 | 1.10 | 1.52 |
| 5 | G | 341 | ALA | CA-CB | -19.90 | 1.10 | 1.52 |
| 4 | L | 453 | TYR | CA-CB | 19.90 | 1.97 | 1.53 |
| 4 | F | 453 | TYR | CA-CB | 19.89 | 1.97 | 1.53 |
| 5 | M | 341 | ALA | CA-CB | -19.88 | 1.10 | 1.52 |
| 4 | X | 453 | TYR | CA-CB | 19.88 | 1.97 | 1.53 |
| 4 | X | 451 | GLU | CA-C | 18.97 | 2.02 | 1.52 |
| 4 | F | 451 | GLU | CA-C | 18.94 | 2.02 | 1.52 |
| 4 | R | 451 | GLU | CA-C | 18.91 | 2.02 | 1.52 |
| 5 | S | 327 | ARG | CA-C | 18.91 | 2.02 | 1.52 |
| 5 | M | 327 | ARG | CA-C | 18.89 | 2.02 | 1.52 |
| 4 | L | 451 | GLU | CA-C | 18.86 | 2.02 | 1.52 |
| 5 | G | 327 | ARG | CA-C | 18.86 | 2.02 | 1.52 |
| 5 | Y | 327 | ARG | CA-C | 18.84 | 2.02 | 1.52 |
| 4 | X | 457 | ALA | N-CA | -18.74 | 1.08 | 1.46 |
| 4 | F | 457 | ALA | N-CA | -18.71 | 1.08 | 1.46 |
| 4 | L | 457 | ALA | N-CA | -18.68 | 1.08 | 1.46 |
| 4 | R | 457 | ALA | N-CA | -18.62 | 1.09 | 1.46 |
| 4 | R | 343 | MET | N-CA | -18.31 | 1.09 | 1.46 |
| 4 | L | 343 | MET | N-CA | -18.30 | 1.09 | 1.46 |
| 4 | F | 343 | MET | N-CA | -18.29 | 1.09 | 1.46 |
| 4 | X | 343 | MET | N-CA | -18.25 | 1.09 | 1.46 |
| 4 | L | 451 | GLU | C-O | 17.85 | 1.57 | 1.23 |
| 4 | F | 451 | GLU | C-O | 17.84 | 1.57 | 1.23 |
| 4 | R | 451 | GLU | C-O | 17.75 | 1.57 | 1.23 |
| 6 | T | 409 | PRO | CA-C | 17.74 | 1.88 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | X | 451 | GLU | C-O | 17.74 | 1.57 | 1.23 |
| 6 | N | 409 | PRO | CA-C | 17.73 | 1.88 | 1.52 |
| 6 | H | 409 | PRO | CA-C | 17.72 | 1.88 | 1.52 |
| 6 | Z | 409 | PRO | CA-C | 17.71 | 1.88 | 1.52 |
| 4 | F | 229 | GLY | CA-C | -17.44 | 1.24 | 1.51 |
| 4 | R | 229 | GLY | CA-C | -17.41 | 1.24 | 1.51 |
| 4 | X | 229 | GLY | CA-C | -17.38 | 1.24 | 1.51 |
| 4 | L | 229 | GLY | CA-C | -17.32 | 1.24 | 1.51 |
| 4 | F | 329 | GLY | N-CA | 17.28 | 1.72 | 1.46 |
| 4 | L | 329 | GLY | N-CA | 17.21 | 1.71 | 1.46 |
| 4 | X | 329 | GLY | N-CA | 17.21 | 1.71 | 1.46 |
| 4 | R | 329 | GLY | N-CA | 17.18 | 1.71 | 1.46 |
| 5 | M | 326 | LEU | N-CA | 17.03 | 1.80 | 1.46 |
| 5 | S | 326 | LEU | N-CA | 17.01 | 1.80 | 1.46 |
| 5 | G | 326 | LEU | N-CA | 17.00 | 1.80 | 1.46 |
| 5 | Y | 326 | LEU | N-CA | 17.00 | 1.80 | 1.46 |
| 5 | M | 339 | TYR | C-N | 16.75 | 1.72 | 1.34 |
| 5 | S | 339 | TYR | C-N | 16.73 | 1.72 | 1.34 |
| 5 | Y | 339 | TYR | C-N | 16.73 | 1.72 | 1.34 |
| 5 | G | 339 | TYR | C-N | 16.68 | 1.72 | 1.34 |
| 4 | L | 458 | ASP | CA-C | 16.08 | 1.94 | 1.52 |
| 4 | X | 458 | ASP | CA-C | 16.07 | 1.94 | 1.52 |
| 4 | F | 458 | ASP | CA-C | 16.05 | 1.94 | 1.52 |
| 4 | R | 458 | ASP | CA-C | 16.05 | 1.94 | 1.52 |
| 5 | S | 352 | GLN | N-CA | -15.77 | 1.14 | 1.46 |
| 5 | G | 352 | GLN | N-CA | -15.77 | 1.14 | 1.46 |
| 5 | M | 352 | GLN | N-CA | -15.77 | 1.14 | 1.46 |
| 5 | Y | 352 | GLN | N-CA | -15.76 | 1.14 | 1.46 |
| 6 | Z | 341 | SER | CA-CB | -15.62 | 1.29 | 1.52 |
| 6 | T | 341 | SER | CA-CB | -15.60 | 1.29 | 1.52 |
| 6 | N | 341 | SER | CA-CB | -15.57 | 1.29 | 1.52 |
| 6 | H | 341 | SER | CA-CB | -15.55 | 1.29 | 1.52 |
| 4 | F | 492 | GLU | C-N | 15.52 | 1.69 | 1.34 |
| 4 | L | 492 | GLU | C-N | 15.51 | 1.69 | 1.34 |
| 5 | S | 327 | ARG | N-CA | 15.50 | 1.77 | 1.46 |
| 5 | M | 327 | ARG | N-CA | 15.49 | 1.77 | 1.46 |
| 4 | R | 492 | GLU | C-N | 15.49 | 1.69 | 1.34 |
| 5 | Y | 327 | ARG | N-CA | 15.49 | 1.77 | 1.46 |
| 4 | X | 492 | GLU | C-N | 15.47 | 1.69 | 1.34 |
| 5 | G | 327 | ARG | N-CA | 15.46 | 1.77 | 1.46 |
| 4 | F | 459 | LEU | C-N | -15.40 | 0.98 | 1.34 |
| 4 | R | 459 | LEU | C-N | -15.38 | 0.98 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | L | 459 | LEU | C-N | -15.37 | 0.98 | 1.34 |
| 4 | X | 459 | LEU | C-N | -15.37 | 0.98 | 1.34 |
| 6 | H | 411 | GLU | C-N | 15.34 | 1.69 | 1.34 |
| 6 | N | 411 | GLU | C-N | 15.31 | 1.69 | 1.34 |
| 6 | Z | 411 | GLU | C-N | 15.30 | 1.69 | 1.34 |
| 6 | T | 411 | GLU | C-N | 15.26 | 1.69 | 1.34 |
| 5 | S | 327 | ARG | CA-CB | 15.24 | 1.87 | 1.53 |
| 5 | G | 327 | ARG | CA-CB | 15.23 | 1.87 | 1.53 |
| 5 | M | 327 | ARG | CA-CB | 15.22 | 1.87 | 1.53 |
| 5 | Y | 327 | ARG | CA-CB | 15.21 | 1.87 | 1.53 |
| 4 | L | 493 | HIS | N-CA | 15.15 | 1.76 | 1.46 |
| 4 | X | 493 | HIS | N-CA | 15.14 | 1.76 | 1.46 |
| 4 | R | 493 | HIS | N-CA | 15.10 | 1.76 | 1.46 |
| 4 | R | 458 | ASP | CA-CB | 15.07 | 1.87 | 1.53 |
| 4 | F | 493 | HIS | N-CA | 15.06 | 1.76 | 1.46 |
| 4 | F | 458 | ASP | CA-CB | 15.04 | 1.87 | 1.53 |
| 5 | S | 379 | HIS | N-CA | 15.04 | 1.76 | 1.46 |
| 4 | L | 458 | ASP | CA-CB | 15.03 | 1.87 | 1.53 |
| 4 | X | 458 | ASP | CA-CB | 15.03 | 1.87 | 1.53 |
| 5 | G | 379 | HIS | N-CA | 15.02 | 1.76 | 1.46 |
| 4 | L | 472 | GLU | N-CA | 15.02 | 1.76 | 1.46 |
| 5 | Y | 379 | HIS | N-CA | 14.99 | 1.76 | 1.46 |
| 4 | R | 472 | GLU | N-CA | 14.97 | 1.76 | 1.46 |
| 4 | R | 455 | ILE | C-N | -14.97 | 0.99 | 1.34 |
| 4 | X | 472 | GLU | N-CA | 14.97 | 1.76 | 1.46 |
| 4 | F | 472 | GLU | N-CA | 14.96 | 1.76 | 1.46 |
| 5 | M | 379 | HIS | N-CA | 14.96 | 1.76 | 1.46 |
| 4 | L | 455 | ILE | C-N | -14.95 | 0.99 | 1.34 |
| 4 | X | 455 | ILE | C-N | -14.92 | 0.99 | 1.34 |
| 4 | F | 455 | ILE | C-N | -14.90 | 0.99 | 1.34 |
| 2 | I | 6 | PHE | CA-CB | -14.78 | 1.21 | 1.53 |
| 2 | O | 6 | PHE | CA-CB | -14.77 | 1.21 | 1.53 |
| 2 | C | 6 | PHE | CA-CB | -14.74 | 1.21 | 1.53 |
| 5 | Y | 340 | ALA | N-CA | -14.71 | 1.17 | 1.46 |
| 2 | U | 6 | PHE | CA-CB | -14.69 | 1.21 | 1.53 |
| 5 | G | 340 | ALA | N-CA | -14.68 | 1.17 | 1.46 |
| 5 | M | 340 | ALA | N-CA | -14.68 | 1.17 | 1.46 |
| 5 | S | 340 | ALA | N-CA | -14.66 | 1.17 | 1.46 |
| 4 | L | 457 | ALA | CA-CB | 14.61 | 1.83 | 1.52 |
| 4 | R | 457 | ALA | CA-CB | 14.60 | 1.83 | 1.52 |
| 4 | F | 457 | ALA | CA-CB | 14.58 | 1.83 | 1.52 |
| 4 | X | 453 | TYR | N-CA | 14.58 | 1.75 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | F | 453 | TYR | N-CA | 14.58 | 1.75 | 1.46 |
| 4 | L | 453 | TYR | N-CA | 14.55 | 1.75 | 1.46 |
| 4 | X | 457 | ALA | CA-CB | 14.55 | 1.83 | 1.52 |
| 4 | R | 453 | TYR | N-CA | 14.55 | 1.75 | 1.46 |
| 4 | L | 453 | TYR | C-O | 14.52 | 1.50 | 1.23 |
| 4 | R | 453 | TYR | C-O | 14.48 | 1.50 | 1.23 |
| 4 | X | 453 | TYR | C-O | 14.46 | 1.50 | 1.23 |
| 4 | F | 453 | TYR | C-O | 14.44 | 1.50 | 1.23 |
| 4 | F | 231 | LYS | CA-C | -14.22 | 1.16 | 1.52 |
| 4 | X | 231 | LYS | CA-C | -14.22 | 1.16 | 1.52 |
| 4 | R | 231 | LYS | CA-C | -14.21 | 1.16 | 1.52 |
| 4 | L | 231 | LYS | CA-C | -14.20 | 1.16 | 1.52 |
| 4 | X | 483 | ASP | CA-CB | 14.19 | 1.85 | 1.53 |
| 4 | L | 483 | ASP | CA-CB | 14.16 | 1.85 | 1.53 |
| 4 | F | 483 | ASP | CA-CB | 14.15 | 1.85 | 1.53 |
| 4 | R | 483 | ASP | CA-CB | 14.13 | 1.85 | 1.53 |
| 4 | X | 402 | ALA | CA-C | 14.11 | 1.89 | 1.52 |
| 4 | R | 402 | ALA | CA-C | 14.11 | 1.89 | 1.52 |
| 6 | Z | 463 | ALA | N-CA | 14.09 | 1.74 | 1.46 |
| 4 | L | 402 | ALA | CA-C | 14.08 | 1.89 | 1.52 |
| 4 | F | 402 | ALA | CA-C | 14.06 | 1.89 | 1.52 |
| 6 | T | 463 | ALA | N-CA | 14.00 | 1.74 | 1.46 |
| 6 | H | 463 | ALA | N-CA | 14.00 | 1.74 | 1.46 |
| 6 | N | 463 | ALA | N-CA | 13.96 | 1.74 | 1.46 |
| 4 | R | 200 | THR | N-CA | -13.90 | 1.18 | 1.46 |
| 4 | L | 200 | THR | N-CA | -13.88 | 1.18 | 1.46 |
| 5 | G | 378 | SER | CA-C | 13.85 | 1.89 | 1.52 |
| 5 | S | 378 | SER | CA-C | 13.85 | 1.89 | 1.52 |
| 4 | X | 200 | THR | N-CA | -13.85 | 1.18 | 1.46 |
| 4 | F | 200 | THR | N-CA | -13.85 | 1.18 | 1.46 |
| 5 | Y | 378 | SER | CA-C | 13.84 | 1.89 | 1.52 |
| 5 | M | 378 | SER | CA-C | 13.82 | 1.88 | 1.52 |
| 4 | X | 328 | VAL | C-N | 13.60 | 1.57 | 1.33 |
| 4 | L | 328 | VAL | C-N | 13.59 | 1.57 | 1.33 |
| 4 | R | 328 | VAL | C-N | 13.59 | 1.57 | 1.33 |
| 3 | D | 1508 | LYS | CA-C | -13.53 | 1.17 | 1.52 |
| 3 | P | 1508 | LYS | CA-C | -13.51 | 1.17 | 1.52 |
| 4 | F | 328 | VAL | C-N | 13.49 | 1.57 | 1.33 |
| 4 | R | 472 | GLU | CA-CB | -13.36 | 1.24 | 1.53 |
| 4 | X | 472 | GLU | CA-CB | -13.32 | 1.24 | 1.53 |
| 4 | L | 472 | GLU | CA-CB | -13.29 | 1.24 | 1.53 |
| 4 | F | 472 | GLU | CA-CB | -13.29 | 1.24 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | F | 222 | THR | CA-C | 13.23 | 1.87 | 1.52 |
| 4 | R | 222 | THR | CA-C | 13.22 | 1.87 | 1.52 |
| 4 | X | 222 | THR | CA-C | 13.19 | 1.87 | 1.52 |
| 4 | L | 222 | THR | CA-C | 13.17 | 1.87 | 1.52 |
| 4 | R | 208 | GLN | CA-CB | -13.10 | 1.25 | 1.53 |
| 4 | X | 208 | GLN | CA-CB | -13.09 | 1.25 | 1.53 |
| 4 | F | 208 | GLN | CA-CB | -13.09 | 1.25 | 1.53 |
| 4 | L | 208 | GLN | CA-CB | -13.08 | 1.25 | 1.53 |
| 4 | R | 459 | LEU | CA-C | 13.08 | 1.86 | 1.52 |
| 4 | F | 459 | LEU | CA-C | 13.08 | 1.86 | 1.52 |
| 4 | X | 459 | LEU | CA-C | 13.06 | 1.86 | 1.52 |
| 4 | F | 211 | GLU | CA-C | -13.04 | 1.19 | 1.52 |
| 4 | F | 445 | GLY | N-CA | -13.04 | 1.26 | 1.46 |
| 4 | L | 402 | ALA | CA-CB | -13.04 | 1.25 | 1.52 |
| 4 | L | 459 | LEU | CA-C | 13.04 | 1.86 | 1.52 |
| 4 | X | 402 | ALA | CA-CB | -13.03 | 1.25 | 1.52 |
| 4 | X | 211 | GLU | CA-C | -13.01 | 1.19 | 1.52 |
| 4 | F | 454 | TYR | C-N | 13.01 | 1.64 | 1.34 |
| 4 | R | 454 | TYR | C-N | 13.01 | 1.64 | 1.34 |
| 4 | R | 211 | GLU | CA-C | -13.01 | 1.19 | 1.52 |
| 4 | F | 402 | ALA | CA-CB | -13.00 | 1.25 | 1.52 |
| 4 | L | 454 | TYR | C-N | 13.00 | 1.64 | 1.34 |
| 4 | R | 402 | ALA | CA-CB | -12.99 | 1.25 | 1.52 |
| 4 | L | 211 | GLU | CA-C | -12.99 | 1.19 | 1.52 |
| 4 | X | 445 | GLY | N-CA | -12.99 | 1.26 | 1.46 |
| 4 | R | 445 | GLY | N-CA | -12.97 | 1.26 | 1.46 |
| 4 | X | 454 | TYR | C-N | 12.95 | 1.63 | 1.34 |
| 4 | L | 445 | GLY | N-CA | -12.92 | 1.26 | 1.46 |
| 6 | Z | 381 | LYS | N-CA | 12.79 | 1.72 | 1.46 |
| 4 | L | 450 | GLU | N-CA | 12.78 | 1.72 | 1.46 |
| 4 | F | 450 | GLU | N-CA | 12.77 | 1.71 | 1.46 |
| 6 | H | 381 | LYS | N-CA | 12.75 | 1.71 | 1.46 |
| 4 | L | 455 | ILE | CA-CB | 12.75 | 1.84 | 1.54 |
| 4 | X | 455 | ILE | CA-CB | 12.74 | 1.84 | 1.54 |
| 4 | R | 455 | ILE | CA-CB | 12.73 | 1.84 | 1.54 |
| 4 | F | 251 | GLY | N-CA | -12.73 | 1.26 | 1.46 |
| 4 | R | 210 | VAL | CA-CB | -12.73 | 1.28 | 1.54 |
| 6 | T | 381 | LYS | N-CA | 12.73 | 1.71 | 1.46 |
| 4 | X | 450 | GLU | N-CA | 12.72 | 1.71 | 1.46 |
| 4 | R | 450 | GLU | N-CA | 12.71 | 1.71 | 1.46 |
| 4 | F | 455 | ILE | CA-CB | 12.71 | 1.84 | 1.54 |
| 6 | N | 381 | LYS | N-CA | 12.70 | 1.71 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 405 | SER | CA-CB | -12.69 | 1.33 | 1.52 |
| 4 | X | 210 | VAL | CA-CB | -12.69 | 1.28 | 1.54 |
| 4 | F | 210 | VAL | CA-CB | -12.65 | 1.28 | 1.54 |
| 4 | L | 210 | VAL | CA-CB | -12.65 | 1.28 | 1.54 |
| 4 | L | 251 | GLY | N-CA | -12.65 | 1.27 | 1.46 |
| 5 | M | 405 | SER | CA-CB | -12.63 | 1.34 | 1.52 |
| 4 | X | 251 | GLY | N-CA | -12.61 | 1.27 | 1.46 |
| 5 | Y | 405 | SER | CA-CB | -12.61 | 1.34 | 1.52 |
| 5 | M | 343 | ALA | CA-C | 12.59 | 1.85 | 1.52 |
| 4 | R | 251 | GLY | N-CA | -12.57 | 1.27 | 1.46 |
| 5 | S | 405 | SER | CA-CB | -12.57 | 1.34 | 1.52 |
| 5 | Y | 343 | ALA | CA-C | 12.57 | 1.85 | 1.52 |
| 5 | S | 343 | ALA | CA-C | 12.57 | 1.85 | 1.52 |
| 4 | L | 367 | THR | CA-C | 12.55 | 1.85 | 1.52 |
| 5 | G | 343 | ALA | CA-C | 12.54 | 1.85 | 1.52 |
| 4 | R | 367 | THR | CA-C | 12.54 | 1.85 | 1.52 |
| 4 | X | 367 | THR | CA-C | 12.54 | 1.85 | 1.52 |
| 4 | F | 367 | THR | CA-C | 12.51 | 1.85 | 1.52 |
| 6 | N | 413 | LEU | N-CA | -12.39 | 1.21 | 1.46 |
| 5 | M | 344 | ASP | CA-C | -12.36 | 1.20 | 1.52 |
| 6 | Z | 413 | LEU | N-CA | -12.36 | 1.21 | 1.46 |
| 6 | H | 413 | LEU | N-CA | -12.34 | 1.21 | 1.46 |
| 5 | G | 344 | ASP | CA-C | -12.31 | 1.21 | 1.52 |
| 5 | S | 344 | ASP | CA-C | -12.31 | 1.21 | 1.52 |
| 6 | N | 494 | LEU | CA-C | -12.30 | 1.21 | 1.52 |
| 6 | T | 413 | LEU | N-CA | -12.30 | 1.21 | 1.46 |
| 5 | Y | 344 | ASP | CA-C | -12.29 | 1.21 | 1.52 |
| 6 | H | 494 | LEU | CA-C | -12.29 | 1.21 | 1.52 |
| 4 | L | 299 | ASN | CA-C | 12.27 | 1.84 | 1.52 |
| 4 | F | 299 | ASN | CA-C | 12.26 | 1.84 | 1.52 |
| 4 | R | 299 | ASN | CA-C | 12.26 | 1.84 | 1.52 |
| 4 | X | 299 | ASN | CA-C | 12.26 | 1.84 | 1.52 |
| 6 | Z | 494 | LEU | CA-C | -12.26 | 1.21 | 1.52 |
| 6 | T | 494 | LEU | CA-C | -12.24 | 1.21 | 1.52 |
| 2 | O | 15 | GLN | CA-C | 12.23 | 1.84 | 1.52 |
| 2 | C | 15 | GLN | CA-C | 12.21 | 1.84 | 1.52 |
| 2 | I | 15 | GLN | CA-C | 12.20 | 1.84 | 1.52 |
| 2 | U | 15 | GLN | CA-C | 12.20 | 1.84 | 1.52 |
| 4 | L | 229 | GLY | N-CA | 12.09 | 1.64 | 1.46 |
| 4 | F | 221 | GLN | C-N | 12.07 | 1.61 | 1.34 |
| 4 | F | 229 | GLY | N-CA | 12.06 | 1.64 | 1.46 |
| 4 | X | 221 | GLN | C-N | 12.06 | 1.61 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 229 | GLY | N-CA | 12.05 | 1.64 | 1.46 |
| 4 | L | 221 | GLN | C-N | 12.03 | 1.61 | 1.34 |
| 4 | R | 221 | GLN | C-N | 12.03 | 1.61 | 1.34 |
| 4 | X | 229 | GLY | N-CA | 12.03 | 1.64 | 1.46 |
| 4 | R | 454 | TYR | CA-C | 11.90 | 1.83 | 1.52 |
| 4 | X | 454 | TYR | CA-C | 11.89 | 1.83 | 1.52 |
| 6 | H | 408 | SER | CA-C | -11.87 | 1.22 | 1.52 |
| 4 | L | 454 | TYR | CA-C | 11.87 | 1.83 | 1.52 |
| 4 | F | 454 | TYR | CA-C | 11.87 | 1.83 | 1.52 |
| 6 | T | 408 | SER | CA-C | -11.85 | 1.22 | 1.52 |
| 6 | N | 408 | SER | CA-C | -11.84 | 1.22 | 1.52 |
| 6 | Z | 408 | SER | CA-C | -11.82 | 1.22 | 1.52 |
| 6 | H | 497 | ARG | N-CA | 11.76 | 1.69 | 1.46 |
| 6 | Z | 497 | ARG | N-CA | 11.75 | 1.69 | 1.46 |
| 6 | N | 497 | ARG | N-CA | 11.71 | 1.69 | 1.46 |
| 6 | T | 497 | ARG | N-CA | 11.71 | 1.69 | 1.46 |
| 5 | Y | 378 | SER | C-N | 11.66 | 1.60 | 1.34 |
| 5 | M | 378 | SER | C-N | 11.65 | 1.60 | 1.34 |
| 5 | G | 378 | SER | C-N | 11.59 | 1.60 | 1.34 |
| 5 | S | 378 | SER | C-N | 11.59 | 1.60 | 1.34 |
| 5 | G | 328 | THR | CA-C | -11.55 | 1.23 | 1.52 |
| 5 | S | 328 | THR | CA-C | -11.55 | 1.23 | 1.52 |
| 5 | Y | 328 | THR | CA-C | -11.52 | 1.23 | 1.52 |
| 5 | M | 328 | THR | CA-C | -11.52 | 1.23 | 1.52 |
| 6 | H | 374 | SER | N-CA | -11.47 | 1.23 | 1.46 |
| 6 | N | 374 | SER | N-CA | -11.47 | 1.23 | 1.46 |
| 6 | T | 374 | SER | N-CA | -11.44 | 1.23 | 1.46 |
| 6 | Z | 374 | SER | N-CA | -11.44 | 1.23 | 1.46 |
| 4 | L | 235 | ASP | CA-CB | 11.42 | 1.79 | 1.53 |
| 4 | F | 235 | ASP | CA-CB | 11.40 | 1.79 | 1.53 |
| 4 | R | 235 | ASP | CA-CB | 11.40 | 1.79 | 1.53 |
| 4 | R | 456 | ASP | N-CA | -11.39 | 1.23 | 1.46 |
| 6 | H | 497 | ARG | CA-CB | -11.39 | 1.28 | 1.53 |
| 6 | Z | 497 | ARG | CA-CB | -11.37 | 1.28 | 1.53 |
| 5 | G | 276 | SER | CA-C | 11.37 | 1.82 | 1.52 |
| 5 | M | 276 | SER | CA-C | 11.36 | 1.82 | 1.52 |
| 6 | T | 497 | ARG | CA-CB | -11.36 | 1.28 | 1.53 |
| 4 | X | 235 | ASP | CA-CB | 11.36 | 1.78 | 1.53 |
| 6 | T | 363 | ARG | CA-C | -11.35 | 1.23 | 1.52 |
| 5 | S | 276 | SER | CA-C | 11.35 | 1.82 | 1.52 |
| 5 | Y | 320 | LYS | N-CA | -11.35 | 1.23 | 1.46 |
| 5 | M | 320 | LYS | N-CA | -11.34 | 1.23 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | S | 320 | LYS | N-CA | -11.34 | 1.23 | 1.46 |
| 4 | L | 456 | ASP | N-CA | -11.34 | 1.23 | 1.46 |
| 6 | N | 363 | ARG | CA-C | -11.34 | 1.23 | 1.52 |
| 6 | H | 363 | ARG | CA-C | -11.33 | 1.23 | 1.52 |
| 6 | N | 497 | ARG | CA-CB | -11.32 | 1.29 | 1.53 |
| 4 | F | 456 | ASP | N-CA | -11.32 | 1.23 | 1.46 |
| 5 | G | 320 | LYS | N-CA | -11.32 | 1.23 | 1.46 |
| 5 | Y | 276 | SER | CA-C | 11.31 | 1.82 | 1.52 |
| 4 | X | 456 | ASP | N-CA | -11.31 | 1.23 | 1.46 |
| 6 | Z | 363 | ARG | CA-C | -11.30 | 1.23 | 1.52 |
| 4 | X | 305 | ASP | CA-CB | -11.30 | 1.29 | 1.53 |
| 4 | X | 447 | VAL | CA-CB | 11.28 | 1.78 | 1.54 |
| 4 | R | 305 | ASP | CA-CB | -11.28 | 1.29 | 1.53 |
| 4 | L | 305 | ASP | CA-CB | -11.27 | 1.29 | 1.53 |
| 4 | F | 305 | ASP | CA-CB | -11.26 | 1.29 | 1.53 |
| 4 | L | 447 | VAL | CA-CB | 11.26 | 1.78 | 1.54 |
| 4 | R | 447 | VAL | CA-CB | 11.26 | 1.78 | 1.54 |
| 3 | D | 1520 | GLY | CA-C | -11.24 | 1.33 | 1.51 |
| 3 | P | 1520 | GLY | CA-C | -11.22 | 1.33 | 1.51 |
| 4 | F | 447 | VAL | CA-CB | 11.20 | 1.78 | 1.54 |
| 4 | L | 249 | PRO | N-CA | -11.18 | 1.28 | 1.47 |
| 4 | X | 249 | PRO | N-CA | -11.16 | 1.28 | 1.47 |
| 3 | D | 1520 | GLY | N-CA | -11.15 | 1.29 | 1.46 |
| 3 | P | 1520 | GLY | N-CA | -11.13 | 1.29 | 1.46 |
| 4 | R | 249 | PRO | N-CA | -11.12 | 1.28 | 1.47 |
| 4 | F | 249 | PRO | N-CA | -11.11 | 1.28 | 1.47 |
| 3 | D | 1517 | SER | CA-C | -11.09 | 1.24 | 1.52 |
| 3 | P | 1517 | SER | CA-C | -11.09 | 1.24 | 1.52 |
| 4 | F | 260 | THR | CA-CB | 11.03 | 1.82 | 1.53 |
| 4 | R | 260 | THR | CA-CB | 11.03 | 1.82 | 1.53 |
| 4 | X | 260 | THR | CA-CB | 11.02 | 1.81 | 1.53 |
| 4 | L | 260 | THR | CA-CB | 11.01 | 1.81 | 1.53 |
| 6 | Z | 408 | SER | C-N | -10.98 | 1.13 | 1.34 |
| 6 | H | 408 | SER | C-N | -10.96 | 1.13 | 1.34 |
| 6 | T | 408 | SER | C-N | -10.96 | 1.13 | 1.34 |
| 6 | N | 408 | SER | C-N | -10.93 | 1.13 | 1.34 |
| 4 | L | 232 | THR | CA-C | -10.86 | 1.24 | 1.52 |
| 4 | R | 232 | THR | CA-C | -10.86 | 1.24 | 1.52 |
| 4 | X | 232 | THR | CA-C | -10.86 | 1.24 | 1.52 |
| 4 | F | 232 | THR | CA-C | -10.84 | 1.24 | 1.52 |
| 2 | U | 28 | HIS | CA-C | -10.74 | 1.25 | 1.52 |
| 4 | R | 454 | TYR | CA-CB | 10.74 | 1.77 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 488 | ILE | N-CA | 10.74 | 1.67 | 1.46 |
| 4 | F | 454 | TYR | CA-CB | 10.74 | 1.77 | 1.53 |
| 2 | C | 28 | HIS | CA-C | -10.73 | 1.25 | 1.52 |
| 3 | D | 1542 | PRO | N-CA | -10.73 | 1.29 | 1.47 |
| 4 | X | 488 | ILE | N-CA | 10.73 | 1.67 | 1.46 |
| 4 | L | 451 | GLU | CA-CB | 10.72 | 1.77 | 1.53 |
| 2 | I | 28 | HIS | CA-C | -10.72 | 1.25 | 1.52 |
| 4 | R | 451 | GLU | CA-CB | 10.72 | 1.77 | 1.53 |
| 4 | X | 454 | TYR | CA-CB | 10.72 | 1.77 | 1.53 |
| 4 | F | 488 | ILE | N-CA | 10.71 | 1.67 | 1.46 |
| 2 | O | 28 | HIS | CA-C | -10.71 | 1.25 | 1.52 |
| 4 | L | 454 | TYR | CA-CB | 10.71 | 1.77 | 1.53 |
| 4 | F | 451 | GLU | CA-CB | 10.68 | 1.77 | 1.53 |
| 4 | L | 488 | ILE | N-CA | 10.68 | 1.67 | 1.46 |
| 3 | P | 1542 | PRO | N-CA | -10.68 | 1.29 | 1.47 |
| 4 | F | 335 | ARG | CA-C | -10.66 | 1.25 | 1.52 |
| 4 | X | 451 | GLU | CA-CB | 10.65 | 1.77 | 1.53 |
| 4 | L | 335 | ARG | CA-C | -10.65 | 1.25 | 1.52 |
| 4 | X | 335 | ARG | CA-C | -10.65 | 1.25 | 1.52 |
| 4 | R | 335 | ARG | CA-C | -10.61 | 1.25 | 1.52 |
| 2 | C | 7 | GLY | N-CA | -10.55 | 1.30 | 1.46 |
| 2 | I | 7 | GLY | N-CA | -10.49 | 1.30 | 1.46 |
| 2 | O | 7 | GLY | N-CA | -10.48 | 1.30 | 1.46 |
| 2 | U | 7 | GLY | N-CA | -10.47 | 1.30 | 1.46 |
| 6 | N | 377 | ARG | CA-C | -10.47 | 1.25 | 1.52 |
| 6 | T | 377 | ARG | CA-C | -10.43 | 1.25 | 1.52 |
| 5 | Y | 393 | TYR | N-CA | 10.43 | 1.67 | 1.46 |
| 6 | Z | 377 | ARG | CA-C | -10.43 | 1.25 | 1.52 |
| 6 | H | 377 | ARG | CA-C | -10.41 | 1.25 | 1.52 |
| 5 | M | 313 | ILE | CA-CB | -10.40 | 1.30 | 1.54 |
| 5 | S | 393 | TYR | N-CA | 10.40 | 1.67 | 1.46 |
| 5 | G | 393 | TYR | N-CA | 10.40 | 1.67 | 1.46 |
| 5 | G | 313 | ILE | CA-CB | -10.39 | 1.30 | 1.54 |
| 6 | T | 462 | GLY | C-N | 10.39 | 1.57 | 1.34 |
| 4 | F | 464 | LYS | CA-C | -10.38 | 1.25 | 1.52 |
| 6 | H | 462 | GLY | C-N | 10.37 | 1.57 | 1.34 |
| 4 | X | 464 | LYS | CA-C | -10.37 | 1.25 | 1.52 |
| 6 | N | 462 | GLY | C-N | 10.37 | 1.57 | 1.34 |
| 5 | S | 313 | ILE | CA-CB | -10.37 | 1.31 | 1.54 |
| 6 | Z | 462 | GLY | C-N | 10.35 | 1.57 | 1.34 |
| 5 | M | 393 | TYR | N-CA | 10.35 | 1.67 | 1.46 |
| 3 | P | 1488 | GLY | CA-C | -10.35 | 1.35 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 464 | LYS | CA-C | -10.33 | 1.26 | 1.52 |
| 3 | D | 1488 | GLY | CA-C | -10.32 | 1.35 | 1.51 |
| 4 | L | 464 | LYS | CA-C | -10.32 | 1.26 | 1.52 |
| 5 | Y | 313 | ILE | CA-CB | -10.32 | 1.31 | 1.54 |
| 5 | Y | 366 | GLU | CA-CB | 10.30 | 1.76 | 1.53 |
| 5 | G | 366 | GLU | CA-CB | 10.29 | 1.76 | 1.53 |
| 5 | S | 366 | GLU | CA-CB | 10.27 | 1.76 | 1.53 |
| 4 | R | 461 | ARG | CA-CB | -10.26 | 1.31 | 1.53 |
| 6 | T | 487 | TRP | N-CA | -10.26 | 1.25 | 1.46 |
| 4 | L | 486 | GLU | CA-CB | -10.25 | 1.31 | 1.53 |
| 5 | S | 331 | THR | CA-C | -10.24 | 1.26 | 1.52 |
| 5 | M | 366 | GLU | CA-CB | 10.24 | 1.76 | 1.53 |
| 6 | N | 487 | TRP | N-CA | -10.24 | 1.25 | 1.46 |
| 5 | M | 331 | THR | CA-C | -10.23 | 1.26 | 1.52 |
| 4 | X | 461 | ARG | CA-CB | -10.23 | 1.31 | 1.53 |
| 6 | H | 373 | THR | CA-CB | -10.22 | 1.26 | 1.53 |
| 6 | T | 373 | THR | CA-CB | -10.22 | 1.26 | 1.53 |
| 6 | H | 487 | TRP | N-CA | -10.22 | 1.25 | 1.46 |
| 4 | X | 486 | GLU | CA-CB | -10.22 | 1.31 | 1.53 |
| 6 | Z | 487 | TRP | N-CA | -10.22 | 1.25 | 1.46 |
| 6 | Z | 373 | THR | CA-CB | -10.22 | 1.26 | 1.53 |
| 4 | R | 486 | GLU | CA-CB | -10.21 | 1.31 | 1.53 |
| 4 | F | 461 | ARG | CA-CB | -10.21 | 1.31 | 1.53 |
| 4 | F | 486 | GLU | CA-CB | -10.21 | 1.31 | 1.53 |
| 4 | R | 461 | ARG | N-CA | 10.20 | 1.66 | 1.46 |
| 5 | Y | 331 | THR | CA-C | -10.21 | 1.26 | 1.52 |
| 5 | G | 331 | THR | CA-C | -10.19 | 1.26 | 1.52 |
| 4 | L | 461 | ARG | CA-CB | -10.18 | 1.31 | 1.53 |
| 6 | N | 373 | THR | CA-CB | -10.18 | 1.26 | 1.53 |
| 4 | F | 368 | SER | N-CA | 10.15 | 1.66 | 1.46 |
| 4 | L | 461 | ARG | N-CA | 10.15 | 1.66 | 1.46 |
| 4 | X | 368 | SER | N-CA | 10.15 | 1.66 | 1.46 |
| 4 | X | 461 | ARG | N-CA | 10.15 | 1.66 | 1.46 |
| 4 | F | 461 | ARG | N-CA | 10.15 | 1.66 | 1.46 |
| 4 | L | 368 | SER | N-CA | 10.10 | 1.66 | 1.46 |
| 4 | R | 368 | SER | N-CA | 10.10 | 1.66 | 1.46 |
| 5 | S | 326 | LEU | CA-C | 10.08 | 1.79 | 1.52 |
| 5 | G | 326 | LEU | CA-C | 10.07 | 1.79 | 1.52 |
| 5 | M | 326 | LEU | CA-C | 10.07 | 1.79 | 1.52 |
| 5 | Y | 326 | LEU | CA-C | 10.06 | 1.79 | 1.52 |
| 6 | Z | 490 | GLN | CA-CB | 9.97 | 1.75 | 1.53 |
| 6 | N | 387 | LYS | CA-C | -9.96 | 1.27 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | H | 490 | GLN | CA-CB | 9.96 | 1.75 | 1.53 |
| 6 | T | 387 | LYS | CA-C | -9.94 | 1.27 | 1.52 |
| 6 | T | 490 | GLN | CA-CB | 9.94 | 1.75 | 1.53 |
| 6 | H | 387 | LYS | CA-C | -9.94 | 1.27 | 1.52 |
| 6 | N | 411 | GLU | C-O | -9.93 | 1.04 | 1.23 |
| 6 | Z | 387 | LYS | CA-C | -9.93 | 1.27 | 1.52 |
| 6 | N | 490 | GLN | CA-CB | 9.93 | 1.75 | 1.53 |
| 5 | S | 327 | ARG | C-N | 9.92 | 1.56 | 1.34 |
| 4 | R | 400 | GLY | CA-C | -9.91 | 1.35 | 1.51 |
| 6 | H | 411 | GLU | C-O | -9.91 | 1.04 | 1.23 |
| 5 | G | 327 | ARG | C-N | 9.90 | 1.56 | 1.34 |
| 5 | M | 327 | ARG | C-N | 9.90 | 1.56 | 1.34 |
| 6 | T | 411 | GLU | C-O | -9.90 | 1.04 | 1.23 |
| 5 | Y | 327 | ARG | C-N | 9.90 | 1.56 | 1.34 |
| 4 | F | 400 | GLY | CA-C | -9.88 | 1.36 | 1.51 |
| 4 | X | 400 | GLY | CA-C | -9.88 | 1.36 | 1.51 |
| 6 | Z | 411 | GLU | C-O | -9.87 | 1.04 | 1.23 |
| 4 | L | 400 | GLY | CA-C | -9.84 | 1.36 | 1.51 |
| 4 | F | 424 | PRO | CA-C | -9.77 | 1.33 | 1.52 |
| 4 | X | 424 | PRO | CA-C | -9.73 | 1.33 | 1.52 |
| 4 | F | 311 | GLN | CA-CB | -9.73 | 1.32 | 1.53 |
| 3 | D | 1512 | TRP | N-CA | -9.70 | 1.26 | 1.46 |
| 4 | R | 424 | PRO | CA-C | -9.70 | 1.33 | 1.52 |
| 4 | X | 311 | GLN | CA-CB | -9.69 | 1.32 | 1.53 |
| 3 | P | 1512 | TRP | N-CA | -9.69 | 1.26 | 1.46 |
| 4 | L | 424 | PRO | CA-C | -9.68 | 1.33 | 1.52 |
| 4 | F | 436 | SER | CA-CB | 9.66 | 1.67 | 1.52 |
| 4 | R | 311 | GLN | CA-CB | -9.66 | 1.32 | 1.53 |
| 4 | L | 311 | GLN | CA-CB | -9.65 | 1.32 | 1.53 |
| 5 | S | 325 | ALA | CA-C | 9.64 | 1.78 | 1.52 |
| 5 | G | 325 | ALA | CA-C | 9.64 | 1.78 | 1.52 |
| 4 | L | 220 | ASN | C-O | 9.63 | 1.41 | 1.23 |
| 5 | Y | 325 | ALA | CA-C | 9.63 | 1.77 | 1.52 |
| 4 | X | 220 | ASN | C-O | 9.61 | 1.41 | 1.23 |
| 5 | M | 325 | ALA | CA-C | 9.61 | 1.77 | 1.52 |
| 4 | L | 436 | SER | CA-CB | 9.60 | 1.67 | 1.52 |
| 4 | R | 220 | ASN | C-O | 9.60 | 1.41 | 1.23 |
| 6 | N | 490 | GLN | N-CA | -9.59 | 1.27 | 1.46 |
| 4 | F | 220 | ASN | C-O | 9.58 | 1.41 | 1.23 |
| 4 | R | 436 | SER | CA-CB | 9.58 | 1.67 | 1.52 |
| 4 | X | 436 | SER | CA-CB | 9.58 | 1.67 | 1.52 |
| 6 | T | 490 | GLN | N-CA | -9.57 | 1.27 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | H | 490 | GLN | N-CA | -9.57 | 1.27 | 1.46 |
| 6 | Z | 490 | GLN | N-CA | -9.54 | 1.27 | 1.46 |
| 4 | R | 201 | GLU | CA-C | -9.50 | 1.28 | 1.52 |
| 4 | F | 201 | GLU | CA-C | -9.49 | 1.28 | 1.52 |
| 2 | C | 12 | GLN | CA-C | -9.49 | 1.28 | 1.52 |
| 4 | L | 201 | GLU | CA-C | -9.49 | 1.28 | 1.52 |
| 2 | I | 12 | GLN | CA-C | -9.48 | 1.28 | 1.52 |
| 4 | X | 201 | GLU | CA-C | -9.47 | 1.28 | 1.52 |
| 2 | U | 12 | GLN | CA-C | -9.46 | 1.28 | 1.52 |
| 2 | O | 12 | GLN | CA-C | -9.44 | 1.28 | 1.52 |
| 4 | X | 311 | GLN | CA-C | 9.38 | 1.77 | 1.52 |
| 4 | F | 311 | GLN | CA-C | 9.38 | 1.77 | 1.52 |
| 4 | L | 311 | GLN | CA-C | 9.36 | 1.77 | 1.52 |
| 4 | R | 311 | GLN | CA-C | 9.34 | 1.77 | 1.52 |
| 4 | X | 243 | TYR | CA-CB | -9.32 | 1.33 | 1.53 |
| 4 | F | 243 | TYR | CA-CB | -9.29 | 1.33 | 1.53 |
| 4 | L | 243 | TYR | CA-CB | -9.27 | 1.33 | 1.53 |
| 4 | R | 243 | TYR | CA-CB | -9.26 | 1.33 | 1.53 |
| 4 | X | 207 | GLN | N-CA | 9.22 | 1.64 | 1.46 |
| 4 | F | 207 | GLN | N-CA | 9.21 | 1.64 | 1.46 |
| 4 | L | 207 | GLN | N-CA | 9.21 | 1.64 | 1.46 |
| 4 | R | 207 | GLN | N-CA | 9.20 | 1.64 | 1.46 |
| 6 | T | 411 | GLU | N-CA | 9.10 | 1.64 | 1.46 |
| 6 | N | 411 | GLU | N-CA | 9.09 | 1.64 | 1.46 |
| 4 | R | 367 | THR | C-N | 9.09 | 1.54 | 1.34 |
| 6 | H | 411 | GLU | N-CA | 9.09 | 1.64 | 1.46 |
| 6 | Z | 411 | GLU | N-CA | 9.07 | 1.64 | 1.46 |
| 4 | F | 367 | THR | C-N | 9.06 | 1.54 | 1.34 |
| 4 | L | 367 | THR | C-N | 9.05 | 1.54 | 1.34 |
| 4 | X | 367 | THR | C-N | 9.05 | 1.54 | 1.34 |
| 6 | H | 388 | ARG | N-CA | -9.04 | 1.28 | 1.46 |
| 6 | Z | 388 | ARG | N-CA | -9.04 | 1.28 | 1.46 |
| 4 | F | 468 | LYS | CA-C | -9.04 | 1.29 | 1.52 |
| 4 | X | 452 | ARG | C-N | 9.03 | 1.54 | 1.34 |
| 4 | R | 452 | ARG | C-N | 9.02 | 1.54 | 1.34 |
| 4 | R | 468 | LYS | CA-C | -9.02 | 1.29 | 1.52 |
| 4 | F | 452 | ARG | C-N | 9.00 | 1.54 | 1.34 |
| 4 | L | 452 | ARG | C-N | 9.00 | 1.54 | 1.34 |
| 4 | L | 468 | LYS | CA-C | -9.00 | 1.29 | 1.52 |
| 4 | X | 468 | LYS | CA-C | -9.00 | 1.29 | 1.52 |
| 6 | T | 388 | ARG | N-CA | -8.99 | 1.28 | 1.46 |
| 6 | H | 409 | PRO | CA-CB | -8.99 | 1.35 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | F | 456 | ASP | CA-C | 8.98 | 1.76 | 1.52 |
| 4 | X | 267 | GLN | CA-C | -8.98 | 1.29 | 1.52 |
| 4 | R | 267 | GLN | CA-C | -8.98 | 1.29 | 1.52 |
| 4 | R | 456 | ASP | CA-C | 8.98 | 1.76 | 1.52 |
| 6 | N | 409 | PRO | CA-CB | -8.97 | 1.35 | 1.53 |
| 4 | L | 267 | GLN | CA-C | -8.97 | 1.29 | 1.52 |
| 4 | L | 452 | ARG | C-O | 8.96 | 1.40 | 1.23 |
| 4 | L | 456 | ASP | CA-C | 8.96 | 1.76 | 1.52 |
| 4 | X | 456 | ASP | CA-C | 8.96 | 1.76 | 1.52 |
| 4 | X | 452 | ARG | C-O | 8.95 | 1.40 | 1.23 |
| 4 | L | 201 | GLU | CA-CB | 8.95 | 1.73 | 1.53 |
| 4 | R | 201 | GLU | CA-CB | 8.95 | 1.73 | 1.53 |
| 4 | F | 267 | GLN | CA-C | -8.95 | 1.29 | 1.52 |
| 6 | N | 388 | ARG | N-CA | -8.95 | 1.28 | 1.46 |
| 4 | F | 201 | GLU | CA-CB | 8.94 | 1.73 | 1.53 |
| 6 | T | 409 | PRO | CA-CB | -8.94 | 1.35 | 1.53 |
| 6 | Z | 409 | PRO | CA-CB | -8.93 | 1.35 | 1.53 |
| 4 | L | 471 | GLN | CA-C | -8.93 | 1.29 | 1.52 |
| 4 | F | 452 | ARG | C-O | 8.91 | 1.40 | 1.23 |
| 4 | R | 452 | ARG | C-O | 8.91 | 1.40 | 1.23 |
| 4 | R | 471 | GLN | CA-C | -8.91 | 1.29 | 1.52 |
| 3 | D | 1474 | GLY | CA-C | -8.91 | 1.37 | 1.51 |
| 4 | X | 201 | GLU | CA-CB | 8.89 | 1.73 | 1.53 |
| 4 | X | 471 | GLN | CA-C | -8.89 | 1.29 | 1.52 |
| 6 | H | 408 | SER | N-CA | -8.88 | 1.28 | 1.46 |
| 5 | S | 348 | ILE | CA-CB | -8.88 | 1.34 | 1.54 |
| 4 | F | 471 | GLN | CA-C | -8.88 | 1.29 | 1.52 |
| 3 | P | 1474 | GLY | CA-C | -8.87 | 1.37 | 1.51 |
| 6 | Z | 408 | SER | N-CA | -8.87 | 1.28 | 1.46 |
| 5 | Y | 348 | ILE | CA-CB | -8.86 | 1.34 | 1.54 |
| 5 | M | 348 | ILE | CA-CB | -8.84 | 1.34 | 1.54 |
| 5 | G | 348 | ILE | CA-CB | -8.84 | 1.34 | 1.54 |
| 6 | T | 356 | THR | N-CA | -8.84 | 1.28 | 1.46 |
| 4 | R | 487 | ASP | CA-CB | 8.84 | 1.73 | 1.53 |
| 4 | L | 487 | ASP | CA-CB | 8.83 | 1.73 | 1.53 |
| 6 | N | 408 | SER | N-CA | -8.83 | 1.28 | 1.46 |
| 4 | F | 487 | ASP | N-CA | -8.83 | 1.28 | 1.46 |
| 6 | T | 408 | SER | N-CA | -8.83 | 1.28 | 1.46 |
| 4 | X | 487 | ASP | CA-CB | 8.83 | 1.73 | 1.53 |
| 6 | H | 356 | THR | N-CA | -8.82 | 1.28 | 1.46 |
| 4 | F | 487 | ASP | CA-CB | 8.82 | 1.73 | 1.53 |
| 3 | D | 1521 | TYR | N-CA | -8.82 | 1.28 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | X | 487 | ASP | N-CA | -8.81 | 1.28 | 1.46 |
| 4 | L | 487 | ASP | N-CA | -8.80 | 1.28 | 1.46 |
| 4 | R | 487 | ASP | N-CA | -8.80 | 1.28 | 1.46 |
| 6 | N | 356 | THR | N-CA | -8.78 | 1.28 | 1.46 |
| 6 | Z | 356 | THR | N-CA | -8.77 | 1.28 | 1.46 |
| 4 | F | 328 | VAL | CA-C | 8.76 | 1.75 | 1.52 |
| 3 | P | 1521 | TYR | N-CA | -8.75 | 1.28 | 1.46 |
| 4 | X | 328 | VAL | CA-C | 8.74 | 1.75 | 1.52 |
| 4 | L | 328 | VAL | CA-C | 8.73 | 1.75 | 1.52 |
| 4 | L | 143 | GLN | N-CA | 8.70 | 1.63 | 1.46 |
| 4 | X | 143 | GLN | N-CA | 8.70 | 1.63 | 1.46 |
| 4 | R | 328 | VAL | CA-C | 8.69 | 1.75 | 1.52 |
| 4 | F | 143 | GLN | N-CA | 8.69 | 1.63 | 1.46 |
| 5 | G | 339 | TYR | CA-CB | -8.67 | 1.34 | 1.53 |
| 6 | Z | 468 | SER | CA-CB | -8.67 | 1.40 | 1.52 |
| 6 | N | 468 | SER | CA-CB | -8.65 | 1.40 | 1.52 |
| 4 | F | 427 | PHE | CA-C | -8.64 | 1.30 | 1.52 |
| 4 | R | 143 | GLN | N-CA | 8.64 | 1.63 | 1.46 |
| 5 | Y | 339 | TYR | CA-CB | -8.64 | 1.34 | 1.53 |
| 2 | U | 7 | GLY | C-N | -8.63 | 1.14 | 1.34 |
| 4 | L | 440 | MET | CA-CB | -8.63 | 1.34 | 1.53 |
| 4 | F | 440 | MET | CA-CB | -8.63 | 1.34 | 1.53 |
| 4 | R | 440 | MET | CA-CB | -8.63 | 1.34 | 1.53 |
| 6 | H | 468 | SER | CA-CB | -8.62 | 1.40 | 1.52 |
| 4 | L | 144 | LEU | CA-CB | 8.62 | 1.73 | 1.53 |
| 4 | R | 427 | PHE | CA-C | -8.62 | 1.30 | 1.52 |
| 4 | F | 449 | SER | CA-CB | -8.62 | 1.40 | 1.52 |
| 2 | I | 7 | GLY | C-N | -8.62 | 1.14 | 1.34 |
| 4 | L | 449 | SER | CA-CB | -8.62 | 1.40 | 1.52 |
| 4 | R | 449 | SER | CA-CB | -8.62 | 1.40 | 1.52 |
| 4 | X | 427 | PHE | CA-C | -8.62 | 1.30 | 1.52 |
| 4 | X | 440 | MET | CA-CB | -8.61 | 1.35 | 1.53 |
| 4 | L | 427 | PHE | CA-C | -8.61 | 1.30 | 1.52 |
| 6 | T | 468 | SER | CA-CB | -8.61 | 1.40 | 1.52 |
| 4 | X | 144 | LEU | CA-CB | 8.61 | 1.73 | 1.53 |
| 5 | M | 339 | TYR | CA-CB | -8.60 | 1.35 | 1.53 |
| 5 | S | 329 | GLN | CA-C | -8.60 | 1.30 | 1.52 |
| 5 | G | 329 | GLN | CA-C | -8.60 | 1.30 | 1.52 |
| 2 | O | 7 | GLY | C-N | -8.60 | 1.14 | 1.34 |
| 2 | C | 7 | GLY | C-N | -8.59 | 1.14 | 1.34 |
| 4 | R | 144 | LEU | CA-CB | 8.59 | 1.73 | 1.53 |
| 6 | H | 408 | SER | CA-CB | 8.59 | 1.65 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 408 | SER | CA-CB | 8.59 | 1.65 | 1.52 |
| 5 | M | 329 | GLN | CA-C | -8.59 | 1.30 | 1.52 |
| 5 | S | 339 | TYR | CA-CB | -8.58 | 1.35 | 1.53 |
| 4 | F | 144 | LEU | CA-CB | 8.57 | 1.73 | 1.53 |
| 5 | Y | 329 | GLN | CA-C | -8.57 | 1.30 | 1.52 |
| 4 | R | 458 | ASP | N-CA | 8.56 | 1.63 | 1.46 |
| 4 | F | 458 | ASP | N-CA | 8.55 | 1.63 | 1.46 |
| 4 | X | 449 | SER | CA-CB | -8.55 | 1.40 | 1.52 |
| 4 | F | 403 | ILE | CA-CB | -8.55 | 1.35 | 1.54 |
| 6 | T | 408 | SER | CA-CB | 8.55 | 1.65 | 1.52 |
| 4 | X | 458 | ASP | N-CA | 8.55 | 1.63 | 1.46 |
| 4 | L | 458 | ASP | N-CA | 8.54 | 1.63 | 1.46 |
| 4 | X | 403 | ILE | CA-CB | -8.54 | 1.35 | 1.54 |
| 4 | R | 403 | ILE | CA-CB | -8.53 | 1.35 | 1.54 |
| 4 | X | 485 | LEU | N-CA | 8.53 | 1.63 | 1.46 |
| 6 | N | 408 | SER | CA-CB | 8.52 | 1.65 | 1.52 |
| 4 | L | 403 | ILE | CA-CB | -8.52 | 1.35 | 1.54 |
| 4 | X | 492 | GLU | CA-C | 8.51 | 1.75 | 1.52 |
| 4 | R | 492 | GLU | CA-C | 8.50 | 1.75 | 1.52 |
| 4 | F | 492 | GLU | CA-C | 8.48 | 1.75 | 1.52 |
| 4 | F | 485 | LEU | N-CA | 8.48 | 1.63 | 1.46 |
| 4 | X | 463 | ILE | N-CA | -8.47 | 1.29 | 1.46 |
| 4 | L | 492 | GLU | CA-C | 8.47 | 1.75 | 1.52 |
| 6 | T | 445 | LYS | N-CA | -8.46 | 1.29 | 1.46 |
| 4 | F | 463 | ILE | N-CA | -8.46 | 1.29 | 1.46 |
| 4 | R | 485 | LEU | N-CA | 8.46 | 1.63 | 1.46 |
| 4 | L | 485 | LEU | N-CA | 8.45 | 1.63 | 1.46 |
| 6 | H | 445 | LYS | N-CA | -8.45 | 1.29 | 1.46 |
| 6 | T | 380 | GLU | CA-CB | 8.44 | 1.72 | 1.53 |
| 4 | L | 463 | ILE | N-CA | -8.44 | 1.29 | 1.46 |
| 6 | N | 445 | LYS | N-CA | -8.44 | 1.29 | 1.46 |
| 6 | Z | 380 | GLU | CA-CB | 8.43 | 1.72 | 1.53 |
| 6 | Z | 445 | LYS | N-CA | -8.42 | 1.29 | 1.46 |
| 6 | H | 380 | GLU | CA-CB | 8.40 | 1.72 | 1.53 |
| 4 | R | 463 | ILE | N-CA | -8.40 | 1.29 | 1.46 |
| 6 | N | 380 | GLU | CA-CB | 8.39 | 1.72 | 1.53 |
| 4 | R | 254 | ARG | N-CA | -8.37 | 1.29 | 1.46 |
| 4 | F | 254 | ARG | N-CA | -8.35 | 1.29 | 1.46 |
| 4 | F | 432 | ASN | N-CA | -8.34 | 1.29 | 1.46 |
| 4 | L | 432 | ASN | N-CA | -8.34 | 1.29 | 1.46 |
| 4 | X | 254 | ARG | N-CA | -8.34 | 1.29 | 1.46 |
| 4 | F | 221 | GLN | N-CA | -8.33 | 1.29 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | X | 221 | GLN | N-CA | -8.32 | 1.29 | 1.46 |
| 4 | L | 221 | GLN | N-CA | -8.32 | 1.29 | 1.46 |
| 4 | L | 254 | ARG | N-CA | -8.32 | 1.29 | 1.46 |
| 4 | R | 221 | GLN | N-CA | -8.31 | 1.29 | 1.46 |
| 4 | X | 432 | ASN | N-CA | -8.30 | 1.29 | 1.46 |
| 4 | R | 432 | ASN | N-CA | -8.29 | 1.29 | 1.46 |
| 3 | D | 1488 | GLY | N-CA | -8.23 | 1.33 | 1.46 |
| 5 | G | 369 | ASN | CA-C | -8.22 | 1.31 | 1.52 |
| 3 | P | 1488 | GLY | N-CA | -8.20 | 1.33 | 1.46 |
| 6 | T | 495 | LEU | N-CA | -8.20 | 1.29 | 1.46 |
| 5 | Y | 369 | ASN | CA-C | -8.19 | 1.31 | 1.52 |
| 4 | R | 463 | ILE | CA-C | 8.19 | 1.74 | 1.52 |
| 4 | X | 223 | LEU | N-CA | 8.19 | 1.62 | 1.46 |
| 4 | X | 463 | ILE | CA-C | 8.18 | 1.74 | 1.52 |
| 6 | H | 495 | LEU | N-CA | -8.18 | 1.29 | 1.46 |
| 6 | N | 495 | LEU | N-CA | -8.16 | 1.30 | 1.46 |
| 4 | L | 463 | ILE | CA-C | 8.16 | 1.74 | 1.52 |
| 5 | Y | 338 | GLU | C-N | 8.16 | 1.52 | 1.34 |
| 6 | Z | 495 | LEU | N-CA | -8.16 | 1.30 | 1.46 |
| 5 | G | 343 | ALA | CA-CB | -8.16 | 1.35 | 1.52 |
| 4 | F | 223 | LEU | N-CA | 8.16 | 1.62 | 1.46 |
| 4 | R | 223 | LEU | N-CA | 8.16 | 1.62 | 1.46 |
| 5 | S | 369 | ASN | CA-C | -8.16 | 1.31 | 1.52 |
| 5 | M | 369 | ASN | CA-C | -8.15 | 1.31 | 1.52 |
| 5 | G | 338 | GLU | C-N | 8.15 | 1.52 | 1.34 |
| 4 | L | 223 | LEU | N-CA | 8.15 | 1.62 | 1.46 |
| 5 | M | 338 | GLU | C-N | 8.15 | 1.52 | 1.34 |
| 5 | Y | 343 | ALA | CA-CB | -8.14 | 1.35 | 1.52 |
| 4 | F | 463 | ILE | CA-C | 8.13 | 1.74 | 1.52 |
| 4 | F | 423 | ALA | CA-C | -8.13 | 1.31 | 1.52 |
| 5 | S | 343 | ALA | CA-CB | -8.12 | 1.35 | 1.52 |
| 6 | N | 420 | THR | CA-C | -8.11 | 1.31 | 1.52 |
| 5 | S | 338 | GLU | C-N | 8.11 | 1.52 | 1.34 |
| 4 | X | 331 | LYS | CA-C | -8.09 | 1.31 | 1.52 |
| 4 | L | 423 | ALA | CA-C | -8.09 | 1.31 | 1.52 |
| 5 | M | 343 | ALA | CA-CB | -8.09 | 1.35 | 1.52 |
| 5 | S | 333 | PRO | N-CA | -8.08 | 1.33 | 1.47 |
| 6 | T | 420 | THR | CA-C | -8.08 | 1.31 | 1.52 |
| 6 | Z | 420 | THR | CA-C | -8.08 | 1.31 | 1.52 |
| 6 | H | 420 | THR | CA-C | -8.07 | 1.31 | 1.52 |
| 4 | R | 423 | ALA | CA-C | -8.07 | 1.31 | 1.52 |
| 3 | D | 1507 | ASP | N-CA | -8.07 | 1.30 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | F | 331 | LYS | CA-C | -8.07 | 1.31 | 1.52 |
| 4 | X | 423 | ALA | CA-C | -8.07 | 1.31 | 1.52 |
| 5 | G | 333 | PRO | N-CA | -8.06 | 1.33 | 1.47 |
| 3 | P | 1507 | ASP | N-CA | -8.06 | 1.30 | 1.46 |
| 5 | Y | 333 | PRO | N-CA | -8.06 | 1.33 | 1.47 |
| 4 | R | 331 | LYS | CA-C | -8.03 | 1.32 | 1.52 |
| 4 | F | 484 | ASP | CA-C | -8.03 | 1.32 | 1.52 |
| 4 | R | 484 | ASP | CA-C | -8.01 | 1.32 | 1.52 |
| 4 | L | 484 | ASP | CA-C | -8.01 | 1.32 | 1.52 |
| 5 | M | 333 | PRO | N-CA | -8.01 | 1.33 | 1.47 |
| 4 | L | 331 | LYS | CA-C | -7.99 | 1.32 | 1.52 |
| 4 | X | 484 | ASP | CA-C | -7.97 | 1.32 | 1.52 |
| 5 | Y | 249 | PRO | N-CA | 7.97 | 1.60 | 1.47 |
| 5 | S | 352 | GLN | CA-CB | 7.96 | 1.71 | 1.53 |
| 5 | G | 249 | PRO | N-CA | 7.94 | 1.60 | 1.47 |
| 5 | Y | 352 | GLN | CA-CB | 7.94 | 1.71 | 1.53 |
| 4 | L | 449 | SER | C-N | 7.92 | 1.52 | 1.34 |
| 5 | S | 328 | THR | CA-CB | 7.92 | 1.74 | 1.53 |
| 4 | R | 299 | ASN | C-N | 7.92 | 1.49 | 1.34 |
| 5 | G | 328 | THR | CA-CB | 7.92 | 1.74 | 1.53 |
| 3 | D | 1511 | GLN | CA-C | -7.91 | 1.32 | 1.52 |
| 5 | Y | 328 | THR | CA-CB | 7.91 | 1.74 | 1.53 |
| 4 | F | 299 | ASN | C-N | 7.91 | 1.49 | 1.34 |
| 5 | M | 328 | THR | CA-CB | 7.91 | 1.74 | 1.53 |
| 4 | X | 299 | ASN | C-N | 7.91 | 1.49 | 1.34 |
| 4 | X | 449 | SER | C-N | 7.91 | 1.52 | 1.34 |
| 5 | G | 352 | GLN | CA-CB | 7.91 | 1.71 | 1.53 |
| 5 | S | 249 | PRO | N-CA | 7.90 | 1.60 | 1.47 |
| 4 | L | 299 | ASN | C-N | 7.90 | 1.49 | 1.34 |
| 6 | T | 385 | ASP | CA-C | -7.90 | 1.32 | 1.52 |
| 5 | M | 249 | PRO | N-CA | 7.90 | 1.60 | 1.47 |
| 5 | M | 352 | GLN | CA-CB | 7.90 | 1.71 | 1.53 |
| 4 | F | 452 | ARG | CA-C | 7.90 | 1.73 | 1.52 |
| 5 | M | 343 | ALA | N-CA | -7.89 | 1.30 | 1.46 |
| 4 | R | 449 | SER | C-N | 7.88 | 1.52 | 1.34 |
| 4 | X | 452 | ARG | CA-C | 7.88 | 1.73 | 1.52 |
| 5 | Y | 343 | ALA | N-CA | -7.87 | 1.30 | 1.46 |
| 6 | N | 385 | ASP | CA-C | -7.87 | 1.32 | 1.52 |
| 4 | X | 235 | ASP | N-CA | 7.87 | 1.62 | 1.46 |
| 3 | P | 1511 | GLN | CA-C | -7.87 | 1.32 | 1.52 |
| 4 | F | 235 | ASP | N-CA | 7.87 | 1.62 | 1.46 |
| 5 | S | 343 | ALA | N-CA | -7.87 | 1.30 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 385 | ASP | CA-C | -7.87 | 1.32 | 1.52 |
| 6 | H | 381 | LYS | CA-CB | 7.86 | 1.71 | 1.53 |
| 6 | H | 414 | VAL | CA-CB | 7.86 | 1.71 | 1.54 |
| 4 | L | 452 | ARG | CA-C | 7.86 | 1.73 | 1.52 |
| 4 | F | 449 | SER | C-N | 7.85 | 1.52 | 1.34 |
| 6 | H | 385 | ASP | CA-C | -7.85 | 1.32 | 1.52 |
| 6 | H | 412 | GLU | C-N | -7.85 | 1.16 | 1.34 |
| 6 | T | 414 | VAL | CA-CB | 7.85 | 1.71 | 1.54 |
| 6 | Z | 414 | VAL | CA-CB | 7.85 | 1.71 | 1.54 |
| 5 | G | 343 | ALA | N-CA | -7.85 | 1.30 | 1.46 |
| 6 | N | 381 | LYS | CA-CB | 7.84 | 1.71 | 1.53 |
| 6 | Z | 381 | LYS | CA-CB | 7.84 | 1.71 | 1.53 |
| 6 | H | 487 | TRP | CA-C | -7.84 | 1.32 | 1.52 |
| 6 | T | 412 | GLU | C-N | -7.84 | 1.16 | 1.34 |
| 6 | N | 414 | VAL | CA-CB | 7.83 | 1.71 | 1.54 |
| 6 | Z | 487 | TRP | CA-C | -7.82 | 1.32 | 1.52 |
| 4 | R | 452 | ARG | CA-C | 7.82 | 1.73 | 1.52 |
| 5 | M | 313 | ILE | N-CA | 7.80 | 1.61 | 1.46 |
| 5 | G | 313 | ILE | N-CA | 7.79 | 1.61 | 1.46 |
| 6 | Z | 412 | GLU | C-N | -7.79 | 1.16 | 1.34 |
| 5 | Y | 313 | ILE | N-CA | 7.79 | 1.61 | 1.46 |
| 4 | R | 235 | ASP | N-CA | 7.79 | 1.61 | 1.46 |
| 6 | N | 487 | TRP | CA-C | -7.78 | 1.32 | 1.52 |
| 6 | T | 381 | LYS | CA-CB | 7.78 | 1.71 | 1.53 |
| 6 | T | 487 | TRP | CA-C | -7.78 | 1.32 | 1.52 |
| 6 | N | 412 | GLU | C-N | -7.78 | 1.16 | 1.34 |
| 4 | L | 235 | ASP | N-CA | 7.78 | 1.61 | 1.46 |
| 4 | L | 144 | LEU | N-CA | -7.77 | 1.30 | 1.46 |
| 4 | R | 144 | LEU | N-CA | -7.76 | 1.30 | 1.46 |
| 4 | F | 485 | LEU | CA-CB | -7.75 | 1.35 | 1.53 |
| 6 | H | 410 | LEU | C-N | 7.75 | 1.51 | 1.34 |
| 4 | F | 144 | LEU | N-CA | -7.74 | 1.30 | 1.46 |
| 4 | X | 144 | LEU | N-CA | -7.73 | 1.30 | 1.46 |
| 6 | N | 410 | LEU | C-N | 7.73 | 1.51 | 1.34 |
| 4 | L | 485 | LEU | CA-CB | -7.73 | 1.35 | 1.53 |
| 5 | S | 313 | ILE | N-CA | 7.73 | 1.61 | 1.46 |
| 4 | X | 485 | LEU | CA-CB | -7.72 | 1.35 | 1.53 |
| 4 | R | 485 | LEU | CA-CB | -7.71 | 1.36 | 1.53 |
| 6 | Z | 335 | SER | CA-C | -7.71 | 1.32 | 1.52 |
| 6 | Z | 410 | LEU | C-N | 7.70 | 1.51 | 1.34 |
| 4 | F | 306 | PRO | CA-C | 7.69 | 1.68 | 1.52 |
| 4 | R | 306 | PRO | CA-C | 7.68 | 1.68 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | T | 410 | LEU | C-N | 7.68 | 1.51 | 1.34 |
| 4 | X | 306 | PRO | CA-C | 7.67 | 1.68 | 1.52 |
| 6 | Z | 402 | GLU | CA-C | -7.66 | 1.33 | 1.52 |
| 6 | H | 402 | GLU | CA-C | -7.65 | 1.33 | 1.52 |
| 6 | T | 335 | SER | CA-C | -7.65 | 1.33 | 1.52 |
| 2 | U | 15 | GLN | N-CA | -7.64 | 1.31 | 1.46 |
| 6 | H | 335 | SER | CA-C | -7.64 | 1.33 | 1.52 |
| 6 | N | 335 | SER | CA-C | -7.64 | 1.33 | 1.52 |
| 2 | C | 15 | GLN | N-CA | -7.63 | 1.31 | 1.46 |
| 6 | T | 402 | GLU | CA-C | -7.63 | 1.33 | 1.52 |
| 6 | N | 402 | GLU | CA-C | -7.62 | 1.33 | 1.52 |
| 2 | I | 15 | GLN | N-CA | -7.61 | 1.31 | 1.46 |
| 2 | O | 15 | GLN | N-CA | -7.61 | 1.31 | 1.46 |
| 4 | F | 231 | LYS | CA-CB | 7.61 | 1.70 | 1.53 |
| 4 | F | 448 | ARG | N-CA | 7.61 | 1.61 | 1.46 |
| 4 | R | 231 | LYS | CA-CB | 7.61 | 1.70 | 1.53 |
| 4 | X | 448 | ARG | N-CA | 7.61 | 1.61 | 1.46 |
| 4 | L | 306 | PRO | CA-C | 7.60 | 1.68 | 1.52 |
| 5 | Y | 346 | PHE | CA-C | -7.59 | 1.33 | 1.52 |
| 4 | L | 448 | ARG | N-CA | 7.59 | 1.61 | 1.46 |
| 4 | R | 448 | ARG | N-CA | 7.58 | 1.61 | 1.46 |
| 4 | L | 252 | THR | CA-CB | 7.58 | 1.73 | 1.53 |
| 5 | G | 346 | PHE | CA-C | -7.58 | 1.33 | 1.52 |
| 6 | T | 370 | GLU | CA-CB | -7.58 | 1.37 | 1.53 |
| 6 | H | 370 | GLU | CA-CB | -7.57 | 1.37 | 1.53 |
| 4 | L | 321 | LYS | N-CA | -7.57 | 1.31 | 1.46 |
| 4 | L | 231 | LYS | CA-CB | 7.57 | 1.70 | 1.53 |
| 6 | N | 370 | GLU | CA-CB | -7.57 | 1.37 | 1.53 |
| 5 | S | 340 | ALA | CA-C | 7.57 | 1.72 | 1.52 |
| 4 | R | 321 | LYS | N-CA | -7.56 | 1.31 | 1.46 |
| 4 | F | 321 | LYS | N-CA | -7.56 | 1.31 | 1.46 |
| 4 | X | 231 | LYS | CA-CB | 7.56 | 1.70 | 1.53 |
| 5 | M | 346 | PHE | CA-C | -7.56 | 1.33 | 1.52 |
| 5 | Y | 340 | ALA | CA-C | 7.56 | 1.72 | 1.52 |
| 5 | S | 346 | PHE | CA-C | -7.55 | 1.33 | 1.52 |
| 4 | R | 252 | THR | CA-CB | 7.55 | 1.73 | 1.53 |
| 5 | M | 340 | ALA | CA-C | 7.55 | 1.72 | 1.52 |
| 3 | D | 1542 | PRO | CA-C | 7.55 | 1.68 | 1.52 |
| 4 | X | 321 | LYS | N-CA | -7.54 | 1.31 | 1.46 |
| 4 | X | 252 | THR | CA-CB | 7.54 | 1.73 | 1.53 |
| 5 | Y | 377 | ASN | N-CA | -7.54 | 1.31 | 1.46 |
| 4 | F | 252 | THR | CA-CB | 7.53 | 1.73 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 370 | GLU | CA-CB | -7.52 | 1.37 | 1.53 |
| 6 | H | 446 | ARG | CA-CB | -7.52 | 1.37 | 1.53 |
| 5 | M | 401 | ALA | CA-CB | -7.52 | 1.36 | 1.52 |
| 5 | G | 340 | ALA | CA-C | 7.52 | 1.72 | 1.52 |
| 4 | R | 420 | GLU | CA-C | -7.51 | 1.33 | 1.52 |
| 6 | T | 446 | ARG | CA-CB | -7.51 | 1.37 | 1.53 |
| 4 | X | 420 | GLU | CA-C | -7.51 | 1.33 | 1.52 |
| 5 | G | 401 | ALA | CA-CB | -7.51 | 1.36 | 1.52 |
| 3 | P | 1542 | PRO | CA-C | 7.51 | 1.67 | 1.52 |
| 5 | G | 377 | ASN | N-CA | -7.51 | 1.31 | 1.46 |
| 4 | L | 420 | GLU | CA-C | -7.51 | 1.33 | 1.52 |
| 5 | M | 377 | ASN | N-CA | -7.51 | 1.31 | 1.46 |
| 5 | S | 341 | ALA | CA-C | 7.51 | 1.72 | 1.52 |
| 6 | N | 446 | ARG | CA-CB | -7.50 | 1.37 | 1.53 |
| 5 | Y | 341 | ALA | CA-C | 7.50 | 1.72 | 1.52 |
| 5 | Y | 401 | ALA | CA-CB | -7.50 | 1.36 | 1.52 |
| 4 | F | 420 | GLU | CA-C | -7.49 | 1.33 | 1.52 |
| 6 | Z | 446 | ARG | CA-CB | -7.49 | 1.37 | 1.53 |
| 4 | L | 450 | GLU | CA-CB | -7.49 | 1.37 | 1.53 |
| 3 | D | 1489 | HIS | N-CA | -7.49 | 1.31 | 1.46 |
| 4 | F | 450 | GLU | CA-CB | -7.48 | 1.37 | 1.53 |
| 5 | S | 377 | ASN | N-CA | -7.48 | 1.31 | 1.46 |
| 3 | P | 1489 | HIS | N-CA | -7.47 | 1.31 | 1.46 |
| 5 | S | 401 | ALA | CA-CB | -7.47 | 1.36 | 1.52 |
| 5 | G | 341 | ALA | CA-C | 7.46 | 1.72 | 1.52 |
| 6 | T | 394 | ASP | CA-C | -7.46 | 1.33 | 1.52 |
| 6 | Z | 394 | ASP | CA-C | -7.46 | 1.33 | 1.52 |
| 6 | N | 394 | ASP | CA-C | -7.45 | 1.33 | 1.52 |
| 4 | X | 450 | GLU | CA-CB | -7.45 | 1.37 | 1.53 |
| 4 | X | 199 | GLU | CA-C | -7.45 | 1.33 | 1.52 |
| 5 | M | 341 | ALA | CA-C | 7.45 | 1.72 | 1.52 |
| 6 | H | 394 | ASP | CA-C | -7.44 | 1.33 | 1.52 |
| 4 | L | 349 | THR | CA-C | -7.42 | 1.33 | 1.52 |
| 4 | R | 450 | GLU | CA-CB | -7.42 | 1.37 | 1.53 |
| 4 | X | 444 | PHE | CA-C | 7.42 | 1.72 | 1.52 |
| 4 | L | 199 | GLU | CA-C | -7.42 | 1.33 | 1.52 |
| 4 | F | 349 | THR | CA-C | -7.40 | 1.33 | 1.52 |
| 4 | F | 444 | PHE | CA-C | 7.40 | 1.72 | 1.52 |
| 4 | F | 199 | GLU | CA-C | -7.38 | 1.33 | 1.52 |
| 4 | X | 349 | THR | CA-C | -7.38 | 1.33 | 1.52 |
| 4 | R | 199 | GLU | CA-C | -7.37 | 1.33 | 1.52 |
| 5 | S | 340 | ALA | C-O | -7.37 | 1.09 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 349 | THR | CA-C | -7.36 | 1.33 | 1.52 |
| 5 | M | 340 | ALA | C-O | -7.35 | 1.09 | 1.23 |
| 5 | Y | 340 | ALA | C-O | -7.35 | 1.09 | 1.23 |
| 4 | R | 444 | PHE | CA-C | 7.34 | 1.72 | 1.52 |
| 4 | L | 444 | PHE | CA-C | 7.34 | 1.72 | 1.52 |
| 4 | R | 405 | ALA | CA-CB | 7.33 | 1.67 | 1.52 |
| 6 | T | 392 | GLU | N-CA | 7.33 | 1.61 | 1.46 |
| 6 | H | 392 | GLU | N-CA | 7.33 | 1.61 | 1.46 |
| 4 | L | 429 | GLY | CA-C | -7.32 | 1.40 | 1.51 |
| 4 | R | 446 | ALA | CA-CB | 7.32 | 1.67 | 1.52 |
| 4 | F | 429 | GLY | CA-C | -7.32 | 1.40 | 1.51 |
| 6 | N | 392 | GLU | N-CA | 7.32 | 1.60 | 1.46 |
| 4 | F | 446 | ALA | CA-CB | 7.31 | 1.67 | 1.52 |
| 4 | R | 429 | GLY | CA-C | -7.30 | 1.40 | 1.51 |
| 5 | G | 340 | ALA | C-O | -7.30 | 1.09 | 1.23 |
| 6 | Z | 392 | GLU | N-CA | 7.29 | 1.60 | 1.46 |
| 4 | F | 405 | ALA | CA-CB | 7.29 | 1.67 | 1.52 |
| 4 | X | 405 | ALA | CA-CB | 7.29 | 1.67 | 1.52 |
| 6 | T | 414 | VAL | CA-C | 7.27 | 1.71 | 1.52 |
| 4 | L | 446 | ALA | CA-CB | 7.27 | 1.67 | 1.52 |
| 4 | R | 439 | ARG | N-CA | -7.27 | 1.31 | 1.46 |
| 5 | S | 248 | PRO | CA-CB | 7.27 | 1.68 | 1.53 |
| 6 | Z | 414 | VAL | CA-C | 7.26 | 1.71 | 1.52 |
| 4 | L | 405 | ALA | CA-CB | 7.26 | 1.67 | 1.52 |
| 6 | N | 414 | VAL | CA-C | 7.26 | 1.71 | 1.52 |
| 4 | X | 446 | ALA | CA-CB | 7.26 | 1.67 | 1.52 |
| 6 | H | 414 | VAL | CA-C | 7.25 | 1.71 | 1.52 |
| 5 | M | 248 | PRO | CA-CB | 7.24 | 1.68 | 1.53 |
| 4 | F | 439 | ARG | N-CA | -7.24 | 1.31 | 1.46 |
| 5 | G | 248 | PRO | CA-CB | 7.23 | 1.68 | 1.53 |
| 4 | X | 429 | GLY | CA-C | -7.23 | 1.40 | 1.51 |
| 5 | M | 277 | SER | N-CA | 7.22 | 1.60 | 1.46 |
| 4 | X | 439 | ARG | N-CA | -7.21 | 1.31 | 1.46 |
| 5 | Y | 248 | PRO | CA-CB | 7.21 | 1.68 | 1.53 |
| 5 | G | 277 | SER | N-CA | 7.18 | 1.60 | 1.46 |
| 3 | P | 1485 | ALA | CA-C | -7.18 | 1.34 | 1.52 |
| 4 | R | 435 | MET | CA-C | 7.18 | 1.71 | 1.52 |
| 4 | X | 235 | ASP | C-N | 7.18 | 1.50 | 1.34 |
| 5 | Y | 277 | SER | N-CA | 7.17 | 1.60 | 1.46 |
| 5 | S | 277 | SER | N-CA | 7.17 | 1.60 | 1.46 |
| 4 | L | 435 | MET | CA-C | 7.16 | 1.71 | 1.52 |
| 3 | D | 1485 | ALA | CA-C | -7.16 | 1.34 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | L | 235 | ASP | C-N | 7.16 | 1.50 | 1.34 |
| 4 | F | 435 | MET | CA-C | 7.16 | 1.71 | 1.52 |
| 4 | L | 439 | ARG | N-CA | -7.16 | 1.32 | 1.46 |
| 4 | F | 235 | ASP | C-N | 7.15 | 1.50 | 1.34 |
| 4 | X | 435 | MET | CA-C | 7.15 | 1.71 | 1.52 |
| 4 | R | 235 | ASP | C-N | 7.13 | 1.50 | 1.34 |
| 3 | P | 1511 | GLN | N-CA | -7.11 | 1.32 | 1.46 |
| 5 | M | 330 | LYS | CA-CB | -7.09 | 1.38 | 1.53 |
| 5 | S | 330 | LYS | CA-CB | -7.09 | 1.38 | 1.53 |
| 4 | X | 320 | GLU | CA-CB | -7.08 | 1.38 | 1.53 |
| 5 | G | 334 | GLY | CA-C | 7.08 | 1.63 | 1.51 |
| 5 | S | 334 | GLY | CA-C | 7.08 | 1.63 | 1.51 |
| 3 | D | 1511 | GLN | N-CA | -7.08 | 1.32 | 1.46 |
| 4 | R | 320 | GLU | CA-CB | -7.08 | 1.38 | 1.53 |
| 5 | Y | 361 | ARG | N-CA | 7.07 | 1.60 | 1.46 |
| 5 | G | 330 | LYS | CA-CB | -7.07 | 1.38 | 1.53 |
| 4 | L | 320 | GLU | CA-CB | -7.06 | 1.38 | 1.53 |
| 5 | M | 334 | GLY | CA-C | 7.06 | 1.63 | 1.51 |
| 4 | F | 320 | GLU | CA-CB | -7.04 | 1.38 | 1.53 |
| 5 | Y | 329 | GLN | N-CA | -7.03 | 1.32 | 1.46 |
| 5 | Y | 330 | LYS | CA-CB | -7.03 | 1.38 | 1.53 |
| 5 | Y | 334 | GLY | CA-C | 7.03 | 1.63 | 1.51 |
| 5 | S | 329 | GLN | N-CA | -7.02 | 1.32 | 1.46 |
| 5 | M | 361 | ARG | N-CA | 7.02 | 1.60 | 1.46 |
| 5 | S | 361 | ARG | N-CA | 7.01 | 1.60 | 1.46 |
| 5 | G | 329 | GLN | N-CA | -7.01 | 1.32 | 1.46 |
| 5 | G | 361 | ARG | N-CA | 7.00 | 1.60 | 1.46 |
| 4 | X | 457 | ALA | CA-C | 7.00 | 1.71 | 1.52 |
| 5 | M | 329 | GLN | N-CA | -6.99 | 1.32 | 1.46 |
| 6 | N | 491 | ASN | N-CA | -6.98 | 1.32 | 1.46 |
| 5 | G | 332 | PRO | CA-CB | 6.97 | 1.67 | 1.53 |
| 5 | M | 332 | PRO | CA-CB | 6.96 | 1.67 | 1.53 |
| 6 | Z | 491 | ASN | N-CA | -6.96 | 1.32 | 1.46 |
| 4 | L | 457 | ALA | CA-C | 6.95 | 1.71 | 1.52 |
| 4 | L | 428 | LYS | CA-C | -6.95 | 1.34 | 1.52 |
| 4 | X | 452 | ARG | CA-CB | 6.95 | 1.69 | 1.53 |
| 4 | F | 457 | ALA | CA-C | 6.95 | 1.71 | 1.52 |
| 5 | M | 322 | ALA | CA-CB | 6.93 | 1.67 | 1.52 |
| 4 | F | 452 | ARG | CA-CB | 6.93 | 1.69 | 1.53 |
| 4 | R | 452 | ARG | CA-CB | 6.93 | 1.69 | 1.53 |
| 4 | X | 428 | LYS | CA-C | -6.93 | 1.34 | 1.52 |
| 4 | F | 428 | LYS | CA-C | -6.93 | 1.34 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 457 | ALA | CA-C | 6.92 | 1.71 | 1.52 |
| 6 | Z | 490 | GLN | CA-C | 6.92 | 1.71 | 1.52 |
| 4 | F | 220 | ASN | C-N | 6.91 | 1.50 | 1.34 |
| 4 | X | 220 | ASN | C-N | 6.91 | 1.50 | 1.34 |
| 5 | Y | 332 | PRO | CA-CB | 6.91 | 1.67 | 1.53 |
| 6 | H | 491 | ASN | N-CA | -6.91 | 1.32 | 1.46 |
| 4 | R | 220 | ASN | C-N | 6.91 | 1.50 | 1.34 |
| 5 | G | 322 | ALA | CA-CB | 6.90 | 1.67 | 1.52 |
| 4 | R | 428 | LYS | CA-C | -6.90 | 1.35 | 1.52 |
| 4 | L | 220 | ASN | C-N | 6.89 | 1.50 | 1.34 |
| 4 | L | 452 | ARG | CA-CB | 6.89 | 1.69 | 1.53 |
| 6 | N | 490 | GLN | CA-C | 6.89 | 1.70 | 1.52 |
| 6 | T | 412 | GLU | CA-C | -6.89 | 1.35 | 1.52 |
| 3 | D | 1450 | GLU | N-CA | -6.89 | 1.32 | 1.46 |
| 6 | Z | 412 | GLU | CA-C | -6.89 | 1.35 | 1.52 |
| 6 | T | 491 | ASN | N-CA | -6.89 | 1.32 | 1.46 |
| 6 | H | 490 | GLN | CA-C | 6.88 | 1.70 | 1.52 |
| 5 | Y | 322 | ALA | CA-CB | 6.88 | 1.67 | 1.52 |
| 6 | T | 490 | GLN | CA-C | 6.88 | 1.70 | 1.52 |
| 5 | S | 332 | PRO | CA-CB | 6.88 | 1.67 | 1.53 |
| 4 | X | 454 | TYR | C-O | 6.88 | 1.36 | 1.23 |
| 5 | S | 322 | ALA | CA-CB | 6.88 | 1.66 | 1.52 |
| 3 | P | 1450 | GLU | N-CA | -6.87 | 1.32 | 1.46 |
| 6 | N | 412 | GLU | CA-C | -6.87 | 1.35 | 1.52 |
| 4 | R | 269 | ASN | CA-CB | -6.87 | 1.35 | 1.53 |
| 4 | F | 454 | TYR | C-O | 6.86 | 1.36 | 1.23 |
| 6 | H | 412 | GLU | CA-C | -6.86 | 1.35 | 1.52 |
| 4 | L | 454 | TYR | C-O | 6.86 | 1.36 | 1.23 |
| 4 | R | 454 | TYR | C-O | 6.86 | 1.36 | 1.23 |
| 5 | M | 324 | ILE | C-O | 6.85 | 1.36 | 1.23 |
| 4 | X | 269 | ASN | CA-CB | -6.84 | 1.35 | 1.53 |
| 4 | L | 269 | ASN | CA-CB | -6.84 | 1.35 | 1.53 |
| 5 | M | 341 | ALA | C-O | -6.83 | 1.10 | 1.23 |
| 5 | S | 264 | GLU | N-CA | 6.83 | 1.60 | 1.46 |
| 4 | L | 429 | GLY | N-CA | -6.83 | 1.35 | 1.46 |
| 5 | S | 341 | ALA | C-O | -6.82 | 1.10 | 1.23 |
| 3 | D | 1546 | LEU | CA-C | -6.82 | 1.35 | 1.52 |
| 4 | L | 459 | LEU | CA-CB | 6.82 | 1.69 | 1.53 |
| 4 | F | 269 | ASN | CA-CB | -6.82 | 1.35 | 1.53 |
| 5 | G | 324 | ILE | C-O | 6.81 | 1.36 | 1.23 |
| 4 | R | 459 | LEU | CA-CB | 6.81 | 1.69 | 1.53 |
| 5 | M | 264 | GLU | N-CA | 6.81 | 1.59 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | P | 1546 | LEU | CA-C | -6.81 | 1.35 | 1.52 |
| 6 | Z | 487 | TRP | CA-CB | 6.80 | 1.69 | 1.53 |
| 4 | F | 459 | LEU | CA-CB | 6.80 | 1.69 | 1.53 |
| 4 | X | 429 | GLY | N-CA | -6.80 | 1.35 | 1.46 |
| 4 | F | 429 | GLY | N-CA | -6.80 | 1.35 | 1.46 |
| 3 | D | 1519 | SER | N-CA | -6.79 | 1.32 | 1.46 |
| 5 | Y | 324 | ILE | C-O | 6.79 | 1.36 | 1.23 |
| 4 | R | 320 | GLU | N-CA | 6.79 | 1.59 | 1.46 |
| 6 | N | 416 | GLU | CA-C | -6.79 | 1.35 | 1.52 |
| 5 | S | 324 | ILE | C-O | 6.79 | 1.36 | 1.23 |
| 5 | Y | 264 | GLU | N-CA | 6.79 | 1.59 | 1.46 |
| 3 | P | 1519 | SER | N-CA | -6.78 | 1.32 | 1.46 |
| 5 | G | 264 | GLU | N-CA | 6.77 | 1.59 | 1.46 |
| 6 | H | 416 | GLU | CA-C | -6.77 | 1.35 | 1.52 |
| 6 | N | 487 | TRP | CA-CB | 6.77 | 1.68 | 1.53 |
| 5 | Y | 341 | ALA | C-O | -6.77 | 1.10 | 1.23 |
| 4 | F | 215 | LYS | CA-CB | 6.77 | 1.68 | 1.53 |
| 6 | H | 487 | TRP | CA-CB | 6.76 | 1.68 | 1.53 |
| 4 | X | 320 | GLU | N-CA | 6.76 | 1.59 | 1.46 |
| 6 | Z | 416 | GLU | CA-C | -6.76 | 1.35 | 1.52 |
| 6 | T | 487 | TRP | CA-CB | 6.75 | 1.68 | 1.53 |
| 3 | D | 1489 | HIS | CA-CB | 6.75 | 1.68 | 1.53 |
| 4 | X | 459 | LEU | CA-CB | 6.75 | 1.69 | 1.53 |
| 4 | L | 215 | LYS | CA-CB | 6.74 | 1.68 | 1.53 |
| 3 | P | 1489 | HIS | CA-CB | 6.74 | 1.68 | 1.53 |
| 6 | T | 416 | GLU | CA-C | -6.74 | 1.35 | 1.52 |
| 6 | Z | 402 | GLU | CA-CB | -6.74 | 1.39 | 1.53 |
| 4 | X | 450 | GLU | C-N | 6.74 | 1.49 | 1.34 |
| 4 | L | 320 | GLU | N-CA | 6.74 | 1.59 | 1.46 |
| 4 | R | 215 | LYS | CA-CB | 6.73 | 1.68 | 1.53 |
| 5 | G | 341 | ALA | C-O | -6.73 | 1.10 | 1.23 |
| 6 | T | 402 | GLU | CA-CB | -6.73 | 1.39 | 1.53 |
| 4 | F | 450 | GLU | C-N | 6.72 | 1.49 | 1.34 |
| 4 | L | 450 | GLU | C-N | 6.72 | 1.49 | 1.34 |
| 2 | U | 28 | HIS | N-CA | 6.72 | 1.59 | 1.46 |
| 6 | H | 402 | GLU | CA-CB | -6.71 | 1.39 | 1.53 |
| 4 | R | 450 | GLU | C-N | 6.71 | 1.49 | 1.34 |
| 6 | H | 415 | LYS | N-CA | 6.71 | 1.59 | 1.46 |
| 4 | F | 320 | GLU | N-CA | 6.70 | 1.59 | 1.46 |
| 6 | N | 415 | LYS | N-CA | 6.70 | 1.59 | 1.46 |
| 4 | R | 429 | GLY | N-CA | -6.70 | 1.35 | 1.46 |
| 4 | X | 215 | LYS | CA-CB | 6.70 | 1.68 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 391 | GLN | C-N | 6.69 | 1.49 | 1.34 |
| 4 | L | 211 | GLU | CA-CB | 6.69 | 1.68 | 1.53 |
| 6 | N | 391 | GLN | C-N | 6.69 | 1.49 | 1.34 |
| 2 | O | 28 | HIS | N-CA | 6.68 | 1.59 | 1.46 |
| 6 | N | 402 | GLU | CA-CB | -6.68 | 1.39 | 1.53 |
| 6 | T | 391 | GLN | C-N | 6.67 | 1.49 | 1.34 |
| 2 | I | 28 | HIS | N-CA | 6.67 | 1.59 | 1.46 |
| 4 | X | 211 | GLU | CA-CB | 6.67 | 1.68 | 1.53 |
| 6 | T | 493 | ALA | CA-C | 6.66 | 1.70 | 1.52 |
| 4 | F | 211 | GLU | CA-CB | 6.66 | 1.68 | 1.53 |
| 6 | Z | 415 | LYS | N-CA | 6.66 | 1.59 | 1.46 |
| 6 | H | 493 | ALA | CA-C | 6.66 | 1.70 | 1.52 |
| 4 | R | 211 | GLU | CA-CB | 6.65 | 1.68 | 1.53 |
| 6 | H | 453 | ASP | CA-CB | 6.65 | 1.68 | 1.53 |
| 6 | T | 415 | LYS | N-CA | 6.65 | 1.59 | 1.46 |
| 2 | C | 28 | HIS | N-CA | 6.64 | 1.59 | 1.46 |
| 4 | F | 303 | GLY | CA-C | 6.64 | 1.62 | 1.51 |
| 6 | Z | 453 | ASP | CA-CB | 6.63 | 1.68 | 1.53 |
| 6 | H | 391 | GLN | C-N | 6.63 | 1.49 | 1.34 |
| 6 | N | 493 | ALA | CA-C | 6.63 | 1.70 | 1.52 |
| 4 | X | 303 | GLY | CA-C | 6.63 | 1.62 | 1.51 |
| 4 | L | 303 | GLY | CA-C | 6.62 | 1.62 | 1.51 |
| 6 | N | 453 | ASP | CA-CB | 6.61 | 1.68 | 1.53 |
| 3 | P | 1510 | GLN | N-CA | -6.60 | 1.33 | 1.46 |
| 5 | M | 366 | GLU | CA-C | -6.59 | 1.35 | 1.52 |
| 5 | Y | 342 | PRO | CA-CB | 6.59 | 1.66 | 1.53 |
| 5 | Y | 366 | GLU | CA-C | -6.59 | 1.35 | 1.52 |
| 6 | Z | 493 | ALA | CA-C | 6.59 | 1.70 | 1.52 |
| 4 | L | 335 | ARG | CA-CB | 6.59 | 1.68 | 1.53 |
| 5 | S | 366 | GLU | CA-C | -6.58 | 1.35 | 1.52 |
| 6 | T | 453 | ASP | CA-CB | 6.57 | 1.68 | 1.53 |
| 4 | X | 335 | ARG | CA-CB | 6.57 | 1.68 | 1.53 |
| 4 | F | 335 | ARG | CA-CB | 6.56 | 1.68 | 1.53 |
| 5 | M | 342 | PRO | CA-CB | 6.56 | 1.66 | 1.53 |
| 5 | S | 342 | PRO | CA-CB | 6.56 | 1.66 | 1.53 |
| 4 | F | 250 | ASN | CA-CB | 6.56 | 1.70 | 1.53 |
| 3 | D | 1510 | GLN | N-CA | -6.55 | 1.33 | 1.46 |
| 4 | R | 303 | GLY | CA-C | 6.55 | 1.62 | 1.51 |
| 5 | M | 252 | CYS | CA-CB | 6.55 | 1.68 | 1.53 |
| 5 | G | 366 | GLU | CA-C | -6.54 | 1.35 | 1.52 |
| 4 | L | 250 | ASN | CA-CB | 6.54 | 1.70 | 1.53 |
| 4 | R | 335 | ARG | CA-CB | 6.53 | 1.68 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | P | 1509 | GLN | N-CA | -6.52 | 1.33 | 1.46 |
| 5 | S | 252 | CYS | CA-CB | 6.52 | 1.68 | 1.53 |
| 3 | D | 1509 | GLN | N-CA | -6.52 | 1.33 | 1.46 |
| 5 | Y | 252 | CYS | CA-CB | 6.51 | 1.68 | 1.53 |
| 5 | G | 342 | PRO | CA-CB | 6.51 | 1.66 | 1.53 |
| 4 | R | 250 | ASN | CA-CB | 6.50 | 1.70 | 1.53 |
| 4 | R | 267 | GLN | CA-CB | 6.49 | 1.68 | 1.53 |
| 4 | L | 422 | ASN | CA-C | -6.49 | 1.36 | 1.52 |
| 4 | X | 250 | ASN | CA-CB | 6.48 | 1.70 | 1.53 |
| 4 | L | 267 | GLN | CA-CB | 6.48 | 1.68 | 1.53 |
| 4 | X | 267 | GLN | CA-CB | 6.48 | 1.68 | 1.53 |
| 4 | L | 419 | GLY | N-CA | 6.47 | 1.55 | 1.46 |
| 6 | T | 409 | PRO | C-N | 6.46 | 1.49 | 1.34 |
| 4 | X | 419 | GLY | N-CA | 6.46 | 1.55 | 1.46 |
| 4 | F | 343 | MET | CA-C | 6.46 | 1.69 | 1.52 |
| 5 | G | 252 | CYS | CA-CB | 6.46 | 1.68 | 1.53 |
| 4 | L | 343 | MET | CA-C | 6.46 | 1.69 | 1.52 |
| 4 | F | 449 | SER | C-O | 6.46 | 1.35 | 1.23 |
| 4 | R | 426 | GLN | CA-C | -6.46 | 1.36 | 1.52 |
| 6 | N | 409 | PRO | C-N | 6.45 | 1.48 | 1.34 |
| 4 | F | 419 | GLY | N-CA | 6.45 | 1.55 | 1.46 |
| 3 | D | 1541 | THR | C-N | -6.45 | 1.22 | 1.34 |
| 6 | H | 409 | PRO | C-N | 6.45 | 1.48 | 1.34 |
| 4 | F | 267 | GLN | CA-CB | 6.45 | 1.68 | 1.53 |
| 6 | Z | 409 | PRO | C-N | 6.44 | 1.48 | 1.34 |
| 4 | F | 422 | ASN | CA-C | -6.44 | 1.36 | 1.52 |
| 2 | O | 5 | GLY | CA-C | -6.44 | 1.41 | 1.51 |
| 4 | F | 426 | GLN | CA-C | -6.43 | 1.36 | 1.52 |
| 4 | R | 343 | MET | CA-C | 6.43 | 1.69 | 1.52 |
| 4 | X | 423 | ALA | N-CA | -6.43 | 1.33 | 1.46 |
| 2 | I | 5 | GLY | CA-C | -6.43 | 1.41 | 1.51 |
| 4 | X | 422 | ASN | CA-C | -6.43 | 1.36 | 1.52 |
| 3 | D | 1547 | LEU | N-CA | -6.43 | 1.33 | 1.46 |
| 3 | P | 1541 | THR | C-N | -6.43 | 1.22 | 1.34 |
| 4 | L | 456 | ASP | C-N | 6.43 | 1.48 | 1.34 |
| 4 | R | 449 | SER | C-O | 6.43 | 1.35 | 1.23 |
| 4 | X | 456 | ASP | C-N | 6.42 | 1.48 | 1.34 |
| 2 | C | 5 | GLY | CA-C | -6.42 | 1.41 | 1.51 |
| 4 | F | 456 | ASP | C-N | 6.42 | 1.48 | 1.34 |
| 4 | R | 422 | ASN | CA-C | -6.42 | 1.36 | 1.52 |
| 4 | X | 343 | MET | CA-C | 6.42 | 1.69 | 1.52 |
| 4 | X | 426 | GLN | CA-C | -6.42 | 1.36 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | L | 426 | GLN | CA-C | -6.41 | 1.36 | 1.52 |
| 2 | U | 5 | GLY | CA-C | -6.40 | 1.41 | 1.51 |
| 3 | P | 1547 | LEU | N-CA | -6.39 | 1.33 | 1.46 |
| 4 | R | 423 | ALA | N-CA | -6.39 | 1.33 | 1.46 |
| 4 | F | 423 | ALA | N-CA | -6.39 | 1.33 | 1.46 |
| 6 | T | 488 | ILE | N-CA | -6.39 | 1.33 | 1.46 |
| 4 | L | 449 | SER | C-O | 6.38 | 1.35 | 1.23 |
| 6 | N | 488 | ILE | N-CA | -6.38 | 1.33 | 1.46 |
| 4 | X | 449 | SER | C-O | 6.38 | 1.35 | 1.23 |
| 4 | L | 423 | ALA | N-CA | -6.38 | 1.33 | 1.46 |
| 6 | H | 488 | ILE | N-CA | -6.37 | 1.33 | 1.46 |
| 4 | R | 456 | ASP | C-N | 6.37 | 1.48 | 1.34 |
| 4 | R | 419 | GLY | N-CA | 6.35 | 1.55 | 1.46 |
| 6 | Z | 488 | ILE | N-CA | -6.33 | 1.33 | 1.46 |
| 6 | H | 370 | GLU | CA-C | 6.32 | 1.69 | 1.52 |
| 4 | F | 443 | HIS | CA-CB | -6.32 | 1.40 | 1.53 |
| 5 | S | 340 | ALA | C-N | 6.32 | 1.48 | 1.34 |
| 4 | L | 443 | HIS | CA-CB | -6.32 | 1.40 | 1.53 |
| 5 | M | 254 | ASP | N-CA | -6.32 | 1.33 | 1.46 |
| 6 | N | 370 | GLU | CA-C | 6.31 | 1.69 | 1.52 |
| 5 | Y | 254 | ASP | N-CA | -6.31 | 1.33 | 1.46 |
| 4 | F | 307 | ILE | N-CA | 6.30 | 1.58 | 1.46 |
| 4 | X | 443 | HIS | CA-CB | -6.30 | 1.40 | 1.53 |
| 5 | G | 254 | ASP | N-CA | -6.29 | 1.33 | 1.46 |
| 4 | F | 300 | PRO | N-CA | 6.28 | 1.57 | 1.47 |
| 4 | X | 307 | ILE | N-CA | 6.28 | 1.58 | 1.46 |
| 5 | G | 340 | ALA | C-N | 6.28 | 1.48 | 1.34 |
| 3 | P | 1516 | LEU | CA-C | -6.28 | 1.36 | 1.52 |
| 4 | R | 443 | HIS | CA-CB | -6.28 | 1.40 | 1.53 |
| 6 | T | 370 | GLU | CA-C | 6.28 | 1.69 | 1.52 |
| 4 | L | 204 | SER | CA-CB | 6.28 | 1.62 | 1.52 |
| 4 | R | 300 | PRO | N-CA | 6.28 | 1.57 | 1.47 |
| 4 | R | 307 | ILE | N-CA | 6.27 | 1.58 | 1.46 |
| 5 | S | 254 | ASP | N-CA | -6.27 | 1.33 | 1.46 |
| 6 | Z | 370 | GLU | CA-C | 6.27 | 1.69 | 1.52 |
| 5 | M | 340 | ALA | C-N | 6.26 | 1.48 | 1.34 |
| 4 | L | 307 | ILE | N-CA | 6.26 | 1.58 | 1.46 |
| 4 | X | 300 | PRO | N-CA | 6.26 | 1.57 | 1.47 |
| 4 | X | 204 | SER | CA-CB | 6.26 | 1.62 | 1.52 |
| 4 | L | 425 | THR | N-CA | -6.26 | 1.33 | 1.46 |
| 3 | D | 1516 | LEU | CA-C | -6.25 | 1.36 | 1.52 |
| 4 | F | 204 | SER | CA-CB | 6.25 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 204 | SER | CA-CB | 6.25 | 1.62 | 1.52 |
| 4 | L | 300 | PRO | N-CA | 6.24 | 1.57 | 1.47 |
| 4 | X | 449 | SER | N-CA | 6.24 | 1.58 | 1.46 |
| 4 | X | 425 | THR | N-CA | -6.24 | 1.33 | 1.46 |
| 4 | F | 483 | ASP | N-CA | -6.24 | 1.33 | 1.46 |
| 5 | S | 393 | TYR | CA-C | 6.24 | 1.69 | 1.52 |
| 4 | R | 483 | ASP | N-CA | -6.23 | 1.33 | 1.46 |
| 3 | D | 1512 | TRP | CA-C | -6.23 | 1.36 | 1.52 |
| 4 | F | 425 | THR | N-CA | -6.23 | 1.33 | 1.46 |
| 5 | Y | 393 | TYR | CA-C | 6.23 | 1.69 | 1.52 |
| 5 | G | 393 | TYR | CA-C | 6.22 | 1.69 | 1.52 |
| 3 | P | 1512 | TRP | CA-C | -6.22 | 1.36 | 1.52 |
| 5 | M | 393 | TYR | CA-C | 6.22 | 1.69 | 1.52 |
| 4 | X | 221 | GLN | CA-CB | 6.22 | 1.67 | 1.53 |
| 4 | X | 465 | GLN | CA-CB | 6.22 | 1.67 | 1.53 |
| 6 | N | 497 | ARG | CA-C | -6.21 | 1.36 | 1.52 |
| 5 | Y | 340 | ALA | C-N | 6.21 | 1.48 | 1.34 |
| 4 | R | 449 | SER | N-CA | 6.20 | 1.58 | 1.46 |
| 4 | X | 483 | ASP | N-CA | -6.20 | 1.33 | 1.46 |
| 4 | L | 483 | ASP | N-CA | -6.20 | 1.33 | 1.46 |
| 4 | F | 465 | GLN | CA-CB | 6.20 | 1.67 | 1.53 |
| 6 | Z | 497 | ARG | CA-C | -6.19 | 1.36 | 1.52 |
| 4 | L | 449 | SER | N-CA | 6.18 | 1.58 | 1.46 |
| 3 | D | 1475 | ALA | N-CA | -6.18 | 1.33 | 1.46 |
| 4 | L | 436 | SER | C-O | 6.18 | 1.35 | 1.23 |
| 4 | L | 465 | GLN | CA-CB | 6.18 | 1.67 | 1.53 |
| 4 | F | 449 | SER | N-CA | 6.18 | 1.58 | 1.46 |
| 4 | R | 425 | THR | N-CA | -6.18 | 1.33 | 1.46 |
| 4 | X | 436 | SER | C-O | 6.18 | 1.35 | 1.23 |
| 4 | L | 221 | GLN | CA-CB | 6.18 | 1.67 | 1.53 |
| 3 | P | 1544 | PRO | CA-C | 6.17 | 1.65 | 1.52 |
| 6 | T | 497 | ARG | CA-C | -6.17 | 1.36 | 1.52 |
| 6 | H | 497 | ARG | CA-C | -6.17 | 1.36 | 1.52 |
| 4 | R | 465 | GLN | CA-CB | 6.17 | 1.67 | 1.53 |
| 4 | R | 221 | GLN | CA-CB | 6.17 | 1.67 | 1.53 |
| 4 | F | 404 | GLN | CA-CB | 6.16 | 1.67 | 1.53 |
| 4 | L | 404 | GLN | CA-CB | 6.16 | 1.67 | 1.53 |
| 4 | F | 436 | SER | C-O | 6.16 | 1.35 | 1.23 |
| 5 | S | 380 | ILE | C-N | 6.16 | 1.48 | 1.34 |
| 3 | P | 1475 | ALA | N-CA | -6.16 | 1.34 | 1.46 |
| 4 | F | 221 | GLN | CA-CB | 6.15 | 1.67 | 1.53 |
| 5 | G | 380 | ILE | C-N | 6.15 | 1.48 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | R | 436 | SER | C-O | 6.15 | 1.35 | 1.23 |
| 5 | G | 338 | GLU | CA-C | -6.13 | 1.37 | 1.52 |
| 5 | Y | 338 | GLU | CA-C | -6.12 | 1.37 | 1.52 |
| 5 | M | 380 | ILE | C-N | 6.11 | 1.48 | 1.34 |
| 3 | D | 1544 | PRO | CA-C | 6.11 | 1.65 | 1.52 |
| 6 | H | 494 | LEU | CA-CB | 6.11 | 1.67 | 1.53 |
| 4 | R | 404 | GLN | CA-CB | 6.10 | 1.67 | 1.53 |
| 5 | Y | 380 | ILE | C-N | 6.10 | 1.48 | 1.34 |
| 4 | F | 222 | THR | C-N | 6.10 | 1.48 | 1.34 |
| 5 | M | 338 | GLU | CA-C | -6.10 | 1.37 | 1.52 |
| 6 | N | 371 | LYS | N-CA | -6.09 | 1.34 | 1.46 |
| 4 | X | 404 | GLN | CA-CB | 6.09 | 1.67 | 1.53 |
| 3 | P | 1451 | ARG | CA-C | -6.09 | 1.37 | 1.52 |
| 4 | R | 222 | THR | C-N | 6.09 | 1.48 | 1.34 |
| 4 | L | 222 | THR | C-N | 6.08 | 1.48 | 1.34 |
| 6 | Z | 494 | LEU | CA-CB | 6.08 | 1.67 | 1.53 |
| 5 | S | 338 | GLU | CA-C | -6.08 | 1.37 | 1.52 |
| 3 | D | 1451 | ARG | CA-C | -6.07 | 1.37 | 1.52 |
| 6 | N | 494 | LEU | CA-CB | 6.07 | 1.67 | 1.53 |
| 4 | R | 405 | ALA | N-CA | -6.07 | 1.34 | 1.46 |
| 4 | X | 222 | THR | C-N | 6.07 | 1.48 | 1.34 |
| 4 | X | 305 | ASP | C-N | -6.07 | 1.22 | 1.34 |
| 4 | F | 405 | ALA | N-CA | -6.07 | 1.34 | 1.46 |
| 6 | H | 371 | LYS | N-CA | -6.06 | 1.34 | 1.46 |
| 6 | T | 371 | LYS | N-CA | -6.05 | 1.34 | 1.46 |
| 6 | T | 494 | LEU | CA-CB | 6.04 | 1.67 | 1.53 |
| 4 | X | 405 | ALA | N-CA | -6.04 | 1.34 | 1.46 |
| 6 | Z | 371 | LYS | N-CA | -6.03 | 1.34 | 1.46 |
| 4 | R | 305 | ASP | C-N | -6.03 | 1.22 | 1.34 |
| 4 | L | 305 | ASP | C-N | -6.02 | 1.22 | 1.34 |
| 5 | G | 276 | SER | N-CA | 6.02 | 1.58 | 1.46 |
| 6 | N | 366 | ILE | N-CA | -6.02 | 1.34 | 1.46 |
| 6 | N | 353 | GLN | CA-CB | 6.02 | 1.67 | 1.53 |
| 4 | L | 405 | ALA | N-CA | -6.01 | 1.34 | 1.46 |
| 4 | X | 428 | LYS | N-CA | -6.01 | 1.34 | 1.46 |
| 6 | Z | 391 | GLN | CA-C | 6.01 | 1.68 | 1.52 |
| 5 | M | 276 | SER | N-CA | 6.00 | 1.58 | 1.46 |
| 6 | T | 353 | GLN | CA-CB | 6.00 | 1.67 | 1.53 |
| 6 | H | 391 | GLN | CA-C | 6.00 | 1.68 | 1.52 |
| 6 | H | 353 | GLN | CA-CB | 5.99 | 1.67 | 1.53 |
| 6 | N | 391 | GLN | CA-C | 5.99 | 1.68 | 1.52 |
| 2 | C | 11 | GLN | CA-CB | -5.99 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | H | 366 | ILE | N-CA | -5.99 | 1.34 | 1.46 |
| 2 | U | 11 | GLN | CA-CB | -5.98 | 1.40 | 1.53 |
| 5 | Y | 276 | SER | N-CA | 5.98 | 1.58 | 1.46 |
| 4 | F | 305 | ASP | C-N | -5.98 | 1.22 | 1.34 |
| 6 | T | 391 | GLN | CA-C | 5.97 | 1.68 | 1.52 |
| 6 | Z | 353 | GLN | CA-CB | 5.97 | 1.67 | 1.53 |
| 4 | X | 408 | GLU | CA-CB | 5.96 | 1.67 | 1.53 |
| 4 | F | 401 | TYR | CA-CB | 5.96 | 1.67 | 1.53 |
| 4 | R | 401 | TYR | CA-CB | 5.96 | 1.67 | 1.53 |
| 3 | D | 1521 | TYR | CA-C | -5.96 | 1.37 | 1.52 |
| 4 | L | 401 | TYR | CA-CB | 5.96 | 1.67 | 1.53 |
| 4 | R | 428 | LYS | N-CA | -5.96 | 1.34 | 1.46 |
| 3 | P | 1521 | TYR | CA-C | -5.95 | 1.37 | 1.52 |
| 6 | Z | 366 | ILE | N-CA | -5.95 | 1.34 | 1.46 |
| 6 | Z | 366 | ILE | CA-CB | -5.95 | 1.41 | 1.54 |
| 4 | L | 408 | GLU | CA-CB | 5.95 | 1.67 | 1.53 |
| 4 | L | 428 | LYS | N-CA | -5.95 | 1.34 | 1.46 |
| 3 | P | 1543 | GLN | C-N | -5.95 | 1.23 | 1.34 |
| 4 | R | 408 | GLU | CA-CB | 5.95 | 1.67 | 1.53 |
| 6 | N | 388 | ARG | CA-C | -5.94 | 1.37 | 1.52 |
| 5 | S | 276 | SER | N-CA | 5.94 | 1.58 | 1.46 |
| 6 | T | 366 | ILE | N-CA | -5.94 | 1.34 | 1.46 |
| 4 | X | 237 | GLN | N-CA | -5.93 | 1.34 | 1.46 |
| 2 | O | 11 | GLN | CA-CB | -5.93 | 1.41 | 1.53 |
| 6 | H | 366 | ILE | CA-CB | -5.92 | 1.41 | 1.54 |
| 4 | F | 428 | LYS | N-CA | -5.92 | 1.34 | 1.46 |
| 4 | F | 408 | GLU | CA-CB | 5.92 | 1.67 | 1.53 |
| 6 | T | 366 | ILE | CA-CB | -5.92 | 1.41 | 1.54 |
| 3 | D | 1543 | GLN | C-N | -5.92 | 1.23 | 1.34 |
| 4 | R | 237 | GLN | N-CA | -5.91 | 1.34 | 1.46 |
| 4 | X | 401 | TYR | CA-CB | 5.91 | 1.67 | 1.53 |
| 4 | L | 237 | GLN | N-CA | -5.91 | 1.34 | 1.46 |
| 2 | I | 11 | GLN | CA-CB | -5.91 | 1.41 | 1.53 |
| 5 | G | 404 | GLN | CA-C | -5.90 | 1.37 | 1.52 |
| 6 | T | 388 | ARG | CA-C | -5.90 | 1.37 | 1.52 |
| 4 | F | 237 | GLN | N-CA | -5.90 | 1.34 | 1.46 |
| 5 | Y | 404 | GLN | CA-C | -5.89 | 1.37 | 1.52 |
| 6 | H | 388 | ARG | CA-C | -5.89 | 1.37 | 1.52 |
| 5 | M | 404 | GLN | CA-C | -5.88 | 1.37 | 1.52 |
| 5 | G | 332 | PRO | CA-C | -5.87 | 1.41 | 1.52 |
| 6 | N | 366 | ILE | CA-CB | -5.87 | 1.41 | 1.54 |
| 6 | N | 412 | GLU | CA-CB | 5.87 | 1.66 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | T | 412 | GLU | CA-CB | 5.87 | 1.66 | 1.53 |
| 5 | S | 404 | GLN | CA-C | -5.87 | 1.37 | 1.52 |
| 6 | Z | 412 | GLU | CA-CB | 5.86 | 1.66 | 1.53 |
| 6 | Z | 388 | ARG | CA-C | -5.86 | 1.37 | 1.52 |
| 5 | Y | 332 | PRO | CA-C | -5.86 | 1.41 | 1.52 |
| 4 | R | 132 | ASP | CA-CB | 5.85 | 1.66 | 1.53 |
| 5 | Y | 381 | THR | N-CA | 5.84 | 1.58 | 1.46 |
| 5 | M | 381 | THR | N-CA | 5.83 | 1.58 | 1.46 |
| 5 | S | 381 | THR | N-CA | 5.83 | 1.58 | 1.46 |
| 6 | H | 412 | GLU | CA-CB | 5.83 | 1.66 | 1.53 |
| 5 | M | 332 | PRO | CA-C | -5.82 | 1.41 | 1.52 |
| 4 | L | 482 | LYS | N-CA | -5.81 | 1.34 | 1.46 |
| 5 | G | 381 | THR | N-CA | 5.80 | 1.57 | 1.46 |
| 4 | F | 132 | ASP | CA-CB | 5.80 | 1.66 | 1.53 |
| 4 | X | 132 | ASP | CA-CB | 5.80 | 1.66 | 1.53 |
| 4 | X | 482 | LYS | N-CA | -5.80 | 1.34 | 1.46 |
| 4 | R | 482 | LYS | N-CA | -5.80 | 1.34 | 1.46 |
| 4 | F | 482 | LYS | N-CA | -5.79 | 1.34 | 1.46 |
| 4 | L | 132 | ASP | CA-CB | 5.79 | 1.66 | 1.53 |
| 3 | P | 1484 | ASP | N-CA | -5.79 | 1.34 | 1.46 |
| 4 | L | 460 | LEU | N-CA | -5.78 | 1.34 | 1.46 |
| 5 | S | 332 | PRO | CA-C | -5.78 | 1.41 | 1.52 |
| 3 | D | 1518 | ASN | N-CA | -5.77 | 1.34 | 1.46 |
| 3 | D | 1484 | ASP | N-CA | -5.77 | 1.34 | 1.46 |
| 3 | P | 1518 | ASN | N-CA | -5.75 | 1.34 | 1.46 |
| 4 | F | 466 | HIS | CA-C | -5.75 | 1.38 | 1.52 |
| 4 | X | 460 | LEU | N-CA | -5.75 | 1.34 | 1.46 |
| 4 | X | 402 | ALA | N-CA | 5.75 | 1.57 | 1.46 |
| 4 | F | 460 | LEU | N-CA | -5.73 | 1.34 | 1.46 |
| 4 | L | 466 | HIS | CA-C | -5.72 | 1.38 | 1.52 |
| 4 | R | 466 | HIS | CA-C | -5.71 | 1.38 | 1.52 |
| 4 | X | 466 | HIS | CA-C | -5.71 | 1.38 | 1.52 |
| 4 | L | 402 | ALA | N-CA | 5.70 | 1.57 | 1.46 |
| 4 | R | 460 | LEU | N-CA | -5.70 | 1.34 | 1.46 |
| 4 | F | 402 | ALA | N-CA | 5.70 | 1.57 | 1.46 |
| 4 | R | 402 | ALA | N-CA | 5.66 | 1.57 | 1.46 |
| 6 | T | 402 | GLU | N-CA | 5.64 | 1.57 | 1.46 |
| 6 | Z | 402 | GLU | N-CA | 5.63 | 1.57 | 1.46 |
| 4 | L | 408 | GLU | CA-C | -5.62 | 1.38 | 1.52 |
| 4 | F | 408 | GLU | CA-C | -5.62 | 1.38 | 1.52 |
| 4 | R | 221 | GLN | CA-C | 5.62 | 1.67 | 1.52 |
| 4 | F | 221 | GLN | CA-C | 5.61 | 1.67 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | X | 221 | GLN | CA-C | 5.60 | 1.67 | 1.52 |
| 4 | F | 306 | PRO | CA-CB | -5.60 | 1.42 | 1.53 |
| 6 | T | 410 | LEU | CA-C | 5.58 | 1.67 | 1.52 |
| 4 | R | 394 | GLU | C-N | 5.58 | 1.46 | 1.34 |
| 6 | N | 402 | GLU | N-CA | 5.58 | 1.57 | 1.46 |
| 4 | L | 221 | GLN | CA-C | 5.58 | 1.67 | 1.52 |
| 6 | H | 402 | GLU | N-CA | 5.57 | 1.57 | 1.46 |
| 4 | X | 408 | GLU | CA-C | -5.57 | 1.38 | 1.52 |
| 4 | R | 408 | GLU | CA-C | -5.56 | 1.38 | 1.52 |
| 4 | X | 394 | GLU | C-N | 5.55 | 1.46 | 1.34 |
| 6 | H | 410 | LEU | CA-C | 5.55 | 1.67 | 1.52 |
| 4 | X | 306 | PRO | CA-CB | -5.55 | 1.42 | 1.53 |
| 4 | R | 400 | GLY | C-N | -5.54 | 1.21 | 1.34 |
| 4 | F | 400 | GLY | C-N | -5.54 | 1.21 | 1.34 |
| 4 | L | 460 | LEU | CA-CB | 5.54 | 1.66 | 1.53 |
| 4 | L | 306 | PRO | CA-CB | -5.53 | 1.42 | 1.53 |
| 6 | N | 410 | LEU | CA-C | 5.52 | 1.67 | 1.52 |
| 6 | Z | 410 | LEU | CA-C | 5.52 | 1.67 | 1.52 |
| 4 | L | 394 | GLU | C-N | 5.52 | 1.46 | 1.34 |
| 6 | T | 403 | LEU | CA-C | -5.52 | 1.38 | 1.52 |
| 4 | F | 420 | GLU | N-CA | 5.51 | 1.57 | 1.46 |
| 4 | X | 420 | GLU | N-CA | 5.51 | 1.57 | 1.46 |
| 4 | F | 394 | GLU | CA-C | 5.51 | 1.67 | 1.52 |
| 4 | R | 306 | PRO | CA-CB | -5.51 | 1.42 | 1.53 |
| 4 | F | 394 | GLU | C-N | 5.50 | 1.46 | 1.34 |
| 4 | X | 400 | GLY | C-N | -5.50 | 1.21 | 1.34 |
| 4 | F | 460 | LEU | CA-CB | 5.50 | 1.66 | 1.53 |
| 4 | L | 400 | GLY | C-N | -5.50 | 1.21 | 1.34 |
| 4 | X | 394 | GLU | CA-C | 5.50 | 1.67 | 1.52 |
| 4 | X | 492 | GLU | CA-CB | 5.50 | 1.66 | 1.53 |
| 4 | X | 460 | LEU | CA-CB | 5.50 | 1.66 | 1.53 |
| 4 | R | 492 | GLU | CA-CB | 5.50 | 1.66 | 1.53 |
| 5 | S | 302 | GLN | CA-CB | -5.50 | 1.41 | 1.53 |
| 4 | X | 435 | MET | C-N | 5.50 | 1.46 | 1.34 |
| 4 | R | 420 | GLU | N-CA | 5.49 | 1.57 | 1.46 |
| 5 | S | 317 | GLN | CA-CB | 5.49 | 1.66 | 1.53 |
| 4 | R | 491 | VAL | CA-CB | 5.49 | 1.66 | 1.54 |
| 4 | X | 491 | VAL | CA-CB | 5.49 | 1.66 | 1.54 |
| 5 | M | 302 | GLN | CA-CB | -5.48 | 1.41 | 1.53 |
| 5 | M | 252 | CYS | CA-C | -5.48 | 1.38 | 1.52 |
| 6 | T | 467 | THR | C-N | 5.48 | 1.46 | 1.34 |
| 4 | F | 435 | MET | C-N | 5.48 | 1.46 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | P | 1516 | LEU | N-CA | -5.48 | 1.35 | 1.46 |
| 3 | D | 1516 | LEU | N-CA | -5.47 | 1.35 | 1.46 |
| 4 | L | 394 | GLU | CA-C | 5.47 | 1.67 | 1.52 |
| 4 | L | 420 | GLU | N-CA | 5.47 | 1.57 | 1.46 |
| 6 | N | 403 | LEU | CA-C | -5.47 | 1.38 | 1.52 |
| 4 | R | 394 | GLU | CA-C | 5.47 | 1.67 | 1.52 |
| 4 | R | 435 | MET | C-N | 5.47 | 1.46 | 1.34 |
| 4 | L | 473 | GLY | CA-C | -5.47 | 1.43 | 1.51 |
| 4 | L | 491 | VAL | CA-CB | 5.47 | 1.66 | 1.54 |
| 4 | R | 460 | LEU | CA-CB | 5.47 | 1.66 | 1.53 |
| 4 | F | 492 | GLU | CA-CB | 5.46 | 1.66 | 1.53 |
| 5 | M | 317 | GLN | CA-CB | 5.46 | 1.66 | 1.53 |
| 5 | G | 302 | GLN | CA-CB | -5.46 | 1.42 | 1.53 |
| 6 | N | 494 | LEU | C-N | -5.46 | 1.21 | 1.34 |
| 3 | D | 1507 | ASP | C-N | 5.46 | 1.46 | 1.34 |
| 6 | Z | 403 | LEU | CA-C | -5.45 | 1.38 | 1.52 |
| 5 | G | 252 | CYS | CA-C | -5.45 | 1.38 | 1.52 |
| 5 | S | 252 | CYS | CA-C | -5.45 | 1.38 | 1.52 |
| 5 | Y | 317 | GLN | CA-CB | 5.45 | 1.66 | 1.53 |
| 4 | L | 469 | GLN | CA-CB | -5.45 | 1.42 | 1.53 |
| 6 | Z | 467 | THR | C-N | 5.44 | 1.46 | 1.34 |
| 6 | H | 403 | LEU | CA-C | -5.44 | 1.38 | 1.52 |
| 6 | H | 386 | GLN | N-CA | -5.44 | 1.35 | 1.46 |
| 5 | Y | 302 | GLN | CA-CB | -5.44 | 1.42 | 1.53 |
| 6 | H | 467 | THR | C-N | 5.43 | 1.46 | 1.34 |
| 4 | L | 492 | GLU | CA-CB | 5.43 | 1.66 | 1.53 |
| 5 | Y | 252 | CYS | CA-C | -5.43 | 1.38 | 1.52 |
| 5 | S | 325 | ALA | C-O | 5.42 | 1.33 | 1.23 |
| 3 | P | 1507 | ASP | C-N | 5.42 | 1.46 | 1.34 |
| 5 | G | 317 | GLN | CA-CB | 5.42 | 1.65 | 1.53 |
| 4 | L | 435 | MET | C-N | 5.42 | 1.46 | 1.34 |
| 6 | N | 467 | THR | C-N | 5.42 | 1.46 | 1.34 |
| 6 | Z | 386 | GLN | N-CA | -5.42 | 1.35 | 1.46 |
| 4 | F | 473 | GLY | CA-C | -5.41 | 1.43 | 1.51 |
| 6 | H | 494 | LEU | C-N | -5.41 | 1.21 | 1.34 |
| 4 | X | 473 | GLY | CA-C | -5.41 | 1.43 | 1.51 |
| 4 | F | 469 | GLN | CA-CB | -5.41 | 1.42 | 1.53 |
| 5 | G | 325 | ALA | C-O | 5.41 | 1.33 | 1.23 |
| 6 | T | 494 | LEU | C-N | -5.41 | 1.21 | 1.34 |
| 6 | Z | 494 | LEU | C-N | -5.41 | 1.21 | 1.34 |
| 5 | M | 321 | ASN | C-N | 5.41 | 1.46 | 1.34 |
| 4 | R | 469 | GLN | CA-CB | -5.40 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | M | 325 | ALA | C-O | 5.40 | 1.33 | 1.23 |
| 5 | Y | 321 | ASN | C-N | 5.40 | 1.46 | 1.34 |
| 4 | F | 491 | VAL | CA-CB | 5.40 | 1.66 | 1.54 |
| 5 | S | 326 | LEU | CA-CB | 5.39 | 1.66 | 1.53 |
| 6 | T | 386 | GLN | N-CA | -5.39 | 1.35 | 1.46 |
| 4 | X | 469 | GLN | CA-CB | -5.39 | 1.42 | 1.53 |
| 6 | N | 386 | GLN | N-CA | -5.39 | 1.35 | 1.46 |
| 4 | L | 328 | VAL | CA-CB | -5.39 | 1.43 | 1.54 |
| 6 | N | 472 | GLN | N-CA | -5.39 | 1.35 | 1.46 |
| 4 | X | 231 | LYS | N-CA | 5.38 | 1.57 | 1.46 |
| 6 | T | 467 | THR | CA-C | -5.38 | 1.39 | 1.52 |
| 4 | F | 419 | GLY | C-N | 5.38 | 1.46 | 1.34 |
| 5 | Y | 325 | ALA | C-O | 5.38 | 1.33 | 1.23 |
| 5 | Y | 326 | LEU | CA-CB | 5.37 | 1.66 | 1.53 |
| 6 | H | 472 | GLN | N-CA | -5.37 | 1.35 | 1.46 |
| 6 | T | 472 | GLN | N-CA | -5.37 | 1.35 | 1.46 |
| 5 | G | 321 | ASN | C-N | 5.37 | 1.46 | 1.34 |
| 4 | R | 419 | GLY | C-N | 5.37 | 1.46 | 1.34 |
| 4 | L | 419 | GLY | C-N | 5.37 | 1.46 | 1.34 |
| 5 | S | 321 | ASN | C-N | 5.37 | 1.46 | 1.34 |
| 4 | X | 328 | VAL | CA-CB | -5.37 | 1.43 | 1.54 |
| 2 | O | 9 | LEU | N-CA | -5.36 | 1.35 | 1.46 |
| 6 | Z | 472 | GLN | N-CA | -5.36 | 1.35 | 1.46 |
| 2 | I | 9 | LEU | N-CA | -5.36 | 1.35 | 1.46 |
| 4 | R | 473 | GLY | CA-C | -5.36 | 1.43 | 1.51 |
| 4 | F | 231 | LYS | N-CA | 5.35 | 1.57 | 1.46 |
| 2 | U | 9 | LEU | N-CA | -5.35 | 1.35 | 1.46 |
| 4 | X | 419 | GLY | C-N | 5.35 | 1.46 | 1.34 |
| 6 | Z | 403 | LEU | N-CA | 5.35 | 1.57 | 1.46 |
| 2 | C | 9 | LEU | N-CA | -5.34 | 1.35 | 1.46 |
| 4 | R | 328 | VAL | CA-CB | -5.34 | 1.43 | 1.54 |
| 5 | G | 274 | ARG | CA-C | -5.34 | 1.39 | 1.52 |
| 6 | H | 467 | THR | CA-C | -5.34 | 1.39 | 1.52 |
| 5 | M | 326 | LEU | CA-CB | 5.34 | 1.66 | 1.53 |
| 4 | L | 231 | LYS | N-CA | 5.34 | 1.57 | 1.46 |
| 4 | R | 231 | LYS | N-CA | 5.34 | 1.57 | 1.46 |
| 5 | Y | 274 | ARG | CA-C | -5.33 | 1.39 | 1.52 |
| 6 | H | 403 | LEU | N-CA | 5.32 | 1.56 | 1.46 |
| 4 | F | 328 | VAL | CA-CB | -5.32 | 1.43 | 1.54 |
| 6 | N | 403 | LEU | N-CA | 5.32 | 1.56 | 1.46 |
| 6 | N | 467 | THR | CA-C | -5.32 | 1.39 | 1.52 |
| 5 | G | 326 | LEU | CA-CB | 5.31 | 1.66 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 276 | SER | C-N | 5.31 | 1.46 | 1.34 |
| 6 | Z | 467 | THR | CA-C | -5.30 | 1.39 | 1.52 |
| 5 | M | 276 | SER | C-N | 5.30 | 1.46 | 1.34 |
| 5 | G | 325 | ALA | N-CA | 5.30 | 1.56 | 1.46 |
| 5 | Y | 276 | SER | C-N | 5.29 | 1.46 | 1.34 |
| 6 | T | 403 | LEU | N-CA | 5.29 | 1.56 | 1.46 |
| 5 | Y | 325 | ALA | N-CA | 5.29 | 1.56 | 1.46 |
| 4 | R | 253 | SER | CA-C | 5.28 | 1.66 | 1.52 |
| 4 | F | 253 | SER | CA-C | 5.28 | 1.66 | 1.52 |
| 4 | X | 253 | SER | CA-C | 5.27 | 1.66 | 1.52 |
| 5 | S | 276 | SER | C-N | 5.27 | 1.46 | 1.34 |
| 4 | X | 252 | THR | N-CA | 5.27 | 1.56 | 1.46 |
| 5 | M | 274 | ARG | CA-C | -5.27 | 1.39 | 1.52 |
| 4 | F | 252 | THR | N-CA | 5.27 | 1.56 | 1.46 |
| 5 | M | 325 | ALA | N-CA | 5.27 | 1.56 | 1.46 |
| 5 | S | 325 | ALA | N-CA | 5.26 | 1.56 | 1.46 |
| 5 | S | 274 | ARG | CA-C | -5.26 | 1.39 | 1.52 |
| 4 | L | 253 | SER | CA-C | 5.26 | 1.66 | 1.52 |
| 5 | G | 327 | ARG | C-O | 5.25 | 1.33 | 1.23 |
| 4 | R | 252 | THR | N-CA | 5.25 | 1.56 | 1.46 |
| 4 | L | 443 | HIS | CA-C | 5.25 | 1.66 | 1.52 |
| 5 | M | 327 | ARG | C-O | 5.25 | 1.33 | 1.23 |
| 4 | F | 443 | HIS | CA-C | 5.24 | 1.66 | 1.52 |
| 4 | L | 404 | GLN | N-CA | -5.24 | 1.35 | 1.46 |
| 5 | Y | 327 | ARG | C-O | 5.23 | 1.33 | 1.23 |
| 4 | L | 252 | THR | N-CA | 5.23 | 1.56 | 1.46 |
| 4 | X | 443 | HIS | CA-C | 5.22 | 1.66 | 1.52 |
| 5 | Y | 380 | ILE | CA-C | 5.22 | 1.66 | 1.52 |
| 5 | G | 380 | ILE | CA-C | 5.22 | 1.66 | 1.52 |
| 5 | S | 380 | ILE | CA-C | 5.21 | 1.66 | 1.52 |
| 2 | C | 234 | LEU | N-CA | -5.20 | 1.35 | 1.46 |
| 6 | T | 469 | ASP | C-N | -5.20 | 1.24 | 1.34 |
| 4 | R | 443 | HIS | CA-C | 5.20 | 1.66 | 1.52 |
| 5 | M | 332 | PRO | N-CA | 5.20 | 1.56 | 1.47 |
| 2 | O | 234 | LEU | N-CA | -5.19 | 1.35 | 1.46 |
| 5 | M | 380 | ILE | CA-C | 5.19 | 1.66 | 1.52 |
| 4 | F | 219 | GLY | C-N | 5.18 | 1.46 | 1.34 |
| 5 | S | 332 | PRO | N-CA | 5.18 | 1.56 | 1.47 |
| 6 | T | 335 | SER | CA-CB | 5.18 | 1.60 | 1.52 |
| 6 | H | 469 | ASP | C-N | -5.18 | 1.24 | 1.34 |
| 2 | U | 234 | LEU | N-CA | -5.18 | 1.35 | 1.46 |
| 4 | X | 404 | GLN | N-CA | -5.18 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 469 | ASP | C-N | -5.18 | 1.24 | 1.34 |
| 4 | F | 404 | GLN | N-CA | -5.17 | 1.36 | 1.46 |
| 2 | I | 234 | LEU | N-CA | -5.17 | 1.36 | 1.46 |
| 5 | Y | 332 | PRO | N-CA | 5.17 | 1.56 | 1.47 |
| 4 | R | 404 | GLN | N-CA | -5.17 | 1.36 | 1.46 |
| 3 | D | 1493 | ARG | CA-C | -5.16 | 1.39 | 1.52 |
| 4 | X | 426 | GLN | N-CA | -5.16 | 1.36 | 1.46 |
| 6 | N | 469 | ASP | C-N | -5.16 | 1.24 | 1.34 |
| 2 | I | 6 | PHE | C-N | -5.15 | 1.23 | 1.33 |
| 5 | S | 327 | ARG | C-O | 5.14 | 1.33 | 1.23 |
| 2 | C | 6 | PHE | C-N | -5.14 | 1.23 | 1.33 |
| 6 | H | 335 | SER | CA-CB | 5.14 | 1.60 | 1.52 |
| 5 | G | 332 | PRO | N-CA | 5.14 | 1.55 | 1.47 |
| 2 | O | 6 | PHE | C-N | -5.13 | 1.23 | 1.33 |
| 4 | R | 132 | ASP | CA-C | -5.13 | 1.39 | 1.52 |
| 4 | L | 219 | GLY | C-N | 5.13 | 1.45 | 1.34 |
| 6 | Z | 335 | SER | CA-CB | 5.13 | 1.60 | 1.52 |
| 4 | L | 426 | GLN | N-CA | -5.12 | 1.36 | 1.46 |
| 4 | X | 219 | GLY | C-N | 5.12 | 1.45 | 1.34 |
| 6 | T | 467 | THR | N-CA | 5.12 | 1.56 | 1.46 |
| 4 | F | 426 | GLN | N-CA | -5.12 | 1.36 | 1.46 |
| 6 | H | 357 | GLN | CA-C | -5.12 | 1.39 | 1.52 |
| 4 | R | 219 | GLY | C-N | 5.11 | 1.45 | 1.34 |
| 6 | Z | 467 | THR | N-CA | 5.11 | 1.56 | 1.46 |
| 6 | Z | 357 | GLN | CA-C | -5.11 | 1.39 | 1.52 |
| 6 | N | 467 | THR | N-CA | 5.10 | 1.56 | 1.46 |
| 6 | N | 335 | SER | CA-CB | 5.10 | 1.60 | 1.52 |
| 3 | P | 1493 | ARG | CA-C | -5.10 | 1.39 | 1.52 |
| 4 | R | 460 | LEU | C-O | 5.09 | 1.33 | 1.23 |
| 4 | X | 398 | LYS | C-O | -5.09 | 1.13 | 1.23 |
| 4 | L | 132 | ASP | CA-C | -5.09 | 1.39 | 1.52 |
| 6 | N | 357 | GLN | CA-C | -5.08 | 1.39 | 1.52 |
| 4 | F | 132 | ASP | CA-C | -5.08 | 1.39 | 1.52 |
| 4 | X | 132 | ASP | CA-C | -5.08 | 1.39 | 1.52 |
| 4 | R | 426 | GLN | N-CA | -5.08 | 1.36 | 1.46 |
| 4 | X | 204 | SER | N-CA | 5.08 | 1.56 | 1.46 |
| 5 | G | 372 | ALA | N-CA | -5.07 | 1.36 | 1.46 |
| 6 | H | 467 | THR | N-CA | 5.07 | 1.56 | 1.46 |
| 6 | T | 357 | GLN | CA-C | -5.07 | 1.39 | 1.52 |
| 3 | D | 1448 | MET | C-N | 5.07 | 1.45 | 1.34 |
| 5 | M | 372 | ALA | N-CA | -5.07 | 1.36 | 1.46 |
| 2 | U | 6 | PHE | C-N | -5.06 | 1.24 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | F | 398 | LYS | C-O | -5.05 | 1.13 | 1.23 |
| 3 | P | 1448 | MET | C-N | 5.05 | 1.45 | 1.34 |
| 4 | X | 460 | LEU | C-O | 5.05 | 1.32 | 1.23 |
| 4 | R | 398 | LYS | C-O | -5.04 | 1.13 | 1.23 |
| 5 | G | 398 | ALA | N-CA | 5.04 | 1.56 | 1.46 |
| 5 | S | 372 | ALA | N-CA | -5.04 | 1.36 | 1.46 |
| 5 | M | 343 | ALA | C-N | 5.03 | 1.45 | 1.34 |
| 5 | Y | 325 | ALA | C-N | 5.03 | 1.45 | 1.34 |
| 3 | D | 1491 | ILE | C-O | 5.03 | 1.32 | 1.23 |
| 4 | L | 460 | LEU | C-O | 5.03 | 1.32 | 1.23 |
| 5 | Y | 372 | ALA | N-CA | -5.03 | 1.36 | 1.46 |
| 5 | S | 398 | ALA | N-CA | 5.02 | 1.56 | 1.46 |
| 5 | Y | 343 | ALA | C-N | 5.02 | 1.45 | 1.34 |
| 4 | F | 460 | LEU | C-O | 5.02 | 1.32 | 1.23 |
| 3 | P | 1449 | TRP | N-CA | 5.01 | 1.56 | 1.46 |
| 4 | X | 421 | LEU | N-CA | -5.01 | 1.36 | 1.46 |
| 5 | S | 325 | ALA | C-N | 5.01 | 1.45 | 1.34 |
| 5 | M | 325 | ALA | C-N | 5.01 | 1.45 | 1.34 |
| 4 | L | 398 | LYS | C-O | -5.00 | 1.13 | 1.23 |
| 5 | Y | 398 | ALA | N-CA | 5.00 | 1.56 | 1.46 |
| 5 | G | 325 | ALA | C-N | 5.00 | 1.45 | 1.34 |

All (2548) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 452 | ARG | CA-C-N | -39.55 | 30.19 | 117.20 |
| 4 | F | 452 | ARG | CA-C-N | -39.54 | 30.20 | 117.20 |
| 4 | R | 452 | ARG | CA-C-N | -39.54 | 30.20 | 117.20 |
| 4 | L | 452 | ARG | CA-C-N | -39.53 | 30.24 | 117.20 |
| 5 | G | 343 | ALA | CB-CA-C | -36.23 | 55.76 | 110.10 |
| 5 | M | 343 | ALA | CB-CA-C | -36.20 | 55.80 | 110.10 |
| 5 | Y | 343 | ALA | CB-CA-C | -36.20 | 55.80 | 110.10 |
| 5 | S | 343 | ALA | CB-CA-C | -36.19 | 55.82 | 110.10 |
| 3 | P | 1449 | TRP | CA-C-N | -32.78 | 45.09 | 117.20 |
| 3 | D | 1449 | TRP | CA-C-N | -32.76 | 45.12 | 117.20 |
| 5 | Y | 340 | ALA | CB-CA-C | 31.37 | 157.15 | 110.10 |
| 5 | M | 340 | ALA | CB-CA-C | 31.36 | 157.14 | 110.10 |
| 5 | S | 340 | ALA | CB-CA-C | 31.35 | 157.12 | 110.10 |
| 5 | G | 340 | ALA | CB-CA-C | 31.35 | 157.12 | 110.10 |
| 4 | F | 450 | GLU | CA-C-N | -29.89 | 51.43 | 117.20 |
| 4 | L | 450 | GLU | CA-C-N | -29.88 | 51.47 | 117.20 |
| 4 | X | 450 | GLU | CA-C-N | -29.87 | 51.48 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 450 | GLU | CA-C-N | -29.86 | 51.51 | 117.20 |
| 3 | D | 1488 | GLY | C-N-CA | -29.72 | 47.39 | 121.70 |
| 3 | P | 1488 | GLY | C-N-CA | -29.71 | 47.42 | 121.70 |
| 5 | M | 340 | ALA | N-CA-C | -29.70 | 30.81 | 111.00 |
| 5 | G | 340 | ALA | N-CA-C | -29.70 | 30.82 | 111.00 |
| 5 | S | 340 | ALA | N-CA-C | -29.68 | 30.85 | 111.00 |
| 5 | Y | 340 | ALA | N-CA-C | -29.67 | 30.88 | 111.00 |
| 4 | R | 454 | TYR | C-N-CA | -27.32 | 53.40 | 121.70 |
| 4 | F | 454 | TYR | C-N-CA | -27.31 | 53.44 | 121.70 |
| 4 | L | 454 | TYR | C-N-CA | -27.30 | 53.45 | 121.70 |
| 4 | X | 454 | TYR | C-N-CA | -27.30 | 53.45 | 121.70 |
| 4 | R | 462 | GLU | C-N-CA | -24.72 | 59.90 | 121.70 |
| 4 | L | 462 | GLU | C-N-CA | -24.72 | 59.91 | 121.70 |
| 4 | F | 462 | GLU | C-N-CA | -24.70 | 59.95 | 121.70 |
| 4 | X | 462 | GLU | C-N-CA | -24.69 | 59.97 | 121.70 |
| 4 | X | 450 | GLU | N-CA-CB | 24.34 | 154.41 | 110.60 |
| 4 | F | 450 | GLU | N-CA-CB | 24.34 | 154.41 | 110.60 |
| 5 | S | 338 | GLU | CA-C-O | -24.33 | 69.00 | 120.10 |
| 4 | L | 450 | GLU | N-CA-CB | 24.32 | 154.38 | 110.60 |
| 5 | M | 338 | GLU | CA-C-O | -24.31 | 69.04 | 120.10 |
| 4 | R | 450 | GLU | N-CA-CB | 24.30 | 154.34 | 110.60 |
| 5 | Y | 338 | GLU | CA-C-O | -24.30 | 69.08 | 120.10 |
| 5 | G | 338 | GLU | CA-C-O | -24.29 | 69.09 | 120.10 |
| 4 | R | 453 | TYR | O-C-N | -23.36 | 85.33 | 122.70 |
| 4 | L | 453 | TYR | O-C-N | -23.36 | 85.33 | 122.70 |
| 4 | X | 453 | TYR | O-C-N | -23.36 | 85.33 | 122.70 |
| 4 | F | 453 | TYR | O-C-N | -23.33 | 85.38 | 122.70 |
| 4 | X | 400 | GLY | CA-C-N | -22.77 | 67.10 | 117.20 |
| 4 | L | 400 | GLY | CA-C-N | -22.77 | 67.11 | 117.20 |
| 4 | R | 400 | GLY | CA-C-N | -22.77 | 67.11 | 117.20 |
| 4 | F | 400 | GLY | CA-C-N | -22.76 | 67.12 | 117.20 |
| 4 | F | 450 | GLU | CA-C-O | 22.69 | 167.74 | 120.10 |
| 4 | X | 450 | GLU | CA-C-O | 22.68 | 167.74 | 120.10 |
| 4 | L | 450 | GLU | CA-C-O | 22.66 | 167.69 | 120.10 |
| 4 | R | 450 | GLU | CA-C-O | 22.66 | 167.68 | 120.10 |
| 5 | M | 340 | ALA | N-CA-CB | 22.42 | 141.49 | 110.10 |
| 5 | Y | 340 | ALA | N-CA-CB | 22.40 | 141.46 | 110.10 |
| 5 | G | 340 | ALA | N-CA-CB | 22.32 | 141.35 | 110.10 |
| 5 | S | 340 | ALA | N-CA-CB | 22.31 | 141.34 | 110.10 |
| 1 | K | 276 | ASP | O-C-N | 21.70 | 157.42 | 122.70 |
| 1 | A | 276 | ASP | O-C-N | 21.70 | 157.42 | 122.70 |
| 1 | E | 276 | ASP | O-C-N | 21.69 | 157.40 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Q | 276 | ASP | O-C-N | 21.69 | 157.40 | 122.70 |
| 1 | B | 276 | ASP | O-C-N | 21.68 | 157.38 | 122.70 |
| 1 | W | 276 | ASP | O-C-N | 21.67 | 157.38 | 122.70 |
| 4 | L | 449 | SER | O-C-N | 21.64 | 157.33 | 122.70 |
| 4 | X | 449 | SER | O-C-N | 21.64 | 157.32 | 122.70 |
| 4 | F | 449 | SER | O-C-N | 21.61 | 157.27 | 122.70 |
| 4 | R | 449 | SER | O-C-N | 21.58 | 157.23 | 122.70 |
| 4 | L | 399 | SER | C-N-CA | -21.32 | 77.52 | 122.30 |
| 4 | X | 399 | SER | C-N-CA | -21.31 | 77.55 | 122.30 |
| 4 | F | 399 | SER | C-N-CA | -21.29 | 77.59 | 122.30 |
| 4 | R | 399 | SER | C-N-CA | -21.29 | 77.60 | 122.30 |
| 4 | R | 400 | GLY | O-C-N | 21.04 | 156.37 | 122.70 |
| 4 | X | 400 | GLY | O-C-N | 21.03 | 156.35 | 122.70 |
| 4 | F | 400 | GLY | O-C-N | 21.02 | 156.33 | 122.70 |
| 4 | L | 400 | GLY | O-C-N | 21.00 | 156.31 | 122.70 |
| 4 | R | 422 | ASN | C-N-CA | -20.44 | 70.61 | 121.70 |
| 4 | F | 422 | ASN | C-N-CA | -20.43 | 70.62 | 121.70 |
| 4 | L | 422 | ASN | C-N-CA | -20.43 | 70.61 | 121.70 |
| 4 | X | 422 | ASN | C-N-CA | -20.41 | 70.67 | 121.70 |
| 4 | X | 402 | ALA | N-CA-C | -20.40 | 55.91 | 111.00 |
| 4 | R | 402 | ALA | N-CA-C | -20.38 | 55.97 | 111.00 |
| 4 | L | 402 | ALA | N-CA-C | -20.38 | 55.98 | 111.00 |
| 4 | F | 402 | ALA | N-CA-C | -20.38 | 55.99 | 111.00 |
| 4 | L | 448 | ARG | CA-C-N | -20.34 | 72.46 | 117.20 |
| 4 | X | 448 | ARG | CA-C-N | -20.34 | 72.46 | 117.20 |
| 4 | F | 448 | ARG | CA-C-N | -20.33 | 72.47 | 117.20 |
| 4 | R | 448 | ARG | CA-C-N | -20.33 | 72.48 | 117.20 |
| 5 | M | 338 | GLU | O-C-N | 19.89 | 154.52 | 122.70 |
| 5 | S | 338 | GLU | O-C-N | 19.87 | 154.50 | 122.70 |
| 4 | L | 450 | GLU | C-N-CA | -19.83 | 72.12 | 121.70 |
| 5 | G | 338 | GLU | O-C-N | 19.83 | 154.43 | 122.70 |
| 5 | Y | 338 | GLU | O-C-N | 19.82 | 154.42 | 122.70 |
| 4 | R | 450 | GLU | C-N-CA | -19.82 | 72.16 | 121.70 |
| 4 | F | 450 | GLU | C-N-CA | -19.81 | 72.17 | 121.70 |
| 4 | X | 450 | GLU | C-N-CA | -19.81 | 72.18 | 121.70 |
| 4 | F | 455 | ILE | C-N-CA | -19.37 | 73.28 | 121.70 |
| 4 | L | 455 | ILE | C-N-CA | -19.36 | 73.30 | 121.70 |
| 4 | X | 455 | ILE | C-N-CA | -19.35 | 73.32 | 121.70 |
| 4 | R | 455 | ILE | C-N-CA | -19.32 | 73.39 | 121.70 |
| 4 | X | 402 | ALA | CB-CA-C | -18.85 | 81.82 | 110.10 |
| 4 | F | 402 | ALA | CB-CA-C | -18.83 | 81.85 | 110.10 |
| 4 | L | 402 | ALA | CB-CA-C | -18.83 | 81.85 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 402 | ALA | CB-CA-C | -18.81 | 81.88 | 110.10 |
| 4 | R | 398 | LYS | O-C-N | -18.72 | 92.74 | 122.70 |
| 4 | F | 398 | LYS | O-C-N | -18.72 | 92.75 | 122.70 |
| 4 | L | 398 | LYS | O-C-N | -18.71 | 92.76 | 122.70 |
| 4 | X | 398 | LYS | O-C-N | -18.65 | 92.85 | 122.70 |
| 6 | H | 494 | LEU | CA-C-N | -18.45 | 76.62 | 117.20 |
| 6 | Z | 494 | LEU | CA-C-N | -18.44 | 76.64 | 117.20 |
| 6 | T | 494 | LEU | CA-C-N | -18.41 | 76.69 | 117.20 |
| 6 | N | 494 | LEU | CA-C-N | -18.39 | 76.74 | 117.20 |
| 1 | K | 276 | ASP | CA-C-N | -18.34 | 76.84 | 117.20 |
| 1 | A | 276 | ASP | CA-C-N | -18.34 | 76.85 | 117.20 |
| 1 | B | 276 | ASP | CA-C-N | -18.33 | 76.87 | 117.20 |
| 1 | Q | 276 | ASP | CA-C-N | -18.33 | 76.86 | 117.20 |
| 1 | E | 276 | ASP | CA-C-N | -18.33 | 76.87 | 117.20 |
| 1 | W | 276 | ASP | CA-C-N | -18.32 | 76.89 | 117.20 |
| 3 | P | 1519 | SER | C-N-CA | -18.04 | 84.43 | 122.30 |
| 3 | D | 1519 | SER | C-N-CA | -18.03 | 84.44 | 122.30 |
| 5 | S | 341 | ALA | CA-C-O | -18.02 | 82.26 | 120.10 |
| 5 | G | 341 | ALA | CA-C-O | -18.01 | 82.28 | 120.10 |
| 5 | Y | 341 | ALA | CA-C-O | -18.00 | 82.30 | 120.10 |
| 5 | M | 341 | ALA | CA-C-O | -17.97 | 82.36 | 120.10 |
| 4 | L | 457 | ALA | N-CA-CB | -17.68 | 85.35 | 110.10 |
| 5 | S | 326 | LEU | CA-C-O | -17.66 | 83.02 | 120.10 |
| 4 | F | 457 | ALA | N-CA-CB | -17.64 | 85.40 | 110.10 |
| 5 | M | 326 | LEU | CA-C-O | -17.64 | 83.06 | 120.10 |
| 4 | R | 457 | ALA | N-CA-CB | -17.64 | 85.41 | 110.10 |
| 4 | X | 458 | ASP | CA-C-N | -17.63 | 78.41 | 117.20 |
| 5 | Y | 326 | LEU | CA-C-O | -17.63 | 83.07 | 120.10 |
| 5 | G | 326 | LEU | CA-C-O | -17.63 | 83.08 | 120.10 |
| 4 | L | 458 | ASP | CA-C-N | -17.62 | 78.43 | 117.20 |
| 4 | R | 458 | ASP | CA-C-N | -17.62 | 78.44 | 117.20 |
| 4 | F | 458 | ASP | CA-C-N | -17.61 | 78.45 | 117.20 |
| 4 | X | 457 | ALA | N-CA-CB | -17.59 | 85.47 | 110.10 |
| 3 | D | 1508 | LYS | C-N-CA | -17.52 | 77.91 | 121.70 |
| 3 | P | 1508 | LYS | C-N-CA | -17.52 | 77.91 | 121.70 |
| 4 | L | 449 | SER | CA-C-N | -17.22 | 79.31 | 117.20 |
| 4 | X | 449 | SER | CA-C-N | -17.21 | 79.33 | 117.20 |
| 4 | R | 449 | SER | CA-C-N | -17.20 | 79.36 | 117.20 |
| 4 | F | 449 | SER | CA-C-N | -17.20 | 79.37 | 117.20 |
| 4 | X | 461 | ARG | CB-CA-C | -17.11 | 76.19 | 110.40 |
| 4 | L | 453 | TYR | CA-C-O | 17.10 | 156.02 | 120.10 |
| 4 | X | 453 | TYR | CA-C-O | 17.10 | 156.02 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 453 | TYR | CA-C-O | 17.10 | 156.01 | 120.10 |
| 4 | R | 461 | ARG | CB-CA-C | -17.10 | 76.21 | 110.40 |
| 4 | R | 453 | TYR | CA-C-O | 17.09 | 155.99 | 120.10 |
| 4 | F | 461 | ARG | CB-CA-C | -17.09 | 76.22 | 110.40 |
| 4 | L | 461 | ARG | CB-CA-C | -17.09 | 76.22 | 110.40 |
| 5 | Y | 379 | HIS | CA-C-N | 16.54 | 153.60 | 117.20 |
| 5 | M | 379 | HIS | CA-C-N | 16.54 | 153.58 | 117.20 |
| 5 | G | 379 | HIS | CA-C-N | 16.53 | 153.57 | 117.20 |
| 5 | S | 379 | HIS | CA-C-N | 16.52 | 153.55 | 117.20 |
| 5 | S | 326 | LEU | CB-CA-C | -16.46 | 78.93 | 110.20 |
| 5 | G | 326 | LEU | CB-CA-C | -16.45 | 78.95 | 110.20 |
| 5 | M | 326 | LEU | CB-CA-C | -16.45 | 78.95 | 110.20 |
| 5 | G | 379 | HIS | C-N-CA | 16.44 | 162.81 | 121.70 |
| 5 | Y | 326 | LEU | CB-CA-C | -16.44 | 78.97 | 110.20 |
| 5 | Y | 379 | HIS | C-N-CA | 16.44 | 162.79 | 121.70 |
| 5 | M | 379 | HIS | C-N-CA | 16.43 | 162.79 | 121.70 |
| 5 | S | 379 | HIS | C-N-CA | 16.43 | 162.76 | 121.70 |
| 4 | R | 454 | TYR | N-CA-C | 16.33 | 155.09 | 111.00 |
| 4 | F | 454 | TYR | N-CA-C | 16.33 | 155.09 | 111.00 |
| 4 | X | 454 | TYR | N-CA-C | 16.32 | 155.08 | 111.00 |
| 4 | L | 454 | TYR | N-CA-C | 16.31 | 155.05 | 111.00 |
| 4 | L | 448 | ARG | O-C-N | -16.26 | 96.68 | 122.70 |
| 4 | F | 448 | ARG | O-C-N | -16.26 | 96.69 | 122.70 |
| 4 | R | 448 | ARG | O-C-N | -16.25 | 96.70 | 122.70 |
| 4 | X | 448 | ARG | O-C-N | -16.22 | 96.74 | 122.70 |
| 4 | F | 457 | ALA | CB-CA-C | 16.01 | 134.12 | 110.10 |
| 4 | R | 457 | ALA | CB-CA-C | 16.01 | 134.12 | 110.10 |
| 4 | X | 457 | ALA | CB-CA-C | 16.00 | 134.10 | 110.10 |
| 4 | L | 457 | ALA | CB-CA-C | 15.99 | 134.08 | 110.10 |
| 4 | F | 454 | TYR | N-CA-CB | -15.97 | 81.86 | 110.60 |
| 4 | X | 454 | TYR | N-CA-CB | -15.96 | 81.88 | 110.60 |
| 4 | L | 454 | TYR | N-CA-CB | -15.95 | 81.88 | 110.60 |
| 4 | R | 454 | TYR | N-CA-CB | -15.95 | 81.90 | 110.60 |
| 5 | M | 342 | PRO | O-C-N | 15.90 | 148.14 | 122.70 |
| 5 | G | 342 | PRO | O-C-N | 15.87 | 148.09 | 122.70 |
| 5 | Y | 342 | PRO | O-C-N | 15.85 | 148.06 | 122.70 |
| 5 | S | 342 | PRO | O-C-N | 15.84 | 148.04 | 122.70 |
| 3 | D | 1506 | VAL | C-N-CA | -15.70 | 82.46 | 121.70 |
| 3 | P | 1506 | VAL | C-N-CA | -15.69 | 82.47 | 121.70 |
| 4 | R | 464 | LYS | CB-CA-C | -15.66 | 79.08 | 110.40 |
| 3 | D | 1509 | GLN | C-N-CA | -15.64 | 82.60 | 121.70 |
| 4 | F | 464 | LYS | CB-CA-C | -15.64 | 79.13 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 464 | LYS | CB-CA-C | -15.63 | 79.14 | 110.40 |
| 4 | X | 464 | LYS | CB-CA-C | -15.63 | 79.14 | 110.40 |
| 3 | P | 1509 | GLN | C-N-CA | -15.62 | 82.65 | 121.70 |
| 4 | F | 455 | ILE | CA-C-O | 15.54 | 152.74 | 120.10 |
| 4 | L | 455 | ILE | CA-C-O | 15.54 | 152.72 | 120.10 |
| 4 | X | 455 | ILE | CA-C-O | 15.53 | 152.72 | 120.10 |
| 4 | R | 455 | ILE | CA-C-O | 15.50 | 152.66 | 120.10 |
| 6 | N | 490 | GLN | CB-CA-C | -15.44 | 79.51 | 110.40 |
| 6 | H | 490 | GLN | CB-CA-C | -15.44 | 79.53 | 110.40 |
| 6 | Z | 490 | GLN | CB-CA-C | -15.44 | 79.53 | 110.40 |
| 6 | T | 490 | GLN | CB-CA-C | -15.42 | 79.55 | 110.40 |
| 5 | M | 340 | ALA | O-C-N | -15.30 | 98.22 | 122.70 |
| 5 | G | 340 | ALA | O-C-N | -15.26 | 98.28 | 122.70 |
| 6 | H | 411 | GLU | O-C-N | -15.26 | 98.29 | 122.70 |
| 6 | N | 412 | GLU | O-C-N | 15.25 | 147.10 | 122.70 |
| 6 | T | 411 | GLU | O-C-N | -15.24 | 98.32 | 122.70 |
| 6 | H | 412 | GLU | O-C-N | 15.23 | 147.07 | 122.70 |
| 6 | T | 412 | GLU | O-C-N | 15.23 | 147.07 | 122.70 |
| 6 | Z | 412 | GLU | O-C-N | 15.23 | 147.06 | 122.70 |
| 5 | S | 340 | ALA | O-C-N | -15.22 | 98.35 | 122.70 |
| 5 | Y | 340 | ALA | O-C-N | -15.22 | 98.35 | 122.70 |
| 6 | Z | 411 | GLU | O-C-N | -15.21 | 98.37 | 122.70 |
| 6 | N | 411 | GLU | O-C-N | -15.21 | 98.37 | 122.70 |
| 3 | P | 1519 | SER | CA-C-N | -15.12 | 85.96 | 116.20 |
| 3 | D | 1519 | SER | CA-C-N | -15.11 | 85.97 | 116.20 |
| 5 | Y | 328 | THR | N-CA-CB | 14.91 | 138.62 | 110.30 |
| 5 | G | 343 | ALA | O-C-N | -14.89 | 98.88 | 122.70 |
| 5 | G | 328 | THR | N-CA-CB | 14.88 | 138.58 | 110.30 |
| 5 | Y | 343 | ALA | O-C-N | -14.88 | 98.89 | 122.70 |
| 5 | S | 328 | THR | N-CA-CB | 14.88 | 138.58 | 110.30 |
| 5 | M | 328 | THR | N-CA-CB | 14.88 | 138.56 | 110.30 |
| 5 | M | 343 | ALA | O-C-N | -14.87 | 98.91 | 122.70 |
| 5 | S | 343 | ALA | O-C-N | -14.86 | 98.93 | 122.70 |
| 5 | S | 333 | PRO | N-CA-CB | 14.79 | 121.05 | 103.30 |
| 5 | Y | 333 | PRO | N-CA-CB | 14.76 | 121.01 | 103.30 |
| 5 | G | 333 | PRO | N-CA-CB | 14.76 | 121.01 | 103.30 |
| 5 | M | 333 | PRO | N-CA-CB | 14.71 | 120.96 | 103.30 |
| 5 | S | 326 | LEU | O-C-N | 14.63 | 146.11 | 122.70 |
| 5 | M | 326 | LEU | O-C-N | 14.58 | 146.03 | 122.70 |
| 5 | G | 326 | LEU | O-C-N | 14.58 | 146.02 | 122.70 |
| 5 | Y | 326 | LEU | O-C-N | 14.57 | 146.01 | 122.70 |
| 4 | R | 451 | GLU | CA-C-N | -14.55 | 85.20 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 451 | GLU | CA-C-N | -14.54 | 85.21 | 117.20 |
| 4 | F | 451 | GLU | CA-C-N | -14.53 | 85.23 | 117.20 |
| 4 | L | 451 | GLU | CA-C-N | -14.50 | 85.30 | 117.20 |
| 4 | X | 457 | ALA | CA-C-N | -14.47 | 85.37 | 117.20 |
| 4 | F | 457 | ALA | CA-C-N | -14.45 | 85.40 | 117.20 |
| 4 | L | 457 | ALA | CA-C-N | -14.46 | 85.40 | 117.20 |
| 4 | R | 457 | ALA | CA-C-N | -14.45 | 85.40 | 117.20 |
| 4 | F | 456 | ASP | CB-CA-C | -14.44 | 81.52 | 110.40 |
| 4 | L | 456 | ASP | CB-CA-C | -14.43 | 81.54 | 110.40 |
| 4 | R | 456 | ASP | CB-CA-C | -14.43 | 81.55 | 110.40 |
| 4 | X | 456 | ASP | CB-CA-C | -14.42 | 81.56 | 110.40 |
| 3 | P | 1546 | LEU | C-N-CA | -14.32 | 85.89 | 121.70 |
| 3 | D | 1546 | LEU | C-N-CA | -14.30 | 85.94 | 121.70 |
| 4 | R | 424 | PRO | C-N-CA | -14.26 | 86.06 | 121.70 |
| 4 | F | 424 | PRO | C-N-CA | -14.25 | 86.07 | 121.70 |
| 4 | X | 424 | PRO | C-N-CA | -14.24 | 86.09 | 121.70 |
| 4 | L | 424 | PRO | C-N-CA | -14.24 | 86.10 | 121.70 |
| 6 | H | 341 | SER | N-CA-CB | 14.12 | 131.68 | 110.50 |
| 6 | Z | 341 | SER | N-CA-CB | 14.12 | 131.68 | 110.50 |
| 6 | N | 341 | SER | N-CA-CB | 14.10 | 131.65 | 110.50 |
| 6 | T | 341 | SER | N-CA-CB | 14.08 | 131.62 | 110.50 |
| 3 | P | 1539 | LEU | C-N-CA | -13.99 | 86.72 | 121.70 |
| 3 | D | 1539 | LEU | C-N-CA | -13.96 | 86.80 | 121.70 |
| 5 | Y | 341 | ALA | C-N-CA | -13.94 | 63.45 | 122.00 |
| 5 | S | 341 | ALA | C-N-CA | -13.94 | 63.47 | 122.00 |
| 5 | G | 341 | ALA | C-N-CA | -13.92 | 63.52 | 122.00 |
| 5 | M | 341 | ALA | C-N-CA | -13.91 | 63.56 | 122.00 |
| 5 | S | 330 | LYS | N-CA-CB | 13.91 | 135.65 | 110.60 |
| 5 | Y | 330 | LYS | N-CA-CB | 13.91 | 135.65 | 110.60 |
| 5 | G | 330 | LYS | N-CA-CB | 13.90 | 135.62 | 110.60 |
| 5 | M | 342 | PRO | CA-C-N | -13.89 | 86.65 | 117.20 |
| 5 | G | 342 | PRO | CA-C-N | -13.88 | 86.67 | 117.20 |
| 5 | M | 330 | LYS | N-CA-CB | 13.87 | 135.56 | 110.60 |
| 5 | Y | 342 | PRO | CA-C-N | -13.86 | 86.70 | 117.20 |
| 5 | S | 342 | PRO | CA-C-N | -13.86 | 86.72 | 117.20 |
| 4 | L | 399 | SER | CA-C-N | -13.79 | 88.63 | 116.20 |
| 4 | R | 399 | SER | CA-C-N | -13.79 | 88.63 | 116.20 |
| 4 | X | 399 | SER | CA-C-N | -13.78 | 88.64 | 116.20 |
| 4 | F | 399 | SER | CA-C-N | -13.78 | 88.64 | 116.20 |
| 4 | R | 400 | GLY | CA-C-O | -13.76 | 95.84 | 120.60 |
| 4 | L | 252 | THR | CB-CA-C | -13.74 | 74.49 | 111.60 |
| 4 | L | 400 | GLY | CA-C-O | -13.74 | 95.86 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 400 | GLY | CA-C-O | -13.74 | 95.86 | 120.60 |
| 4 | R | 252 | THR | CB-CA-C | -13.74 | 74.50 | 111.60 |
| 4 | F | 252 | THR | CB-CA-C | -13.73 | 74.52 | 111.60 |
| 4 | F | 400 | GLY | CA-C-O | -13.73 | 95.88 | 120.60 |
| 4 | X | 252 | THR | CB-CA-C | -13.73 | 74.52 | 111.60 |
| 5 | S | 327 | ARG | N-CA-CB | 13.71 | 135.28 | 110.60 |
| 5 | M | 327 | ARG | N-CA-CB | 13.70 | 135.26 | 110.60 |
| 5 | G | 327 | ARG | N-CA-CB | 13.70 | 135.25 | 110.60 |
| 5 | Y | 327 | ARG | N-CA-CB | 13.68 | 135.23 | 110.60 |
| 4 | F | 448 | ARG | CB-CA-C | -13.66 | 83.08 | 110.40 |
| 4 | X | 459 | LEU | N-CA-CB | 13.65 | 137.71 | 110.40 |
| 4 | R | 448 | ARG | CB-CA-C | -13.65 | 83.11 | 110.40 |
| 4 | L | 448 | ARG | CB-CA-C | -13.64 | 83.11 | 110.40 |
| 4 | X | 448 | ARG | CB-CA-C | -13.64 | 83.11 | 110.40 |
| 4 | R | 459 | LEU | N-CA-CB | 13.63 | 137.66 | 110.40 |
| 6 | N | 446 | ARG | CB-CA-C | 13.61 | 137.63 | 110.40 |
| 4 | L | 459 | LEU | N-CA-CB | 13.61 | 137.62 | 110.40 |
| 4 | F | 459 | LEU | N-CA-CB | 13.60 | 137.60 | 110.40 |
| 6 | T | 446 | ARG | CB-CA-C | 13.59 | 137.58 | 110.40 |
| 6 | H | 446 | ARG | CB-CA-C | 13.58 | 137.57 | 110.40 |
| 6 | Z | 446 | ARG | CB-CA-C | 13.57 | 137.53 | 110.40 |
| 4 | R | 463 | ILE | N-CA-CB | -13.39 | 80.01 | 110.80 |
| 4 | L | 463 | ILE | N-CA-CB | -13.38 | 80.02 | 110.80 |
| 4 | X | 463 | ILE | N-CA-CB | -13.37 | 80.04 | 110.80 |
| 4 | F | 463 | ILE | N-CA-CB | -13.37 | 80.06 | 110.80 |
| 3 | D | 1449 | TRP | O-C-N | -13.32 | 101.39 | 122.70 |
| 4 | L | 487 | ASP | O-C-N | -13.29 | 101.44 | 122.70 |
| 4 | R | 487 | ASP | O-C-N | -13.28 | 101.45 | 122.70 |
| 3 | P | 1449 | TRP | O-C-N | -13.28 | 101.46 | 122.70 |
| 4 | X | 487 | ASP | O-C-N | -13.28 | 101.46 | 122.70 |
| 4 | F | 487 | ASP | O-C-N | -13.26 | 101.48 | 122.70 |
| 4 | L | 452 | ARG | CA-C-O | 13.15 | 147.72 | 120.10 |
| 4 | R | 452 | ARG | CA-C-O | 13.15 | 147.71 | 120.10 |
| 4 | F | 452 | ARG | CA-C-O | 13.13 | 147.67 | 120.10 |
| 4 | X | 452 | ARG | CA-C-O | 13.13 | 147.66 | 120.10 |
| 4 | F | 452 | ARG | N-CA-CB | 13.05 | 134.08 | 110.60 |
| 4 | L | 452 | ARG | N-CA-CB | 13.03 | 134.05 | 110.60 |
| 4 | X | 452 | ARG | N-CA-CB | 13.02 | 134.04 | 110.60 |
| 4 | R | 452 | ARG | N-CA-CB | 13.02 | 134.03 | 110.60 |
| 5 | S | 341 | ALA | CA-C-N | -12.97 | 80.77 | 117.10 |
| 5 | Y | 341 | ALA | CA-C-N | -12.97 | 80.79 | 117.10 |
| 5 | G | 341 | ALA | CA-C-N | -12.96 | 80.81 | 117.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 341 | ALA | CA-C-N | -12.96 | 80.82 | 117.10 |
| 6 | Z | 408 | SER | C-N-CA | -12.91 | 67.77 | 122.00 |
| 6 | N | 408 | SER | C-N-CA | -12.91 | 67.80 | 122.00 |
| 6 | T | 408 | SER | C-N-CA | -12.91 | 67.80 | 122.00 |
| 3 | D | 1541 | THR | C-N-CA | -12.90 | 67.81 | 122.00 |
| 3 | P | 1541 | THR | C-N-CA | -12.90 | 67.82 | 122.00 |
| 6 | H | 408 | SER | C-N-CA | -12.89 | 67.87 | 122.00 |
| 4 | F | 450 | GLU | N-CA-C | -12.63 | 76.90 | 111.00 |
| 4 | F | 221 | GLN | CB-CA-C | -12.62 | 85.15 | 110.40 |
| 4 | L | 221 | GLN | CB-CA-C | -12.62 | 85.16 | 110.40 |
| 4 | L | 450 | GLU | N-CA-C | -12.62 | 76.93 | 111.00 |
| 4 | R | 450 | GLU | N-CA-C | -12.62 | 76.93 | 111.00 |
| 4 | X | 450 | GLU | N-CA-C | -12.61 | 76.94 | 111.00 |
| 4 | X | 221 | GLN | CB-CA-C | -12.61 | 85.17 | 110.40 |
| 4 | R | 221 | GLN | CB-CA-C | -12.60 | 85.19 | 110.40 |
| 5 | G | 339 | TYR | O-C-N | 12.52 | 142.72 | 122.70 |
| 5 | S | 339 | TYR | O-C-N | 12.50 | 142.71 | 122.70 |
| 5 | Y | 339 | TYR | O-C-N | 12.50 | 142.69 | 122.70 |
| 5 | M | 339 | TYR | O-C-N | 12.49 | 142.69 | 122.70 |
| 4 | L | 400 | GLY | C-N-CA | -12.49 | 90.48 | 121.70 |
| 4 | X | 400 | GLY | C-N-CA | -12.49 | 90.47 | 121.70 |
| 4 | R | 400 | GLY | C-N-CA | -12.49 | 90.48 | 121.70 |
| 4 | F | 400 | GLY | C-N-CA | -12.48 | 90.51 | 121.70 |
| 4 | L | 401 | TYR | O-C-N | -12.45 | 102.78 | 122.70 |
| 4 | R | 401 | TYR | O-C-N | -12.42 | 102.82 | 122.70 |
| 4 | X | 453 | TYR | N-CA-C | -12.38 | 77.59 | 111.00 |
| 4 | F | 401 | TYR | O-C-N | -12.37 | 102.91 | 122.70 |
| 4 | X | 401 | TYR | O-C-N | -12.37 | 102.91 | 122.70 |
| 4 | L | 453 | TYR | N-CA-C | -12.37 | 77.61 | 111.00 |
| 4 | F | 453 | TYR | N-CA-C | -12.37 | 77.62 | 111.00 |
| 4 | R | 453 | TYR | N-CA-C | -12.35 | 77.64 | 111.00 |
| 3 | P | 1504 | VAL | C-N-CA | -12.22 | 91.15 | 121.70 |
| 3 | D | 1504 | VAL | C-N-CA | -12.22 | 91.16 | 121.70 |
| 5 | M | 343 | ALA | CA-C-O | 12.13 | 145.58 | 120.10 |
| 4 | L | 456 | ASP | CA-C-O | 12.13 | 145.58 | 120.10 |
| 4 | R | 456 | ASP | CA-C-O | 12.13 | 145.57 | 120.10 |
| 4 | X | 456 | ASP | CA-C-O | 12.13 | 145.58 | 120.10 |
| 4 | F | 456 | ASP | CA-C-O | 12.12 | 145.56 | 120.10 |
| 5 | S | 343 | ALA | CA-C-O | 12.12 | 145.55 | 120.10 |
| 5 | Y | 343 | ALA | CA-C-O | 12.11 | 145.54 | 120.10 |
| 5 | G | 343 | ALA | CA-C-O | 12.10 | 145.51 | 120.10 |
| 6 | H | 494 | LEU | CA-C-O | 12.05 | 145.41 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | T | 494 | LEU | CA-C-O | 12.01 | 145.33 | 120.10 |
| 6 | Z | 494 | LEU | CA-C-O | 12.00 | 145.30 | 120.10 |
| 6 | N | 494 | LEU | CA-C-O | 11.98 | 145.27 | 120.10 |
| 3 | D | 1493 | ARG | C-N-CA | -11.92 | 91.90 | 121.70 |
| 3 | P | 1493 | ARG | C-N-CA | -11.92 | 91.90 | 121.70 |
| 4 | F | 452 | ARG | CB-CA-C | -11.88 | 86.64 | 110.40 |
| 4 | F | 456 | ASP | O-C-N | -11.88 | 103.70 | 122.70 |
| 4 | L | 452 | ARG | CB-CA-C | -11.87 | 86.65 | 110.40 |
| 4 | L | 456 | ASP | O-C-N | -11.87 | 103.71 | 122.70 |
| 3 | D | 1541 | THR | CA-C-N | -11.86 | 83.89 | 117.10 |
| 4 | R | 452 | ARG | CB-CA-C | -11.86 | 86.68 | 110.40 |
| 3 | P | 1541 | THR | CA-C-N | -11.85 | 83.92 | 117.10 |
| 4 | X | 456 | ASP | O-C-N | -11.85 | 103.74 | 122.70 |
| 4 | X | 452 | ARG | CB-CA-C | -11.85 | 86.70 | 110.40 |
| 4 | R | 456 | ASP | O-C-N | -11.84 | 103.75 | 122.70 |
| 4 | R | 493 | HIS | N-CA-C | 11.77 | 142.76 | 111.00 |
| 4 | X | 493 | HIS | N-CA-C | 11.76 | 142.76 | 111.00 |
| 4 | L | 493 | HIS | N-CA-C | 11.76 | 142.76 | 111.00 |
| 4 | F | 493 | HIS | N-CA-C | 11.76 | 142.75 | 111.00 |
| 4 | L | 293 | ILE | CB-CA-C | -11.74 | 88.12 | 111.60 |
| 4 | X | 293 | ILE | CB-CA-C | -11.73 | 88.15 | 111.60 |
| 4 | F | 293 | ILE | CB-CA-C | -11.71 | 88.18 | 111.60 |
| 4 | R | 293 | ILE | CB-CA-C | -11.71 | 88.18 | 111.60 |
| 6 | N | 467 | THR | C-N-CA | 11.68 | 150.89 | 121.70 |
| 3 | P | 1449 | TRP | CA-C-O | 11.67 | 144.61 | 120.10 |
| 4 | X | 455 | ILE | CA-C-N | -11.67 | 91.53 | 117.20 |
| 6 | T | 467 | THR | C-N-CA | 11.66 | 150.84 | 121.70 |
| 6 | H | 467 | THR | C-N-CA | 11.65 | 150.83 | 121.70 |
| 4 | L | 455 | ILE | CA-C-N | -11.65 | 91.57 | 117.20 |
| 3 | D | 1449 | TRP | CA-C-O | 11.64 | 144.56 | 120.10 |
| 4 | F | 455 | ILE | CA-C-N | -11.64 | 91.58 | 117.20 |
| 6 | Z | 467 | THR | C-N-CA | 11.62 | 150.76 | 121.70 |
| 4 | X | 423 | ALA | CA-C-N | -11.62 | 84.57 | 117.10 |
| 4 | R | 423 | ALA | CA-C-N | -11.62 | 84.57 | 117.10 |
| 4 | L | 423 | ALA | CA-C-N | -11.61 | 84.59 | 117.10 |
| 4 | F | 423 | ALA | CA-C-N | -11.61 | 84.60 | 117.10 |
| 4 | R | 455 | ILE | CA-C-N | -11.59 | 91.70 | 117.20 |
| 6 | T | 410 | LEU | O-C-N | 11.59 | 141.25 | 122.70 |
| 4 | F | 456 | ASP | CA-C-N | -11.58 | 91.72 | 117.20 |
| 4 | X | 455 | ILE | N-CA-C | 11.58 | 142.26 | 111.00 |
| 3 | P | 1544 | PRO | N-CA-C | 11.58 | 142.20 | 112.10 |
| 4 | L | 455 | ILE | N-CA-C | 11.57 | 142.25 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 1544 | PRO | N-CA-C | 11.57 | 142.19 | 112.10 |
| 4 | F | 455 | ILE | N-CA-C | 11.57 | 142.24 | 111.00 |
| 4 | R | 455 | ILE | N-CA-C | 11.57 | 142.24 | 111.00 |
| 4 | L | 456 | ASP | CA-C-N | -11.56 | 91.76 | 117.20 |
| 4 | R | 456 | ASP | CA-C-N | -11.56 | 91.76 | 117.20 |
| 4 | R | 220 | ASN | O-C-N | 11.55 | 141.19 | 122.70 |
| 4 | X | 456 | ASP | CA-C-N | -11.55 | 91.78 | 117.20 |
| 4 | F | 220 | ASN | O-C-N | 11.54 | 141.17 | 122.70 |
| 7 | V | 1473 | LEU | C-N-CA | 11.54 | 150.55 | 121.70 |
| 6 | N | 410 | LEU | O-C-N | 11.53 | 141.16 | 122.70 |
| 6 | H | 410 | LEU | O-C-N | 11.53 | 141.14 | 122.70 |
| 7 | J | 1473 | LEU | C-N-CA | 11.52 | 150.51 | 121.70 |
| 4 | X | 220 | ASN | O-C-N | 11.52 | 141.14 | 122.70 |
| 4 | L | 220 | ASN | O-C-N | 11.51 | 141.12 | 122.70 |
| 6 | Z | 410 | LEU | CB-CA-C | 11.50 | 132.05 | 110.20 |
| 6 | Z | 410 | LEU | O-C-N | 11.50 | 141.10 | 122.70 |
| 6 | H | 410 | LEU | CB-CA-C | 11.49 | 132.03 | 110.20 |
| 6 | N | 410 | LEU | CB-CA-C | 11.48 | 132.01 | 110.20 |
| 6 | T | 410 | LEU | CB-CA-C | 11.46 | 131.97 | 110.20 |
| 4 | F | 458 | ASP | C-N-CA | -11.46 | 93.06 | 121.70 |
| 4 | R | 458 | ASP | C-N-CA | -11.45 | 93.07 | 121.70 |
| 4 | X | 458 | ASP | C-N-CA | -11.45 | 93.07 | 121.70 |
| 4 | L | 458 | ASP | C-N-CA | -11.43 | 93.13 | 121.70 |
| 4 | L | 460 | LEU | N-CA-CB | 11.42 | 133.25 | 110.40 |
| 4 | X | 460 | LEU | N-CA-CB | 11.41 | 133.22 | 110.40 |
| 4 | R | 460 | LEU | N-CA-CB | 11.40 | 133.20 | 110.40 |
| 3 | D | 1518 | ASN | CA-C-N | -11.39 | 92.13 | 117.20 |
| 5 | M | 339 | TYR | C-N-CA | -11.39 | 93.23 | 121.70 |
| 4 | F | 460 | LEU | N-CA-CB | 11.39 | 133.17 | 110.40 |
| 3 | P | 1518 | ASN | CA-C-N | -11.38 | 92.16 | 117.20 |
| 5 | Y | 334 | GLY | C-N-CA | 11.38 | 150.14 | 121.70 |
| 5 | G | 334 | GLY | C-N-CA | 11.37 | 150.13 | 121.70 |
| 5 | Y | 339 | TYR | C-N-CA | -11.37 | 93.27 | 121.70 |
| 5 | S | 339 | TYR | C-N-CA | -11.36 | 93.29 | 121.70 |
| 5 | G | 339 | TYR | C-N-CA | -11.36 | 93.31 | 121.70 |
| 5 | S | 334 | GLY | C-N-CA | 11.36 | 150.09 | 121.70 |
| 5 | M | 334 | GLY | C-N-CA | 11.35 | 150.08 | 121.70 |
| 2 | U | 15 | GLN | CB-CA-C | -11.35 | 87.70 | 110.40 |
| 2 | O | 15 | GLN | CB-CA-C | -11.33 | 87.74 | 110.40 |
| 4 | R | 487 | ASP | CB-CA-C | -11.33 | 87.75 | 110.40 |
| 2 | C | 15 | GLN | CB-CA-C | -11.32 | 87.75 | 110.40 |
| 2 | I | 15 | GLN | CB-CA-C | -11.32 | 87.75 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 487 | ASP | CB-CA-C | -11.32 | 87.77 | 110.40 |
| 4 | L | 420 | GLU | O-C-N | 11.31 | 140.80 | 122.70 |
| 4 | X | 487 | ASP | CB-CA-C | -11.31 | 87.78 | 110.40 |
| 4 | F | 487 | ASP | CB-CA-C | -11.30 | 87.79 | 110.40 |
| 4 | X | 420 | GLU | O-C-N | 11.29 | 140.76 | 122.70 |
| 4 | F | 420 | GLU | O-C-N | 11.29 | 140.76 | 122.70 |
| 4 | X | 249 | PRO | N-CA-CB | 11.27 | 116.83 | 103.30 |
| 4 | R | 249 | PRO | N-CA-CB | 11.27 | 116.82 | 103.30 |
| 4 | R | 420 | GLU | O-C-N | 11.26 | 140.71 | 122.70 |
| 4 | F | 249 | PRO | N-CA-CB | 11.26 | 116.81 | 103.30 |
| 3 | D | 400 | LEU | CB-CA-C | -11.25 | 88.82 | 110.20 |
| 3 | D | 1487 | ASP | CA-C-N | -11.22 | 93.76 | 116.20 |
| 3 | P | 1487 | ASP | CA-C-N | -11.22 | 93.77 | 116.20 |
| 3 | P | 400 | LEU | CB-CA-C | -11.21 | 88.90 | 110.20 |
| 5 | M | 405 | SER | CB-CA-C | 11.19 | 131.37 | 110.10 |
| 4 | L | 249 | PRO | N-CA-CB | 11.19 | 116.73 | 103.30 |
| 6 | H | 373 | THR | N-CA-CB | 11.18 | 131.53 | 110.30 |
| 5 | G | 405 | SER | CB-CA-C | 11.17 | 131.33 | 110.10 |
| 5 | S | 405 | SER | CB-CA-C | 11.17 | 131.33 | 110.10 |
| 5 | Y | 405 | SER | CB-CA-C | 11.15 | 131.29 | 110.10 |
| 6 | T | 373 | THR | N-CA-CB | 11.15 | 131.48 | 110.30 |
| 3 | P | 1520 | GLY | CA-C-N | -11.15 | 92.68 | 117.20 |
| 3 | D | 1520 | GLY | CA-C-N | -11.14 | 92.69 | 117.20 |
| 6 | N | 373 | THR | N-CA-CB | 11.14 | 131.46 | 110.30 |
| 6 | Z | 373 | THR | N-CA-CB | 11.14 | 131.46 | 110.30 |
| 4 | R | 424 | PRO | CA-C-N | -11.13 | 92.71 | 117.20 |
| 4 | L | 424 | PRO | CA-C-N | -11.13 | 92.72 | 117.20 |
| 4 | X | 424 | PRO | CA-C-N | -11.12 | 92.73 | 117.20 |
| 6 | H | 462 | GLY | CA-C-N | 11.12 | 141.66 | 117.20 |
| 4 | L | 450 | GLU | O-C-N | 11.11 | 140.48 | 122.70 |
| 6 | T | 462 | GLY | CA-C-N | 11.11 | 141.65 | 117.20 |
| 6 | Z | 462 | GLY | CA-C-N | 11.11 | 141.64 | 117.20 |
| 4 | F | 424 | PRO | CA-C-N | -11.11 | 92.77 | 117.20 |
| 4 | F | 450 | GLU | O-C-N | 11.11 | 140.47 | 122.70 |
| 6 | N | 462 | GLY | CA-C-N | 11.10 | 141.62 | 117.20 |
| 4 | R | 460 | LEU | CA-C-O | -11.10 | 96.79 | 120.10 |
| 4 | R | 450 | GLU | O-C-N | 11.09 | 140.44 | 122.70 |
| 5 | M | 327 | ARG | CB-CA-C | -11.09 | 88.23 | 110.40 |
| 4 | X | 343 | MET | N-CA-CB | 11.09 | 130.56 | 110.60 |
| 4 | F | 460 | LEU | CA-C-O | -11.09 | 96.82 | 120.10 |
| 5 | S | 327 | ARG | CB-CA-C | -11.08 | 88.23 | 110.40 |
| 4 | X | 450 | GLU | O-C-N | 11.08 | 140.43 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | G | 327 | ARG | CB-CA-C | -11.08 | 88.24 | 110.40 |
| 4 | R | 343 | MET | N-CA-CB | 11.08 | 130.55 | 110.60 |
| 4 | L | 343 | MET | N-CA-CB | 11.08 | 130.54 | 110.60 |
| 4 | X | 460 | LEU | CA-C-O | -11.08 | 96.83 | 120.10 |
| 5 | Y | 327 | ARG | CB-CA-C | -11.08 | 88.25 | 110.40 |
| 4 | L | 486 | GLU | N-CA-CB | 11.06 | 130.52 | 110.60 |
| 4 | L | 243 | TYR | N-CA-CB | 11.06 | 130.51 | 110.60 |
| 4 | F | 343 | MET | N-CA-CB | 11.05 | 130.50 | 110.60 |
| 4 | L | 460 | LEU | CA-C-O | -11.05 | 96.89 | 120.10 |
| 4 | X | 486 | GLU | N-CA-CB | 11.05 | 130.49 | 110.60 |
| 4 | X | 243 | TYR | N-CA-CB | 11.04 | 130.48 | 110.60 |
| 4 | F | 243 | TYR | N-CA-CB | 11.04 | 130.46 | 110.60 |
| 4 | L | 451 | GLU | CA-C-O | 11.03 | 143.26 | 120.10 |
| 4 | X | 451 | GLU | CA-C-O | 11.03 | 143.26 | 120.10 |
| 4 | R | 243 | TYR | N-CA-CB | 11.03 | 130.45 | 110.60 |
| 4 | F | 451 | GLU | CA-C-O | 11.02 | 143.24 | 120.10 |
| 4 | R | 486 | GLU | N-CA-CB | 11.02 | 130.43 | 110.60 |
| 4 | R | 451 | GLU | CA-C-O | 11.01 | 143.23 | 120.10 |
| 4 | F | 486 | GLU | N-CA-CB | 11.01 | 130.42 | 110.60 |
| 6 | Z | 494 | LEU | C-N-CA | -11.00 | 94.20 | 121.70 |
| 6 | H | 494 | LEU | C-N-CA | -10.99 | 94.22 | 121.70 |
| 6 | N | 494 | LEU | C-N-CA | -10.98 | 94.24 | 121.70 |
| 6 | T | 494 | LEU | C-N-CA | -10.98 | 94.24 | 121.70 |
| 3 | P | 1491 | ILE | N-CA-C | 10.96 | 140.59 | 111.00 |
| 3 | D | 1491 | ILE | N-CA-C | 10.96 | 140.59 | 111.00 |
| 4 | R | 420 | GLU | CA-C-N | -10.93 | 93.15 | 117.20 |
| 4 | F | 235 | ASP | C-N-CA | 10.92 | 149.00 | 121.70 |
| 4 | L | 420 | GLU | CA-C-N | -10.92 | 93.17 | 117.20 |
| 4 | F | 420 | GLU | CA-C-N | -10.92 | 93.18 | 117.20 |
| 4 | X | 420 | GLU | CA-C-N | -10.91 | 93.19 | 117.20 |
| 4 | X | 235 | ASP | C-N-CA | 10.90 | 148.96 | 121.70 |
| 4 | R | 235 | ASP | C-N-CA | 10.90 | 148.94 | 121.70 |
| 4 | L | 235 | ASP | C-N-CA | 10.89 | 148.92 | 121.70 |
| 4 | R | 328 | VAL | CA-C-N | 10.88 | 137.97 | 116.20 |
| 4 | L | 328 | VAL | CA-C-N | 10.87 | 137.93 | 116.20 |
| 4 | X | 328 | VAL | CA-C-N | 10.85 | 137.91 | 116.20 |
| 4 | F | 328 | VAL | CA-C-N | 10.84 | 137.88 | 116.20 |
| 4 | X | 423 | ALA | C-N-CA | -10.84 | 76.49 | 122.00 |
| 4 | R | 423 | ALA | C-N-CA | -10.83 | 76.50 | 122.00 |
| 4 | F | 423 | ALA | C-N-CA | -10.83 | 76.51 | 122.00 |
| 4 | L | 423 | ALA | C-N-CA | -10.83 | 76.51 | 122.00 |
| 5 | G | 379 | HIS | O-C-N | -10.81 | 105.40 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 379 | HIS | O-C-N | -10.81 | 105.40 | 122.70 |
| 5 | Y | 379 | HIS | O-C-N | -10.80 | 105.42 | 122.70 |
| 2 | U | 6 | PHE | CB-CA-C | 10.80 | 132.00 | 110.40 |
| 5 | S | 379 | HIS | O-C-N | -10.80 | 105.42 | 122.70 |
| 2 | C | 6 | PHE | CB-CA-C | 10.79 | 131.99 | 110.40 |
| 2 | I | 6 | PHE | CB-CA-C | 10.79 | 131.98 | 110.40 |
| 2 | O | 6 | PHE | CB-CA-C | 10.78 | 131.97 | 110.40 |
| 4 | L | 462 | GLU | N-CA-CB | 10.77 | 129.99 | 110.60 |
| 4 | F | 462 | GLU | N-CA-CB | 10.76 | 129.97 | 110.60 |
| 4 | X | 462 | GLU | N-CA-CB | 10.74 | 129.94 | 110.60 |
| 4 | R | 462 | GLU | N-CA-CB | 10.73 | 129.92 | 110.60 |
| 2 | O | 11 | GLN | CB-CA-C | 10.72 | 131.85 | 110.40 |
| 2 | C | 11 | GLN | CB-CA-C | 10.71 | 131.82 | 110.40 |
| 2 | I | 11 | GLN | CB-CA-C | 10.71 | 131.81 | 110.40 |
| 2 | U | 11 | GLN | CB-CA-C | 10.69 | 131.78 | 110.40 |
| 4 | L | 144 | LEU | CB-CA-C | -10.69 | 89.89 | 110.20 |
| 4 | R | 144 | LEU | CB-CA-C | -10.67 | 89.93 | 110.20 |
| 5 | Y | 378 | SER | CA-C-N | 10.66 | 140.66 | 117.20 |
| 4 | F | 144 | LEU | CB-CA-C | -10.66 | 89.95 | 110.20 |
| 5 | M | 378 | SER | CA-C-N | 10.65 | 140.64 | 117.20 |
| 5 | S | 378 | SER | CA-C-N | 10.65 | 140.64 | 117.20 |
| 5 | G | 378 | SER | CA-C-N | 10.65 | 140.63 | 117.20 |
| 4 | X | 144 | LEU | CB-CA-C | -10.65 | 89.97 | 110.20 |
| 2 | U | 7 | GLY | CA-C-O | -10.60 | 101.52 | 120.60 |
| 2 | I | 7 | GLY | CA-C-O | -10.59 | 101.54 | 120.60 |
| 2 | C | 7 | GLY | CA-C-O | -10.56 | 101.59 | 120.60 |
| 2 | O | 7 | GLY | CA-C-O | -10.55 | 101.62 | 120.60 |
| 4 | X | 208 | GLN | N-CA-CB | 10.54 | 129.57 | 110.60 |
| 4 | L | 208 | GLN | N-CA-CB | 10.54 | 129.57 | 110.60 |
| 6 | Z | 405 | ASP | CB-CA-C | -10.54 | 89.33 | 110.40 |
| 6 | N | 405 | ASP | CB-CA-C | -10.53 | 89.34 | 110.40 |
| 6 | H | 405 | ASP | CB-CA-C | -10.52 | 89.37 | 110.40 |
| 6 | T | 405 | ASP | CB-CA-C | -10.52 | 89.37 | 110.40 |
| 4 | R | 208 | GLN | N-CA-CB | 10.48 | 129.46 | 110.60 |
| 4 | F | 208 | GLN | N-CA-CB | 10.47 | 129.45 | 110.60 |
| 3 | P | 1508 | LYS | CA-C-N | -10.46 | 94.18 | 117.20 |
| 5 | Y | 341 | ALA | O-C-N | 10.46 | 140.98 | 121.10 |
| 3 | D | 1508 | LYS | CA-C-N | -10.46 | 94.19 | 117.20 |
| 4 | L | 466 | HIS | C-N-CA | -10.46 | 95.56 | 121.70 |
| 4 | X | 448 | ARG | CA-C-O | 10.45 | 142.05 | 120.10 |
| 4 | R | 466 | HIS | C-N-CA | -10.45 | 95.58 | 121.70 |
| 4 | F | 448 | ARG | CA-C-O | 10.44 | 142.03 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 341 | ALA | O-C-N | 10.44 | 140.94 | 121.10 |
| 4 | F | 466 | HIS | C-N-CA | -10.44 | 95.60 | 121.70 |
| 4 | X | 466 | HIS | C-N-CA | -10.43 | 95.62 | 121.70 |
| 5 | G | 341 | ALA | O-C-N | 10.43 | 140.91 | 121.10 |
| 4 | R | 448 | ARG | CA-C-O | 10.42 | 141.99 | 120.10 |
| 4 | L | 448 | ARG | CA-C-O | 10.42 | 141.98 | 120.10 |
| 6 | Z | 493 | ALA | C-N-CA | 10.42 | 147.75 | 121.70 |
| 6 | N | 493 | ALA | C-N-CA | 10.41 | 147.73 | 121.70 |
| 6 | T | 493 | ALA | C-N-CA | 10.40 | 147.71 | 121.70 |
| 6 | H | 493 | ALA | C-N-CA | 10.40 | 147.69 | 121.70 |
| 5 | S | 341 | ALA | O-C-N | 10.39 | 140.85 | 121.10 |
| 4 | L | 222 | THR | C-N-CA | 10.30 | 147.46 | 121.70 |
| 4 | R | 222 | THR | C-N-CA | 10.30 | 147.46 | 121.70 |
| 4 | L | 402 | ALA | CA-C-O | 10.30 | 141.73 | 120.10 |
| 4 | F | 222 | THR | C-N-CA | 10.29 | 147.42 | 121.70 |
| 4 | X | 222 | THR | C-N-CA | 10.29 | 147.42 | 121.70 |
| 4 | X | 402 | ALA | CA-C-O | 10.28 | 141.69 | 120.10 |
| 4 | R | 402 | ALA | CA-C-O | 10.25 | 141.63 | 120.10 |
| 4 | X | 484 | ASP | C-N-CA | -10.25 | 96.07 | 121.70 |
| 4 | F | 402 | ALA | CA-C-O | 10.24 | 141.62 | 120.10 |
| 4 | L | 484 | ASP | C-N-CA | -10.23 | 96.12 | 121.70 |
| 4 | F | 484 | ASP | C-N-CA | -10.23 | 96.14 | 121.70 |
| 4 | R | 484 | ASP | C-N-CA | -10.22 | 96.14 | 121.70 |
| 3 | P | 1541 | THR | CA-C-O | 10.21 | 141.54 | 120.10 |
| 3 | D | 1541 | THR | CA-C-O | 10.20 | 141.53 | 120.10 |
| 4 | X | 235 | ASP | CA-C-N | 10.17 | 139.57 | 117.20 |
| 4 | F | 235 | ASP | CA-C-N | 10.15 | 139.54 | 117.20 |
| 4 | L | 235 | ASP | CA-C-N | 10.15 | 139.53 | 117.20 |
| 6 | Z | 487 | TRP | CA-C-N | -10.12 | 94.93 | 117.20 |
| 6 | N | 487 | TRP | CA-C-N | -10.12 | 94.94 | 117.20 |
| 3 | P | 1486 | CYS | C-N-CA | -10.11 | 96.43 | 121.70 |
| 3 | D | 1486 | CYS | C-N-CA | -10.10 | 96.44 | 121.70 |
| 4 | R | 397 | ARG | O-C-N | -10.10 | 106.54 | 122.70 |
| 4 | R | 235 | ASP | CA-C-N | 10.09 | 139.41 | 117.20 |
| 6 | H | 487 | TRP | CA-C-N | -10.09 | 95.00 | 117.20 |
| 6 | T | 487 | TRP | CA-C-N | -10.09 | 95.00 | 117.20 |
| 4 | L | 397 | ARG | O-C-N | -10.08 | 106.58 | 122.70 |
| 1 | K | 259 | SER | O-C-N | -10.07 | 106.59 | 122.70 |
| 4 | X | 397 | ARG | O-C-N | -10.07 | 106.59 | 122.70 |
| 3 | D | 1520 | GLY | O-C-N | 10.07 | 138.81 | 122.70 |
| 3 | P | 1520 | GLY | O-C-N | 10.06 | 138.80 | 122.70 |
| 1 | B | 259 | SER | O-C-N | -10.06 | 106.60 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 397 | ARG | O-C-N | -10.06 | 106.60 | 122.70 |
| 4 | R | 320 | GLU | C-N-CA | -10.06 | 96.55 | 121.70 |
| 1 | E | 259 | SER | O-C-N | -10.06 | 106.61 | 122.70 |
| 4 | F | 320 | GLU | C-N-CA | -10.05 | 96.58 | 121.70 |
| 4 | X | 320 | GLU | C-N-CA | -10.05 | 96.58 | 121.70 |
| 1 | W | 259 | SER | O-C-N | -10.05 | 106.62 | 122.70 |
| 1 | Q | 259 | SER | O-C-N | -10.04 | 106.63 | 122.70 |
| 4 | L | 320 | GLU | C-N-CA | -10.03 | 96.62 | 121.70 |
| 1 | A | 259 | SER | O-C-N | -10.03 | 106.65 | 122.70 |
| 4 | R | 443 | HIS | CA-C-O | 10.02 | 141.13 | 120.10 |
| 4 | X | 305 | ASP | CB-CA-C | 10.01 | 130.42 | 110.40 |
| 5 | G | 330 | LYS | O-C-N | -10.00 | 106.70 | 122.70 |
| 4 | X | 443 | HIS | CA-C-O | 10.00 | 141.10 | 120.10 |
| 5 | S | 330 | LYS | O-C-N | -10.00 | 106.70 | 122.70 |
| 5 | Y | 330 | LYS | O-C-N | -9.99 | 106.71 | 122.70 |
| 4 | F | 443 | HIS | CA-C-O | 9.99 | 141.08 | 120.10 |
| 4 | L | 443 | HIS | CA-C-O | 9.99 | 141.07 | 120.10 |
| 3 | P | 1513 | LEU | C-N-CA | -9.99 | 96.74 | 121.70 |
| 3 | D | 1513 | LEU | C-N-CA | -9.98 | 96.74 | 121.70 |
| 4 | L | 305 | ASP | CB-CA-C | 9.98 | 130.36 | 110.40 |
| 4 | L | 456 | ASP | C-N-CA | -9.98 | 96.75 | 121.70 |
| 4 | R | 305 | ASP | CB-CA-C | 9.98 | 130.36 | 110.40 |
| 4 | F | 305 | ASP | CB-CA-C | 9.98 | 130.36 | 110.40 |
| 5 | M | 330 | LYS | O-C-N | -9.98 | 106.73 | 122.70 |
| 4 | F | 456 | ASP | C-N-CA | -9.97 | 96.78 | 121.70 |
| 4 | R | 456 | ASP | C-N-CA | -9.96 | 96.80 | 121.70 |
| 4 | X | 456 | ASP | C-N-CA | -9.96 | 96.80 | 121.70 |
| 4 | X | 399 | SER | CA-C-O | 9.95 | 140.99 | 120.10 |
| 4 | F | 399 | SER | CA-C-O | 9.94 | 140.97 | 120.10 |
| 4 | L | 399 | SER | CA-C-O | 9.93 | 140.96 | 120.10 |
| 4 | R | 399 | SER | CA-C-O | 9.93 | 140.94 | 120.10 |
| 6 | T | 490 | GLN | C-N-CA | -9.91 | 96.93 | 121.70 |
| 4 | R | 328 | VAL | C-N-CA | 9.90 | 143.10 | 122.30 |
| 6 | Z | 490 | GLN | C-N-CA | -9.90 | 96.94 | 121.70 |
| 6 | N | 490 | GLN | C-N-CA | -9.90 | 96.95 | 121.70 |
| 6 | H | 490 | GLN | C-N-CA | -9.89 | 96.97 | 121.70 |
| 4 | X | 328 | VAL | C-N-CA | 9.89 | 143.06 | 122.30 |
| 4 | L | 328 | VAL | C-N-CA | 9.88 | 143.05 | 122.30 |
| 4 | F | 328 | VAL | C-N-CA | 9.88 | 143.05 | 122.30 |
| 6 | N | 356 | THR | N-CA-CB | 9.85 | 129.02 | 110.30 |
| 6 | H | 356 | THR | N-CA-CB | 9.85 | 129.01 | 110.30 |
| 6 | T | 356 | THR | N-CA-CB | 9.85 | 129.01 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 356 | THR | N-CA-CB | 9.84 | 128.99 | 110.30 |
| 6 | H | 409 | PRO | N-CA-CB | 9.83 | 115.10 | 103.30 |
| 6 | Z | 409 | PRO | N-CA-CB | 9.83 | 115.10 | 103.30 |
| 3 | D | 1510 | GLN | CA-C-N | -9.82 | 95.59 | 117.20 |
| 6 | T | 409 | PRO | N-CA-CB | 9.82 | 115.08 | 103.30 |
| 3 | P | 1510 | GLN | CA-C-N | -9.82 | 95.60 | 117.20 |
| 6 | N | 409 | PRO | N-CA-CB | 9.80 | 115.06 | 103.30 |
| 5 | G | 339 | TYR | N-CA-CB | 9.79 | 128.22 | 110.60 |
| 5 | S | 339 | TYR | N-CA-CB | 9.78 | 128.21 | 110.60 |
| 5 | Y | 339 | TYR | N-CA-CB | 9.78 | 128.21 | 110.60 |
| 4 | R | 395 | ILE | O-C-N | -9.76 | 107.09 | 122.70 |
| 4 | F | 395 | ILE | O-C-N | -9.75 | 107.10 | 122.70 |
| 5 | M | 339 | TYR | N-CA-CB | 9.75 | 128.15 | 110.60 |
| 4 | L | 395 | ILE | O-C-N | -9.75 | 107.10 | 122.70 |
| 4 | X | 395 | ILE | O-C-N | -9.74 | 107.11 | 122.70 |
| 4 | L | 235 | ASP | N-CA-CB | -9.72 | 93.10 | 110.60 |
| 4 | X | 235 | ASP | N-CA-CB | -9.72 | 93.11 | 110.60 |
| 3 | D | 1488 | GLY | CA-C-N | -9.71 | 95.83 | 117.20 |
| 4 | F | 235 | ASP | N-CA-CB | -9.71 | 93.12 | 110.60 |
| 3 | P | 1488 | GLY | CA-C-N | -9.71 | 95.84 | 117.20 |
| 4 | F | 394 | GLU | CB-CA-C | -9.70 | 91.00 | 110.40 |
| 4 | R | 235 | ASP | N-CA-CB | -9.69 | 93.16 | 110.60 |
| 4 | R | 394 | GLU | CB-CA-C | -9.69 | 91.02 | 110.40 |
| 4 | X | 394 | GLU | CB-CA-C | -9.68 | 91.03 | 110.40 |
| 6 | H | 411 | GLU | C-N-CA | 9.68 | 145.90 | 121.70 |
| 6 | N | 411 | GLU | C-N-CA | 9.68 | 145.90 | 121.70 |
| 4 | L | 394 | GLU | CB-CA-C | -9.68 | 91.05 | 110.40 |
| 6 | T | 411 | GLU | C-N-CA | 9.67 | 145.88 | 121.70 |
| 3 | P | 1511 | GLN | O-C-N | 9.67 | 138.17 | 122.70 |
| 5 | Y | 320 | LYS | N-CA-C | 9.67 | 137.10 | 111.00 |
| 5 | M | 320 | LYS | N-CA-C | 9.66 | 137.09 | 111.00 |
| 5 | S | 320 | LYS | N-CA-C | 9.66 | 137.08 | 111.00 |
| 6 | Z | 411 | GLU | C-N-CA | 9.66 | 145.84 | 121.70 |
| 5 | G | 320 | LYS | N-CA-C | 9.65 | 137.05 | 111.00 |
| 3 | D | 1511 | GLN | O-C-N | 9.64 | 138.13 | 122.70 |
| 6 | Z | 462 | GLY | C-N-CA | 9.61 | 145.72 | 121.70 |
| 4 | R | 487 | ASP | N-CA-C | -9.61 | 85.06 | 111.00 |
| 4 | F | 487 | ASP | N-CA-C | -9.61 | 85.07 | 111.00 |
| 4 | X | 487 | ASP | N-CA-C | -9.60 | 85.07 | 111.00 |
| 6 | H | 462 | GLY | C-N-CA | 9.60 | 145.69 | 121.70 |
| 6 | T | 462 | GLY | C-N-CA | 9.60 | 145.69 | 121.70 |
| 6 | N | 462 | GLY | C-N-CA | 9.59 | 145.69 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 487 | ASP | N-CA-C | -9.59 | 85.11 | 111.00 |
| 6 | N | 374 | SER | CB-CA-C | -9.56 | 91.93 | 110.10 |
| 6 | H | 374 | SER | CB-CA-C | -9.55 | 91.96 | 110.10 |
| 6 | Z | 374 | SER | CB-CA-C | -9.54 | 91.97 | 110.10 |
| 5 | G | 339 | TYR | CA-C-O | -9.53 | 100.09 | 120.10 |
| 6 | T | 374 | SER | CB-CA-C | -9.53 | 92.00 | 110.10 |
| 3 | D | 1506 | VAL | CA-C-N | -9.52 | 96.27 | 117.20 |
| 3 | P | 1511 | GLN | CA-C-N | -9.51 | 96.28 | 117.20 |
| 3 | P | 1485 | ALA | C-N-CA | -9.51 | 97.93 | 121.70 |
| 3 | D | 1485 | ALA | C-N-CA | -9.51 | 97.94 | 121.70 |
| 3 | D | 1511 | GLN | CA-C-N | -9.50 | 96.29 | 117.20 |
| 4 | L | 462 | GLU | CB-CA-C | -9.49 | 91.41 | 110.40 |
| 5 | S | 339 | TYR | CA-C-O | -9.49 | 100.17 | 120.10 |
| 4 | F | 462 | GLU | CB-CA-C | -9.49 | 91.42 | 110.40 |
| 3 | P | 1506 | VAL | CA-C-N | -9.49 | 96.32 | 117.20 |
| 5 | M | 339 | TYR | CA-C-O | -9.48 | 100.19 | 120.10 |
| 5 | Y | 339 | TYR | CA-C-O | -9.48 | 100.19 | 120.10 |
| 3 | P | 1484 | ASP | O-C-N | 9.47 | 137.85 | 122.70 |
| 4 | R | 462 | GLU | CB-CA-C | -9.47 | 91.46 | 110.40 |
| 3 | D | 1484 | ASP | O-C-N | 9.46 | 137.84 | 122.70 |
| 4 | X | 462 | GLU | CB-CA-C | -9.44 | 91.52 | 110.40 |
| 4 | R | 327 | MET | CB-CA-C | -9.43 | 91.54 | 110.40 |
| 6 | Z | 405 | ASP | N-CA-C | -9.43 | 85.55 | 111.00 |
| 4 | X | 398 | LYS | C-N-CA | -9.43 | 98.13 | 121.70 |
| 6 | N | 405 | ASP | N-CA-C | -9.43 | 85.55 | 111.00 |
| 6 | T | 405 | ASP | N-CA-C | -9.42 | 85.56 | 111.00 |
| 4 | X | 327 | MET | CB-CA-C | -9.42 | 91.56 | 110.40 |
| 4 | F | 327 | MET | CB-CA-C | -9.41 | 91.57 | 110.40 |
| 4 | L | 327 | MET | CB-CA-C | -9.41 | 91.58 | 110.40 |
| 4 | L | 367 | THR | CA-C-N | 9.41 | 137.91 | 117.20 |
| 4 | F | 367 | THR | CA-C-N | 9.41 | 137.90 | 117.20 |
| 6 | H | 405 | ASP | N-CA-C | -9.41 | 85.60 | 111.00 |
| 4 | X | 367 | THR | CA-C-N | 9.41 | 137.90 | 117.20 |
| 4 | F | 398 | LYS | C-N-CA | -9.40 | 98.19 | 121.70 |
| 4 | R | 398 | LYS | C-N-CA | -9.40 | 98.19 | 121.70 |
| 4 | X | 221 | GLN | N-CA-C | 9.40 | 136.38 | 111.00 |
| 4 | L | 221 | GLN | N-CA-C | 9.39 | 136.36 | 111.00 |
| 4 | R | 367 | THR | CA-C-N | 9.39 | 137.86 | 117.20 |
| 4 | L | 398 | LYS | C-N-CA | -9.38 | 98.24 | 121.70 |
| 4 | F | 423 | ALA | N-CA-C | 9.38 | 136.32 | 111.00 |
| 4 | R | 221 | GLN | N-CA-C | 9.38 | 136.32 | 111.00 |
| 3 | P | 1474 | GLY | C-N-CA | -9.37 | 98.27 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 423 | ALA | N-CA-C | 9.37 | 136.29 | 111.00 |
| 4 | F | 221 | GLN | N-CA-C | 9.36 | 136.28 | 111.00 |
| 3 | D | 1474 | GLY | C-N-CA | -9.36 | 98.29 | 121.70 |
| 4 | X | 210 | VAL | CB-CA-C | 9.36 | 129.19 | 111.40 |
| 4 | R | 210 | VAL | CB-CA-C | 9.35 | 129.17 | 111.40 |
| 4 | X | 423 | ALA | N-CA-C | 9.35 | 136.25 | 111.00 |
| 4 | F | 210 | VAL | CB-CA-C | 9.33 | 129.13 | 111.40 |
| 4 | R | 423 | ALA | N-CA-C | 9.33 | 136.19 | 111.00 |
| 4 | X | 419 | GLY | CA-C-O | -9.33 | 103.81 | 120.60 |
| 4 | L | 210 | VAL | CB-CA-C | 9.32 | 129.10 | 111.40 |
| 4 | R | 402 | ALA | CA-C-N | -9.31 | 96.71 | 117.20 |
| 4 | X | 402 | ALA | CA-C-N | -9.31 | 96.71 | 117.20 |
| 5 | Y | 401 | ALA | N-CA-CB | 9.31 | 123.14 | 110.10 |
| 4 | L | 402 | ALA | CA-C-N | -9.31 | 96.73 | 117.20 |
| 4 | F | 221 | GLN | CA-C-O | -9.30 | 100.57 | 120.10 |
| 4 | L | 419 | GLY | CA-C-O | -9.30 | 103.86 | 120.60 |
| 4 | F | 419 | GLY | CA-C-O | -9.30 | 103.86 | 120.60 |
| 4 | R | 419 | GLY | CA-C-O | -9.29 | 103.88 | 120.60 |
| 4 | X | 221 | GLN | CA-C-O | -9.29 | 100.59 | 120.10 |
| 4 | L | 221 | GLN | CA-C-O | -9.29 | 100.60 | 120.10 |
| 4 | R | 405 | ALA | CB-CA-C | -9.29 | 96.17 | 110.10 |
| 4 | F | 402 | ALA | CA-C-N | -9.28 | 96.78 | 117.20 |
| 4 | R | 221 | GLN | CA-C-O | -9.28 | 100.60 | 120.10 |
| 5 | S | 401 | ALA | N-CA-CB | 9.28 | 123.09 | 110.10 |
| 4 | F | 405 | ALA | CB-CA-C | -9.28 | 96.19 | 110.10 |
| 4 | X | 405 | ALA | CB-CA-C | -9.27 | 96.20 | 110.10 |
| 5 | M | 401 | ALA | N-CA-CB | 9.26 | 123.06 | 110.10 |
| 5 | G | 401 | ALA | N-CA-CB | 9.25 | 123.05 | 110.10 |
| 4 | L | 405 | ALA | CB-CA-C | -9.24 | 96.23 | 110.10 |
| 5 | G | 385 | LEU | CB-CA-C | -9.21 | 92.71 | 110.20 |
| 5 | M | 385 | LEU | CB-CA-C | -9.19 | 92.74 | 110.20 |
| 5 | S | 385 | LEU | CB-CA-C | -9.17 | 92.77 | 110.20 |
| 5 | Y | 385 | LEU | CB-CA-C | -9.17 | 92.78 | 110.20 |
| 6 | H | 412 | GLU | CB-CA-C | -9.16 | 92.07 | 110.40 |
| 6 | N | 412 | GLU | CB-CA-C | -9.15 | 92.11 | 110.40 |
| 6 | Z | 412 | GLU | CB-CA-C | -9.14 | 92.11 | 110.40 |
| 6 | T | 412 | GLU | CB-CA-C | -9.13 | 92.13 | 110.40 |
| 6 | N | 366 | ILE | N-CA-CB | 9.12 | 131.77 | 110.80 |
| 6 | H | 374 | SER | N-CA-CB | -9.11 | 96.83 | 110.50 |
| 6 | H | 366 | ILE | N-CA-CB | 9.10 | 131.73 | 110.80 |
| 5 | Y | 379 | HIS | CA-C-O | -9.10 | 100.99 | 120.10 |
| 6 | N | 374 | SER | N-CA-CB | -9.10 | 96.86 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 366 | ILE | N-CA-CB | 9.09 | 131.72 | 110.80 |
| 6 | Z | 374 | SER | N-CA-CB | -9.09 | 96.86 | 110.50 |
| 6 | T | 366 | ILE | N-CA-CB | 9.09 | 131.70 | 110.80 |
| 5 | M | 379 | HIS | CA-C-O | -9.09 | 101.02 | 120.10 |
| 7 | V | 1387 | SER | N-CA-C | -9.09 | 86.47 | 111.00 |
| 5 | S | 379 | HIS | CA-C-O | -9.08 | 101.03 | 120.10 |
| 5 | G | 379 | HIS | CA-C-O | -9.08 | 101.03 | 120.10 |
| 7 | J | 1387 | SER | N-CA-C | -9.07 | 86.51 | 111.00 |
| 5 | Y | 337 | HIS | O-C-N | -9.04 | 108.23 | 122.70 |
| 4 | F | 303 | GLY | N-CA-C | -9.03 | 90.53 | 113.10 |
| 5 | S | 337 | HIS | O-C-N | -9.02 | 108.26 | 122.70 |
| 4 | X | 303 | GLY | N-CA-C | -9.02 | 90.55 | 113.10 |
| 5 | G | 337 | HIS | O-C-N | -9.02 | 108.28 | 122.70 |
| 2 | I | 5 | GLY | O-C-N | -9.02 | 108.28 | 122.70 |
| 6 | T | 374 | SER | N-CA-CB | -9.02 | 96.97 | 110.50 |
| 2 | U | 5 | GLY | O-C-N | -9.02 | 108.27 | 122.70 |
| 5 | M | 337 | HIS | O-C-N | -9.01 | 108.28 | 122.70 |
| 4 | R | 303 | GLY | N-CA-C | -9.00 | 90.59 | 113.10 |
| 4 | F | 401 | TYR | N-CA-CB | 8.99 | 126.79 | 110.60 |
| 2 | O | 5 | GLY | O-C-N | -8.99 | 108.31 | 122.70 |
| 4 | X | 486 | GLU | O-C-N | 8.99 | 137.09 | 122.70 |
| 2 | C | 5 | GLY | O-C-N | -8.99 | 108.32 | 122.70 |
| 4 | L | 451 | GLU | N-CA-C | 8.98 | 135.26 | 111.00 |
| 4 | R | 451 | GLU | N-CA-C | 8.98 | 135.26 | 111.00 |
| 4 | F | 486 | GLU | O-C-N | 8.98 | 137.07 | 122.70 |
| 4 | L | 303 | GLY | N-CA-C | -8.98 | 90.65 | 113.10 |
| 4 | X | 401 | TYR | N-CA-CB | 8.98 | 126.77 | 110.60 |
| 4 | R | 486 | GLU | O-C-N | 8.98 | 137.06 | 122.70 |
| 4 | L | 486 | GLU | O-C-N | 8.97 | 137.06 | 122.70 |
| 4 | L | 401 | TYR | N-CA-CB | 8.97 | 126.75 | 110.60 |
| 4 | R | 401 | TYR | N-CA-CB | 8.97 | 126.75 | 110.60 |
| 4 | L | 424 | PRO | O-C-N | 8.96 | 137.04 | 122.70 |
| 4 | R | 423 | ALA | O-C-N | 8.96 | 138.13 | 121.10 |
| 4 | F | 451 | GLU | N-CA-C | 8.95 | 135.17 | 111.00 |
| 6 | Z | 411 | GLU | CA-C-O | -8.95 | 101.30 | 120.10 |
| 4 | X | 451 | GLU | N-CA-C | 8.95 | 135.17 | 111.00 |
| 5 | M | 347 | ARG | C-N-CA | -8.94 | 99.35 | 121.70 |
| 6 | T | 411 | GLU | CA-C-O | -8.94 | 101.33 | 120.10 |
| 6 | N | 411 | GLU | CA-C-O | -8.94 | 101.33 | 120.10 |
| 5 | S | 347 | ARG | C-N-CA | -8.94 | 99.36 | 121.70 |
| 5 | G | 347 | ARG | C-N-CA | -8.93 | 99.37 | 121.70 |
| 4 | F | 305 | ASP | N-CA-CB | 8.93 | 126.67 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 305 | ASP | N-CA-CB | 8.93 | 126.67 | 110.60 |
| 4 | X | 424 | PRO | O-C-N | 8.93 | 136.99 | 122.70 |
| 5 | Y | 347 | ARG | C-N-CA | -8.93 | 99.38 | 121.70 |
| 4 | R | 424 | PRO | O-C-N | 8.93 | 136.98 | 122.70 |
| 4 | X | 423 | ALA | O-C-N | 8.93 | 138.06 | 121.10 |
| 4 | F | 424 | PRO | O-C-N | 8.92 | 136.98 | 122.70 |
| 6 | H | 411 | GLU | CA-C-O | -8.92 | 101.36 | 120.10 |
| 4 | R | 305 | ASP | N-CA-CB | 8.92 | 126.66 | 110.60 |
| 4 | X | 305 | ASP | N-CA-CB | 8.92 | 126.66 | 110.60 |
| 4 | L | 423 | ALA | O-C-N | 8.90 | 138.01 | 121.10 |
| 5 | S | 324 | ILE | CB-CA-C | -8.90 | 93.80 | 111.60 |
| 3 | P | 1509 | GLN | CA-C-N | -8.90 | 97.63 | 117.20 |
| 3 | D | 1509 | GLN | CA-C-N | -8.89 | 97.63 | 117.20 |
| 5 | M | 324 | ILE | CB-CA-C | -8.89 | 93.81 | 111.60 |
| 5 | G | 324 | ILE | CB-CA-C | -8.89 | 93.82 | 111.60 |
| 2 | I | 5 | GLY | N-CA-C | 8.89 | 135.32 | 113.10 |
| 4 | F | 423 | ALA | O-C-N | 8.88 | 137.98 | 121.10 |
| 5 | Y | 324 | ILE | CB-CA-C | -8.88 | 93.84 | 111.60 |
| 5 | G | 329 | GLN | CA-C-O | -8.88 | 101.45 | 120.10 |
| 4 | R | 454 | TYR | CA-C-N | -8.88 | 97.67 | 117.20 |
| 5 | S | 324 | ILE | O-C-N | 8.88 | 136.91 | 122.70 |
| 5 | Y | 329 | GLN | CA-C-O | -8.88 | 101.46 | 120.10 |
| 2 | C | 5 | GLY | N-CA-C | 8.88 | 135.29 | 113.10 |
| 5 | M | 329 | GLN | CA-C-O | -8.88 | 101.46 | 120.10 |
| 5 | S | 329 | GLN | CA-C-O | -8.87 | 101.46 | 120.10 |
| 3 | P | 1511 | GLN | C-N-CA | -8.87 | 99.52 | 121.70 |
| 3 | D | 1511 | GLN | C-N-CA | -8.87 | 99.53 | 121.70 |
| 2 | O | 5 | GLY | N-CA-C | 8.87 | 135.27 | 113.10 |
| 4 | F | 454 | TYR | CA-C-N | -8.86 | 97.70 | 117.20 |
| 2 | U | 5 | GLY | N-CA-C | 8.86 | 135.25 | 113.10 |
| 5 | G | 324 | ILE | O-C-N | 8.85 | 136.86 | 122.70 |
| 4 | L | 454 | TYR | CA-C-N | -8.85 | 97.73 | 117.20 |
| 4 | R | 431 | LEU | C-N-CA | -8.85 | 99.57 | 121.70 |
| 4 | L | 431 | LEU | C-N-CA | -8.85 | 99.58 | 121.70 |
| 4 | F | 431 | LEU | C-N-CA | -8.85 | 99.58 | 121.70 |
| 4 | X | 454 | TYR | CA-C-N | -8.85 | 97.74 | 117.20 |
| 5 | Y | 324 | ILE | O-C-N | 8.84 | 136.84 | 122.70 |
| 5 | M | 324 | ILE | O-C-N | 8.84 | 136.84 | 122.70 |
| 4 | X | 431 | LEU | C-N-CA | -8.83 | 99.62 | 121.70 |
| 4 | X | 493 | HIS | N-CA-CB | -8.78 | 94.80 | 110.60 |
| 4 | F | 341 | ASP | N-CA-CB | 8.77 | 126.39 | 110.60 |
| 4 | L | 341 | ASP | N-CA-CB | 8.77 | 126.39 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 1542 | PRO | CA-C-O | -8.77 | 99.16 | 120.20 |
| 3 | D | 1542 | PRO | CA-C-O | -8.76 | 99.17 | 120.20 |
| 4 | R | 341 | ASP | N-CA-CB | 8.76 | 126.37 | 110.60 |
| 4 | F | 493 | HIS | N-CA-CB | -8.76 | 94.83 | 110.60 |
| 4 | X | 341 | ASP | N-CA-CB | 8.76 | 126.36 | 110.60 |
| 4 | L | 493 | HIS | N-CA-CB | -8.75 | 94.85 | 110.60 |
| 4 | R | 493 | HIS | N-CA-CB | -8.75 | 94.85 | 110.60 |
| 4 | L | 425 | THR | O-C-N | 8.73 | 136.66 | 122.70 |
| 6 | H | 487 | TRP | N-CA-C | 8.71 | 134.52 | 111.00 |
| 4 | F | 220 | ASN | CA-C-O | -8.71 | 101.81 | 120.10 |
| 4 | L | 220 | ASN | CA-C-O | -8.70 | 101.82 | 120.10 |
| 6 | Z | 487 | TRP | N-CA-C | 8.70 | 134.50 | 111.00 |
| 4 | F | 425 | THR | O-C-N | 8.70 | 136.61 | 122.70 |
| 6 | N | 487 | TRP | N-CA-C | 8.69 | 134.46 | 111.00 |
| 4 | R | 425 | THR | O-C-N | 8.68 | 136.59 | 122.70 |
| 6 | T | 487 | TRP | N-CA-C | 8.68 | 134.43 | 111.00 |
| 4 | X | 220 | ASN | CA-C-O | -8.68 | 101.88 | 120.10 |
| 4 | R | 220 | ASN | CA-C-O | -8.67 | 101.89 | 120.10 |
| 4 | X | 425 | THR | O-C-N | 8.66 | 136.56 | 122.70 |
| 3 | D | 1510 | GLN | C-N-CA | -8.65 | 100.07 | 121.70 |
| 3 | P | 1510 | GLN | C-N-CA | -8.64 | 100.10 | 121.70 |
| 6 | H | 352 | LEU | N-CA-CB | 8.64 | 127.67 | 110.40 |
| 5 | S | 330 | LYS | CB-CA-C | 8.62 | 127.65 | 110.40 |
| 5 | M | 330 | LYS | CB-CA-C | 8.62 | 127.64 | 110.40 |
| 6 | N | 352 | LEU | N-CA-CB | 8.60 | 127.61 | 110.40 |
| 6 | T | 352 | LEU | N-CA-CB | 8.60 | 127.60 | 110.40 |
| 5 | Y | 330 | LYS | CB-CA-C | 8.59 | 127.59 | 110.40 |
| 5 | G | 330 | LYS | CB-CA-C | 8.59 | 127.58 | 110.40 |
| 3 | D | 1490 | GLU | C-N-CA | -8.59 | 100.23 | 121.70 |
| 2 | C | 234 | LEU | N-CA-C | -8.58 | 87.83 | 111.00 |
| 3 | P | 1490 | GLU | C-N-CA | -8.58 | 100.24 | 121.70 |
| 2 | I | 234 | LEU | N-CA-C | -8.58 | 87.83 | 111.00 |
| 2 | U | 234 | LEU | N-CA-C | -8.58 | 87.83 | 111.00 |
| 2 | O | 234 | LEU | N-CA-C | -8.58 | 87.84 | 111.00 |
| 6 | Z | 352 | LEU | N-CA-CB | 8.58 | 127.56 | 110.40 |
| 5 | S | 335 | LEU | O-C-N | -8.56 | 109.01 | 122.70 |
| 2 | C | 15 | GLN | N-CA-CB | 8.54 | 125.98 | 110.60 |
| 3 | D | 1472 | SER | CA-C-N | -8.54 | 98.40 | 117.20 |
| 2 | O | 28 | HIS | CB-CA-C | 8.54 | 127.48 | 110.40 |
| 2 | U | 28 | HIS | CB-CA-C | 8.54 | 127.48 | 110.40 |
| 2 | O | 15 | GLN | N-CA-CB | 8.54 | 125.97 | 110.60 |
| 3 | P | 1472 | SER | CA-C-N | -8.54 | 98.41 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 28 | HIS | CB-CA-C | 8.54 | 127.47 | 110.40 |
| 2 | I | 28 | HIS | CB-CA-C | 8.53 | 127.47 | 110.40 |
| 2 | I | 15 | GLN | N-CA-CB | 8.53 | 125.96 | 110.60 |
| 5 | Y | 378 | SER | C-N-CA | 8.52 | 143.01 | 121.70 |
| 4 | F | 199 | GLU | CA-C-N | -8.52 | 98.45 | 117.20 |
| 5 | G | 335 | LEU | O-C-N | -8.52 | 109.06 | 122.70 |
| 5 | M | 335 | LEU | O-C-N | -8.52 | 109.07 | 122.70 |
| 4 | R | 199 | GLU | CA-C-N | -8.52 | 98.46 | 117.20 |
| 2 | U | 15 | GLN | N-CA-CB | 8.52 | 125.93 | 110.60 |
| 5 | G | 378 | SER | C-N-CA | 8.52 | 142.99 | 121.70 |
| 5 | S | 378 | SER | C-N-CA | 8.52 | 142.99 | 121.70 |
| 5 | Y | 335 | LEU | O-C-N | -8.50 | 109.10 | 122.70 |
| 5 | M | 378 | SER | C-N-CA | 8.49 | 142.94 | 121.70 |
| 4 | X | 199 | GLU | CA-C-N | -8.49 | 98.52 | 117.20 |
| 4 | L | 199 | GLU | CA-C-N | -8.48 | 98.54 | 117.20 |
| 5 | M | 331 | THR | CA-C-O | 8.48 | 137.91 | 120.10 |
| 3 | D | 1519 | SER | CA-C-O | 8.47 | 137.90 | 120.10 |
| 3 | D | 1538 | SER | C-N-CA | 8.47 | 142.89 | 121.70 |
| 2 | I | 250 | VAL | N-CA-CB | -8.47 | 92.86 | 111.50 |
| 2 | C | 250 | VAL | N-CA-CB | -8.46 | 92.88 | 111.50 |
| 2 | O | 250 | VAL | N-CA-CB | -8.46 | 92.89 | 111.50 |
| 3 | P | 1519 | SER | CA-C-O | 8.46 | 137.85 | 120.10 |
| 5 | Y | 331 | THR | CA-C-O | 8.46 | 137.86 | 120.10 |
| 2 | U | 250 | VAL | N-CA-CB | -8.45 | 92.91 | 111.50 |
| 6 | T | 387 | LYS | C-N-CA | -8.45 | 100.59 | 121.70 |
| 5 | G | 331 | THR | CA-C-O | 8.44 | 137.83 | 120.10 |
| 4 | F | 485 | LEU | O-C-N | -8.43 | 109.21 | 122.70 |
| 6 | N | 387 | LYS | C-N-CA | -8.43 | 100.62 | 121.70 |
| 3 | P | 1538 | SER | C-N-CA | 8.42 | 142.76 | 121.70 |
| 6 | Z | 497 | ARG | CB-CA-C | 8.42 | 127.25 | 110.40 |
| 5 | S | 331 | THR | CA-C-O | 8.42 | 137.78 | 120.10 |
| 6 | H | 387 | LYS | C-N-CA | -8.41 | 100.67 | 121.70 |
| 4 | X | 485 | LEU | O-C-N | -8.41 | 109.24 | 122.70 |
| 6 | H | 497 | ARG | CB-CA-C | 8.41 | 127.21 | 110.40 |
| 4 | L | 485 | LEU | O-C-N | -8.41 | 109.25 | 122.70 |
| 4 | R | 485 | LEU | O-C-N | -8.40 | 109.26 | 122.70 |
| 3 | P | 1506 | VAL | CA-C-O | 8.40 | 137.73 | 120.10 |
| 6 | T | 497 | ARG | CB-CA-C | 8.40 | 127.20 | 110.40 |
| 6 | N | 497 | ARG | CB-CA-C | 8.39 | 127.18 | 110.40 |
| 3 | D | 1506 | VAL | CA-C-O | 8.39 | 137.71 | 120.10 |
| 3 | P | 1450 | GLU | C-N-CA | 8.39 | 142.67 | 121.70 |
| 3 | D | 1450 | GLU | C-N-CA | 8.39 | 142.66 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 387 | LYS | C-N-CA | -8.39 | 100.73 | 121.70 |
| 2 | C | 382 | ASN | C-N-CA | 8.38 | 142.64 | 121.70 |
| 4 | L | 367 | THR | C-N-CA | 8.37 | 142.62 | 121.70 |
| 3 | D | 1520 | GLY | C-N-CA | -8.37 | 100.79 | 121.70 |
| 4 | R | 367 | THR | C-N-CA | 8.37 | 142.61 | 121.70 |
| 4 | F | 367 | THR | C-N-CA | 8.36 | 142.61 | 121.70 |
| 2 | U | 382 | ASN | C-N-CA | 8.36 | 142.60 | 121.70 |
| 3 | P | 1492 | GLY | C-N-CA | 8.35 | 142.58 | 121.70 |
| 3 | P | 1520 | GLY | C-N-CA | -8.35 | 100.81 | 121.70 |
| 6 | N | 412 | GLU | CA-C-N | -8.35 | 98.83 | 117.20 |
| 2 | O | 382 | ASN | C-N-CA | 8.35 | 142.58 | 121.70 |
| 3 | D | 1492 | GLY | C-N-CA | 8.35 | 142.57 | 121.70 |
| 4 | X | 367 | THR | C-N-CA | 8.35 | 142.57 | 121.70 |
| 2 | U | 7 | GLY | N-CA-C | -8.35 | 92.24 | 113.10 |
| 4 | X | 484 | ASP | O-C-N | 8.35 | 136.05 | 122.70 |
| 2 | I | 382 | ASN | C-N-CA | 8.34 | 142.56 | 121.70 |
| 4 | F | 222 | THR | CB-CA-C | -8.34 | 89.09 | 111.60 |
| 2 | O | 7 | GLY | N-CA-C | -8.34 | 92.26 | 113.10 |
| 2 | I | 7 | GLY | N-CA-C | -8.34 | 92.26 | 113.10 |
| 6 | Z | 412 | GLU | CA-C-N | -8.33 | 98.87 | 117.20 |
| 6 | H | 412 | GLU | CA-C-N | -8.33 | 98.88 | 117.20 |
| 6 | T | 412 | GLU | CA-C-N | -8.33 | 98.87 | 117.20 |
| 4 | R | 222 | THR | CB-CA-C | -8.32 | 89.14 | 111.60 |
| 2 | C | 7 | GLY | N-CA-C | -8.31 | 92.33 | 113.10 |
| 4 | R | 484 | ASP | O-C-N | 8.31 | 135.99 | 122.70 |
| 4 | X | 222 | THR | CB-CA-C | -8.30 | 89.18 | 111.60 |
| 4 | L | 484 | ASP | O-C-N | 8.30 | 135.98 | 122.70 |
| 4 | F | 484 | ASP | O-C-N | 8.29 | 135.97 | 122.70 |
| 4 | L | 222 | THR | CB-CA-C | -8.29 | 89.22 | 111.60 |
| 6 | N | 416 | GLU | N-CA-CB | 8.21 | 125.37 | 110.60 |
| 6 | H | 416 | GLU | N-CA-CB | 8.20 | 125.35 | 110.60 |
| 6 | H | 468 | SER | N-CA-CB | 8.19 | 122.78 | 110.50 |
| 6 | T | 416 | GLU | N-CA-CB | 8.18 | 125.33 | 110.60 |
| 6 | Z | 416 | GLU | N-CA-CB | 8.17 | 125.31 | 110.60 |
| 6 | T | 468 | SER | N-CA-CB | 8.17 | 122.75 | 110.50 |
| 3 | P | 1517 | SER | C-N-CA | -8.17 | 101.28 | 121.70 |
| 3 | D | 1517 | SER | C-N-CA | -8.16 | 101.29 | 121.70 |
| 6 | N | 468 | SER | N-CA-CB | 8.15 | 122.73 | 110.50 |
| 6 | Z | 468 | SER | N-CA-CB | 8.13 | 122.70 | 110.50 |
| 6 | H | 494 | LEU | N-CA-C | 8.13 | 132.95 | 111.00 |
| 6 | Z | 494 | LEU | N-CA-C | 8.12 | 132.93 | 111.00 |
| 6 | N | 494 | LEU | N-CA-C | 8.12 | 132.91 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | T | 494 | LEU | N-CA-C | 8.11 | 132.89 | 111.00 |
| 3 | D | 1507 | ASP | CA-C-O | -8.10 | 103.08 | 120.10 |
| 3 | P | 1507 | ASP | CA-C-O | -8.10 | 103.09 | 120.10 |
| 4 | R | 443 | HIS | O-C-N | -8.06 | 109.80 | 122.70 |
| 6 | H | 408 | SER | N-CA-C | 8.06 | 132.76 | 111.00 |
| 6 | Z | 408 | SER | N-CA-C | 8.05 | 132.74 | 111.00 |
| 6 | T | 408 | SER | N-CA-C | 8.04 | 132.72 | 111.00 |
| 4 | X | 443 | HIS | O-C-N | -8.04 | 109.83 | 122.70 |
| 3 | P | 1488 | GLY | CA-C-O | 8.04 | 135.07 | 120.60 |
| 3 | P | 1545 | PRO | C-N-CA | 8.04 | 141.79 | 121.70 |
| 4 | L | 427 | PHE | C-N-CA | -8.03 | 101.62 | 121.70 |
| 3 | P | 1510 | GLN | N-CA-C | 8.03 | 132.69 | 111.00 |
| 4 | F | 443 | HIS | O-C-N | -8.03 | 109.86 | 122.70 |
| 3 | D | 1510 | GLN | N-CA-C | 8.03 | 132.67 | 111.00 |
| 3 | D | 1545 | PRO | C-N-CA | 8.02 | 141.76 | 121.70 |
| 4 | F | 427 | PHE | C-N-CA | -8.02 | 101.64 | 121.70 |
| 6 | T | 473 | GLN | CB-CA-C | -8.02 | 94.35 | 110.40 |
| 3 | D | 1488 | GLY | CA-C-O | 8.02 | 135.04 | 120.60 |
| 3 | D | 1487 | ASP | N-CA-C | 8.02 | 132.64 | 111.00 |
| 6 | H | 473 | GLN | CB-CA-C | -8.02 | 94.37 | 110.40 |
| 3 | P | 1489 | HIS | CA-C-O | -8.02 | 103.27 | 120.10 |
| 3 | D | 1489 | HIS | N-CA-CB | -8.01 | 96.17 | 110.60 |
| 3 | D | 1489 | HIS | CA-C-O | -8.01 | 103.27 | 120.10 |
| 6 | N | 408 | SER | N-CA-C | 8.01 | 132.63 | 111.00 |
| 4 | R | 427 | PHE | C-N-CA | -8.01 | 101.67 | 121.70 |
| 6 | Z | 473 | GLN | CB-CA-C | -8.01 | 94.38 | 110.40 |
| 3 | P | 1489 | HIS | N-CA-CB | -8.01 | 96.19 | 110.60 |
| 4 | L | 443 | HIS | O-C-N | -8.00 | 109.89 | 122.70 |
| 6 | N | 473 | GLN | CB-CA-C | -8.00 | 94.39 | 110.40 |
| 5 | S | 331 | THR | CB-CA-C | 8.00 | 133.21 | 111.60 |
| 4 | R | 252 | THR | N-CA-CB | 8.00 | 125.50 | 110.30 |
| 4 | X | 427 | PHE | C-N-CA | -8.00 | 101.70 | 121.70 |
| 6 | N | 411 | GLU | CA-C-N | 8.00 | 134.80 | 117.20 |
| 3 | P | 1487 | ASP | N-CA-C | 8.00 | 132.60 | 111.00 |
| 5 | G | 331 | THR | CB-CA-C | 7.99 | 133.19 | 111.60 |
| 6 | T | 411 | GLU | CA-C-N | 7.99 | 134.78 | 117.20 |
| 5 | M | 331 | THR | CB-CA-C | 7.99 | 133.16 | 111.60 |
| 5 | Y | 328 | THR | C-N-CA | 7.99 | 141.66 | 121.70 |
| 4 | X | 252 | THR | N-CA-CB | 7.98 | 125.47 | 110.30 |
| 6 | Z | 411 | GLU | CA-C-N | 7.98 | 134.76 | 117.20 |
| 4 | L | 252 | THR | N-CA-CB | 7.98 | 125.46 | 110.30 |
| 4 | X | 493 | HIS | CA-C-O | -7.98 | 103.35 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 411 | GLU | CA-C-N | 7.97 | 134.74 | 117.20 |
| 4 | L | 221 | GLN | C-N-CA | 7.97 | 141.63 | 121.70 |
| 5 | Y | 331 | THR | CB-CA-C | 7.97 | 133.12 | 111.60 |
| 4 | F | 221 | GLN | C-N-CA | 7.96 | 141.60 | 121.70 |
| 4 | X | 221 | GLN | C-N-CA | 7.96 | 141.60 | 121.70 |
| 5 | G | 328 | THR | C-N-CA | 7.95 | 141.58 | 121.70 |
| 1 | Q | 259 | SER | C-N-CA | 7.95 | 141.58 | 121.70 |
| 4 | R | 221 | GLN | C-N-CA | 7.95 | 141.57 | 121.70 |
| 5 | S | 328 | THR | C-N-CA | 7.94 | 141.56 | 121.70 |
| 4 | F | 252 | THR | N-CA-CB | 7.94 | 125.39 | 110.30 |
| 4 | R | 493 | HIS | CA-C-O | -7.94 | 103.42 | 120.10 |
| 1 | B | 259 | SER | C-N-CA | 7.94 | 141.55 | 121.70 |
| 5 | M | 328 | THR | C-N-CA | 7.94 | 141.55 | 121.70 |
| 1 | W | 259 | SER | C-N-CA | 7.94 | 141.55 | 121.70 |
| 1 | K | 259 | SER | C-N-CA | 7.94 | 141.54 | 121.70 |
| 1 | E | 259 | SER | C-N-CA | 7.94 | 141.54 | 121.70 |
| 1 | A | 259 | SER | C-N-CA | 7.93 | 141.54 | 121.70 |
| 6 | Z | 381 | LYS | N-CA-CB | -7.93 | 96.32 | 110.60 |
| 6 | N | 381 | LYS | N-CA-CB | -7.93 | 96.32 | 110.60 |
| 4 | X | 439 | ARG | N-CA-CB | 7.93 | 124.88 | 110.60 |
| 6 | H | 381 | LYS | N-CA-CB | -7.93 | 96.33 | 110.60 |
| 4 | F | 439 | ARG | N-CA-CB | 7.92 | 124.86 | 110.60 |
| 4 | R | 439 | ARG | N-CA-CB | 7.92 | 124.86 | 110.60 |
| 6 | T | 381 | LYS | N-CA-CB | -7.92 | 96.35 | 110.60 |
| 4 | X | 485 | LEU | N-CA-CB | -7.91 | 94.57 | 110.40 |
| 4 | L | 493 | HIS | CA-C-O | -7.91 | 103.49 | 120.10 |
| 5 | S | 338 | GLU | CA-C-N | 7.91 | 134.59 | 117.20 |
| 5 | Y | 338 | GLU | CA-C-N | 7.89 | 134.57 | 117.20 |
| 4 | F | 485 | LEU | N-CA-CB | -7.89 | 94.63 | 110.40 |
| 4 | F | 493 | HIS | CA-C-O | -7.88 | 103.54 | 120.10 |
| 4 | L | 439 | ARG | N-CA-CB | 7.88 | 124.79 | 110.60 |
| 5 | G | 338 | GLU | CA-C-N | 7.88 | 134.53 | 117.20 |
| 4 | L | 426 | GLN | O-C-N | 7.87 | 135.29 | 122.70 |
| 4 | R | 485 | LEU | N-CA-CB | -7.87 | 94.66 | 110.40 |
| 4 | L | 485 | LEU | N-CA-CB | -7.87 | 94.66 | 110.40 |
| 5 | M | 338 | GLU | CA-C-N | 7.87 | 134.51 | 117.20 |
| 2 | C | 455 | VAL | N-CA-C | -7.87 | 89.76 | 111.00 |
| 6 | N | 462 | GLY | N-CA-C | 7.86 | 132.75 | 113.10 |
| 4 | L | 425 | THR | CA-C-N | -7.86 | 99.91 | 117.20 |
| 4 | R | 425 | THR | CA-C-N | -7.86 | 99.91 | 117.20 |
| 4 | X | 426 | GLN | O-C-N | 7.86 | 135.27 | 122.70 |
| 2 | I | 455 | VAL | N-CA-C | -7.84 | 89.82 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | O | 455 | VAL | N-CA-C | -7.84 | 89.82 | 111.00 |
| 4 | F | 433 | GLU | CB-CA-C | -7.84 | 94.72 | 110.40 |
| 2 | U | 455 | VAL | N-CA-C | -7.84 | 89.83 | 111.00 |
| 6 | H | 462 | GLY | N-CA-C | 7.84 | 132.69 | 113.10 |
| 5 | G | 326 | LEU | C-N-CA | -7.83 | 102.12 | 121.70 |
| 4 | X | 433 | GLU | CB-CA-C | -7.83 | 94.73 | 110.40 |
| 6 | Z | 462 | GLY | N-CA-C | 7.83 | 132.68 | 113.10 |
| 6 | T | 462 | GLY | N-CA-C | 7.83 | 132.68 | 113.10 |
| 4 | X | 425 | THR | CA-C-N | -7.83 | 99.97 | 117.20 |
| 5 | Y | 326 | LEU | C-N-CA | -7.83 | 102.13 | 121.70 |
| 3 | D | 1518 | ASN | C-N-CA | -7.83 | 102.13 | 121.70 |
| 4 | F | 425 | THR | CA-C-N | -7.83 | 99.98 | 117.20 |
| 5 | G | 366 | GLU | CB-CA-C | -7.82 | 94.75 | 110.40 |
| 4 | L | 433 | GLU | CB-CA-C | -7.82 | 94.75 | 110.40 |
| 4 | F | 426 | GLN | O-C-N | 7.82 | 135.21 | 122.70 |
| 5 | M | 326 | LEU | C-N-CA | -7.82 | 102.15 | 121.70 |
| 3 | P | 1518 | ASN | C-N-CA | -7.82 | 102.15 | 121.70 |
| 5 | S | 326 | LEU | C-N-CA | -7.81 | 102.17 | 121.70 |
| 4 | R | 426 | GLN | O-C-N | 7.80 | 135.19 | 122.70 |
| 5 | Y | 366 | GLU | CB-CA-C | -7.80 | 94.79 | 110.40 |
| 4 | R | 433 | GLU | CB-CA-C | -7.80 | 94.80 | 110.40 |
| 5 | M | 366 | GLU | CB-CA-C | -7.78 | 94.84 | 110.40 |
| 3 | D | 1449 | TRP | C-N-CA | 7.78 | 141.14 | 121.70 |
| 3 | P | 1449 | TRP | C-N-CA | 7.78 | 141.14 | 121.70 |
| 5 | S | 366 | GLU | CB-CA-C | -7.77 | 94.85 | 110.40 |
| 5 | S | 324 | ILE | CA-C-N | -7.77 | 100.11 | 117.20 |
| 5 | Y | 324 | ILE | CA-C-N | -7.77 | 100.11 | 117.20 |
| 5 | G | 324 | ILE | CA-C-N | -7.76 | 100.12 | 117.20 |
| 5 | M | 324 | ILE | CA-C-N | -7.73 | 100.19 | 117.20 |
| 4 | L | 436 | SER | CA-C-O | 7.73 | 136.32 | 120.10 |
| 5 | S | 342 | PRO | C-N-CA | -7.72 | 102.39 | 121.70 |
| 5 | M | 342 | PRO | C-N-CA | -7.71 | 102.42 | 121.70 |
| 5 | G | 342 | PRO | C-N-CA | -7.71 | 102.43 | 121.70 |
| 4 | F | 436 | SER | CA-C-O | 7.71 | 136.28 | 120.10 |
| 5 | Y | 342 | PRO | C-N-CA | -7.70 | 102.45 | 121.70 |
| 4 | L | 482 | LYS | N-CA-CB | 7.70 | 124.45 | 110.60 |
| 4 | F | 482 | LYS | N-CA-CB | 7.70 | 124.45 | 110.60 |
| 4 | X | 436 | SER | CA-C-O | 7.69 | 136.25 | 120.10 |
| 4 | R | 422 | ASN | CA-C-N | -7.68 | 100.31 | 117.20 |
| 4 | L | 422 | ASN | CA-C-N | -7.67 | 100.32 | 117.20 |
| 4 | R | 436 | SER | CA-C-O | 7.67 | 136.22 | 120.10 |
| 4 | X | 482 | LYS | N-CA-CB | 7.67 | 124.42 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 482 | LYS | N-CA-CB | 7.67 | 124.41 | 110.60 |
| 4 | F | 422 | ASN | CA-C-N | -7.66 | 100.35 | 117.20 |
| 4 | L | 211 | GLU | CA-C-N | -7.65 | 100.36 | 117.20 |
| 4 | X | 422 | ASN | CA-C-N | -7.65 | 100.36 | 117.20 |
| 4 | X | 211 | GLU | CA-C-N | -7.64 | 100.38 | 117.20 |
| 6 | Z | 487 | TRP | C-N-CA | -7.62 | 102.64 | 121.70 |
| 6 | N | 487 | TRP | C-N-CA | -7.62 | 102.65 | 121.70 |
| 4 | R | 320 | GLU | CB-CA-C | 7.62 | 125.63 | 110.40 |
| 4 | F | 320 | GLU | CB-CA-C | 7.61 | 125.62 | 110.40 |
| 4 | F | 211 | GLU | CA-C-N | -7.61 | 100.47 | 117.20 |
| 6 | T | 410 | LEU | CA-C-O | -7.61 | 104.12 | 120.10 |
| 4 | R | 211 | GLU | CA-C-N | -7.59 | 100.50 | 117.20 |
| 4 | R | 457 | ALA | CA-C-O | -7.59 | 104.16 | 120.10 |
| 4 | L | 211 | GLU | N-CA-C | 7.58 | 131.48 | 111.00 |
| 5 | S | 331 | THR | N-CA-CB | -7.58 | 95.89 | 110.30 |
| 4 | X | 320 | GLU | CB-CA-C | 7.58 | 125.57 | 110.40 |
| 4 | X | 457 | ALA | CA-C-O | -7.58 | 104.17 | 120.10 |
| 6 | H | 487 | TRP | C-N-CA | -7.58 | 102.75 | 121.70 |
| 6 | T | 487 | TRP | C-N-CA | -7.58 | 102.75 | 121.70 |
| 4 | L | 448 | ARG | N-CA-C | 7.58 | 131.46 | 111.00 |
| 4 | L | 457 | ALA | CA-C-O | -7.58 | 104.19 | 120.10 |
| 4 | F | 448 | ARG | N-CA-C | 7.58 | 131.46 | 111.00 |
| 3 | P | 1542 | PRO | CA-C-N | 7.58 | 133.87 | 117.20 |
| 4 | R | 448 | ARG | N-CA-C | 7.57 | 131.45 | 111.00 |
| 4 | F | 211 | GLU | N-CA-C | 7.57 | 131.45 | 111.00 |
| 4 | X | 211 | GLU | N-CA-C | 7.57 | 131.44 | 111.00 |
| 6 | H | 410 | LEU | CA-C-O | -7.57 | 104.20 | 120.10 |
| 6 | Z | 410 | LEU | CA-C-O | -7.57 | 104.20 | 120.10 |
| 4 | L | 320 | GLU | CB-CA-C | 7.57 | 125.53 | 110.40 |
| 6 | N | 410 | LEU | CA-C-O | -7.57 | 104.21 | 120.10 |
| 5 | Y | 331 | THR | N-CA-CB | -7.57 | 95.93 | 110.30 |
| 5 | G | 333 | PRO | CB-CA-C | -7.56 | 93.09 | 112.00 |
| 5 | M | 333 | PRO | CB-CA-C | -7.56 | 93.10 | 112.00 |
| 4 | F | 457 | ALA | CA-C-O | -7.56 | 104.23 | 120.10 |
| 4 | R | 211 | GLU | N-CA-C | 7.55 | 131.39 | 111.00 |
| 4 | X | 448 | ARG | N-CA-C | 7.55 | 131.39 | 111.00 |
| 5 | S | 333 | PRO | CB-CA-C | -7.55 | 93.13 | 112.00 |
| 5 | Y | 333 | PRO | CB-CA-C | -7.55 | 93.13 | 112.00 |
| 3 | D | 1542 | PRO | CA-C-N | 7.54 | 133.79 | 117.20 |
| 3 | D | 1510 | GLN | O-C-N | 7.54 | 134.76 | 122.70 |
| 5 | G | 331 | THR | N-CA-CB | -7.54 | 95.98 | 110.30 |
| 5 | M | 331 | THR | N-CA-CB | -7.54 | 95.98 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 384 | LEU | N-CA-C | -7.54 | 90.65 | 111.00 |
| 6 | N | 384 | LEU | N-CA-C | -7.54 | 90.66 | 111.00 |
| 3 | P | 1510 | GLN | O-C-N | 7.53 | 134.75 | 122.70 |
| 6 | Z | 462 | GLY | CA-C-O | -7.53 | 107.05 | 120.60 |
| 6 | T | 384 | LEU | N-CA-C | -7.52 | 90.69 | 111.00 |
| 6 | H | 462 | GLY | CA-C-O | -7.52 | 107.07 | 120.60 |
| 6 | T | 462 | GLY | CA-C-O | -7.52 | 107.06 | 120.60 |
| 6 | H | 384 | LEU | N-CA-C | -7.51 | 90.71 | 111.00 |
| 6 | Z | 409 | PRO | CB-CA-C | -7.51 | 93.21 | 112.00 |
| 5 | M | 253 | GLN | CA-C-N | -7.51 | 100.68 | 117.20 |
| 6 | H | 409 | PRO | CB-CA-C | -7.51 | 93.23 | 112.00 |
| 6 | N | 409 | PRO | CB-CA-C | -7.51 | 93.23 | 112.00 |
| 6 | N | 487 | TRP | O-C-N | 7.50 | 134.70 | 122.70 |
| 6 | T | 409 | PRO | CB-CA-C | -7.50 | 93.25 | 112.00 |
| 6 | N | 462 | GLY | CA-C-O | -7.50 | 107.10 | 120.60 |
| 5 | G | 253 | GLN | CA-C-N | -7.48 | 100.74 | 117.20 |
| 5 | S | 253 | GLN | CA-C-N | -7.48 | 100.74 | 117.20 |
| 5 | Y | 253 | GLN | CA-C-N | -7.47 | 100.76 | 117.20 |
| 6 | T | 487 | TRP | O-C-N | 7.46 | 134.64 | 122.70 |
| 6 | Z | 487 | TRP | O-C-N | 7.45 | 134.62 | 122.70 |
| 3 | D | 1487 | ASP | CA-C-O | 7.45 | 135.74 | 120.10 |
| 3 | P | 1487 | ASP | CA-C-O | 7.45 | 135.73 | 120.10 |
| 5 | M | 406 | ILE | CB-CA-C | -7.44 | 96.72 | 111.60 |
| 4 | R | 398 | LYS | N-CA-CB | 7.43 | 123.98 | 110.60 |
| 4 | X | 398 | LYS | N-CA-CB | 7.42 | 123.96 | 110.60 |
| 6 | H | 487 | TRP | O-C-N | 7.41 | 134.56 | 122.70 |
| 4 | L | 398 | LYS | N-CA-CB | 7.41 | 123.93 | 110.60 |
| 4 | F | 398 | LYS | N-CA-CB | 7.40 | 123.93 | 110.60 |
| 5 | G | 406 | ILE | CB-CA-C | -7.40 | 96.79 | 111.60 |
| 4 | R | 394 | GLU | O-C-N | -7.40 | 110.86 | 122.70 |
| 2 | U | 454 | THR | C-N-CA | 7.40 | 140.21 | 121.70 |
| 6 | Z | 494 | LEU | O-C-N | 7.40 | 134.54 | 122.70 |
| 5 | S | 406 | ILE | CB-CA-C | -7.39 | 96.81 | 111.60 |
| 2 | I | 454 | THR | C-N-CA | 7.39 | 140.17 | 121.70 |
| 2 | O | 454 | THR | C-N-CA | 7.39 | 140.17 | 121.70 |
| 4 | X | 394 | GLU | O-C-N | -7.39 | 110.88 | 122.70 |
| 2 | C | 454 | THR | C-N-CA | 7.38 | 140.14 | 121.70 |
| 4 | L | 215 | LYS | CB-CA-C | -7.37 | 95.66 | 110.40 |
| 6 | H | 418 | SER | CB-CA-C | 7.37 | 124.10 | 110.10 |
| 4 | L | 394 | GLU | O-C-N | -7.37 | 110.91 | 122.70 |
| 6 | N | 494 | LEU | O-C-N | 7.36 | 134.48 | 122.70 |
| 4 | X | 215 | LYS | CB-CA-C | -7.36 | 95.67 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 399 | SER | N-CA-CB | -7.36 | 99.46 | 110.50 |
| 6 | N | 418 | SER | CB-CA-C | 7.36 | 124.09 | 110.10 |
| 4 | R | 399 | SER | N-CA-CB | -7.36 | 99.47 | 110.50 |
| 5 | Y | 406 | ILE | CB-CA-C | -7.36 | 96.89 | 111.60 |
| 6 | Z | 418 | SER | CB-CA-C | 7.35 | 124.07 | 110.10 |
| 6 | T | 494 | LEU | O-C-N | 7.35 | 134.46 | 122.70 |
| 6 | T | 418 | SER | CB-CA-C | 7.34 | 124.05 | 110.10 |
| 4 | F | 215 | LYS | CB-CA-C | -7.34 | 95.72 | 110.40 |
| 4 | F | 394 | GLU | O-C-N | -7.34 | 110.96 | 122.70 |
| 4 | L | 399 | SER | N-CA-CB | -7.33 | 99.50 | 110.50 |
| 4 | R | 215 | LYS | CB-CA-C | -7.33 | 95.73 | 110.40 |
| 4 | X | 399 | SER | N-CA-CB | -7.33 | 99.50 | 110.50 |
| 6 | Z | 408 | SER | CB-CA-C | -7.33 | 96.18 | 110.10 |
| 6 | H | 494 | LEU | O-C-N | 7.33 | 134.42 | 122.70 |
| 5 | Y | 393 | TYR | CA-C-O | -7.33 | 104.71 | 120.10 |
| 6 | H | 408 | SER | CB-CA-C | -7.32 | 96.19 | 110.10 |
| 3 | P | 1546 | LEU | CA-C-N | -7.31 | 101.11 | 117.20 |
| 6 | T | 408 | SER | CB-CA-C | -7.31 | 96.21 | 110.10 |
| 4 | X | 487 | ASP | C-N-CA | 7.31 | 139.97 | 121.70 |
| 5 | G | 393 | TYR | CA-C-O | -7.30 | 104.76 | 120.10 |
| 4 | R | 487 | ASP | C-N-CA | 7.30 | 139.96 | 121.70 |
| 5 | S | 393 | TYR | CA-C-O | -7.30 | 104.76 | 120.10 |
| 4 | L | 487 | ASP | C-N-CA | 7.30 | 139.94 | 121.70 |
| 6 | N | 338 | ASN | CB-CA-C | -7.30 | 95.81 | 110.40 |
| 4 | F | 487 | ASP | C-N-CA | 7.29 | 139.94 | 121.70 |
| 6 | Z | 338 | ASN | CB-CA-C | -7.29 | 95.82 | 110.40 |
| 6 | T | 477 | ILE | CB-CA-C | 7.29 | 126.18 | 111.60 |
| 6 | N | 408 | SER | CB-CA-C | -7.29 | 96.25 | 110.10 |
| 5 | M | 344 | ASP | CB-CA-C | 7.29 | 124.97 | 110.40 |
| 4 | X | 454 | TYR | O-C-N | 7.28 | 134.35 | 122.70 |
| 3 | D | 1546 | LEU | CA-C-N | -7.28 | 101.18 | 117.20 |
| 6 | Z | 477 | ILE | CB-CA-C | 7.28 | 126.16 | 111.60 |
| 3 | P | 1487 | ASP | C-N-CA | -7.28 | 107.01 | 122.30 |
| 2 | C | 4 | GLU | C-N-CA | -7.28 | 107.02 | 122.30 |
| 6 | H | 477 | ILE | CB-CA-C | 7.28 | 126.16 | 111.60 |
| 6 | T | 338 | ASN | CB-CA-C | -7.28 | 95.85 | 110.40 |
| 6 | N | 477 | ILE | CB-CA-C | 7.28 | 126.15 | 111.60 |
| 6 | H | 338 | ASN | CB-CA-C | -7.27 | 95.85 | 110.40 |
| 3 | D | 1487 | ASP | C-N-CA | -7.27 | 107.03 | 122.30 |
| 2 | I | 4 | GLU | C-N-CA | -7.27 | 107.03 | 122.30 |
| 5 | M | 296 | LEU | CB-CA-C | -7.27 | 96.38 | 110.20 |
| 2 | O | 4 | GLU | C-N-CA | -7.27 | 107.03 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 393 | TYR | CA-C-O | -7.27 | 104.83 | 120.10 |
| 4 | R | 454 | TYR | O-C-N | 7.27 | 134.33 | 122.70 |
| 3 | P | 1512 | TRP | CA-C-O | -7.27 | 104.84 | 120.10 |
| 2 | U | 4 | GLU | C-N-CA | -7.26 | 107.05 | 122.30 |
| 6 | Z | 406 | LEU | O-C-N | -7.26 | 111.09 | 122.70 |
| 4 | F | 467 | LEU | CA-C-O | -7.26 | 104.86 | 120.10 |
| 5 | G | 344 | ASP | CB-CA-C | 7.26 | 124.91 | 110.40 |
| 5 | S | 344 | ASP | CB-CA-C | 7.25 | 124.91 | 110.40 |
| 3 | D | 878 | PRO | C-N-CA | 7.25 | 139.82 | 121.70 |
| 3 | P | 1473 | TYR | C-N-CA | 7.25 | 137.52 | 122.30 |
| 5 | Y | 344 | ASP | CB-CA-C | 7.25 | 124.89 | 110.40 |
| 4 | F | 454 | TYR | O-C-N | 7.25 | 134.29 | 122.70 |
| 3 | D | 1512 | TRP | CA-C-O | -7.24 | 104.89 | 120.10 |
| 5 | Y | 296 | LEU | CB-CA-C | -7.24 | 96.44 | 110.20 |
| 5 | S | 296 | LEU | CB-CA-C | -7.24 | 96.44 | 110.20 |
| 3 | P | 878 | PRO | C-N-CA | 7.24 | 139.80 | 121.70 |
| 4 | X | 467 | LEU | CA-C-O | -7.24 | 104.90 | 120.10 |
| 5 | G | 296 | LEU | CB-CA-C | -7.23 | 96.46 | 110.20 |
| 6 | T | 406 | LEU | O-C-N | -7.23 | 111.13 | 122.70 |
| 4 | L | 454 | TYR | O-C-N | 7.22 | 134.26 | 122.70 |
| 6 | N | 406 | LEU | O-C-N | -7.22 | 111.14 | 122.70 |
| 3 | D | 1473 | TYR | C-N-CA | 7.21 | 137.44 | 122.30 |
| 6 | H | 406 | LEU | O-C-N | -7.21 | 111.17 | 122.70 |
| 6 | H | 462 | GLY | O-C-N | -7.20 | 111.18 | 122.70 |
| 4 | L | 235 | ASP | CA-C-O | -7.20 | 104.98 | 120.10 |
| 4 | L | 467 | LEU | CA-C-O | -7.20 | 104.98 | 120.10 |
| 4 | F | 460 | LEU | O-C-N | 7.20 | 134.22 | 122.70 |
| 4 | R | 460 | LEU | O-C-N | 7.20 | 134.22 | 122.70 |
| 6 | N | 462 | GLY | O-C-N | -7.20 | 111.18 | 122.70 |
| 6 | T | 462 | GLY | O-C-N | -7.19 | 111.19 | 122.70 |
| 4 | X | 235 | ASP | CA-C-O | -7.19 | 104.99 | 120.10 |
| 4 | R | 341 | ASP | CB-CA-C | 7.19 | 124.78 | 110.40 |
| 4 | R | 467 | LEU | CA-C-O | -7.19 | 105.00 | 120.10 |
| 4 | L | 464 | LYS | O-C-N | 7.18 | 134.19 | 122.70 |
| 6 | Z | 462 | GLY | O-C-N | -7.18 | 111.21 | 122.70 |
| 4 | F | 475 | SER | N-CA-CB | 7.18 | 121.27 | 110.50 |
| 4 | X | 460 | LEU | O-C-N | 7.18 | 134.19 | 122.70 |
| 4 | L | 341 | ASP | CB-CA-C | 7.17 | 124.75 | 110.40 |
| 4 | R | 475 | SER | N-CA-CB | 7.17 | 121.26 | 110.50 |
| 4 | L | 460 | LEU | O-C-N | 7.17 | 134.17 | 122.70 |
| 4 | X | 475 | SER | N-CA-CB | 7.17 | 121.25 | 110.50 |
| 4 | F | 235 | ASP | CA-C-O | -7.16 | 105.06 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 341 | ASP | CB-CA-C | 7.16 | 124.72 | 110.40 |
| 4 | L | 475 | SER | N-CA-CB | 7.15 | 121.23 | 110.50 |
| 6 | Z | 394 | ASP | C-N-CA | -7.14 | 103.84 | 121.70 |
| 4 | R | 235 | ASP | CA-C-O | -7.14 | 105.11 | 120.10 |
| 4 | R | 464 | LYS | O-C-N | 7.14 | 134.12 | 122.70 |
| 4 | X | 341 | ASP | CB-CA-C | 7.14 | 124.68 | 110.40 |
| 4 | X | 464 | LYS | O-C-N | 7.13 | 134.12 | 122.70 |
| 4 | R | 452 | ARG | N-CA-C | 7.13 | 130.26 | 111.00 |
| 4 | R | 492 | GLU | N-CA-CB | 7.13 | 123.44 | 110.60 |
| 4 | F | 464 | LYS | O-C-N | 7.13 | 134.11 | 122.70 |
| 7 | V | 157 | GLU | N-CA-CB | 7.13 | 123.43 | 110.60 |
| 4 | F | 452 | ARG | N-CA-C | 7.12 | 130.23 | 111.00 |
| 4 | X | 492 | GLU | N-CA-CB | 7.12 | 123.42 | 110.60 |
| 7 | J | 157 | GLU | N-CA-CB | 7.12 | 123.42 | 110.60 |
| 4 | L | 398 | LYS | CB-CA-C | -7.12 | 96.16 | 110.40 |
| 4 | F | 492 | GLU | N-CA-CB | 7.12 | 123.41 | 110.60 |
| 6 | H | 394 | ASP | C-N-CA | -7.12 | 103.91 | 121.70 |
| 4 | L | 452 | ARG | N-CA-C | 7.12 | 130.21 | 111.00 |
| 6 | N | 394 | ASP | C-N-CA | -7.11 | 103.92 | 121.70 |
| 6 | N | 407 | LEU | CB-CA-C | -7.11 | 96.68 | 110.20 |
| 6 | H | 407 | LEU | CB-CA-C | -7.11 | 96.69 | 110.20 |
| 6 | Z | 407 | LEU | CB-CA-C | -7.11 | 96.69 | 110.20 |
| 4 | F | 398 | LYS | CB-CA-C | -7.11 | 96.19 | 110.40 |
| 4 | L | 427 | PHE | O-C-N | 7.11 | 134.07 | 122.70 |
| 4 | X | 452 | ARG | N-CA-C | 7.11 | 130.19 | 111.00 |
| 4 | L | 492 | GLU | N-CA-CB | 7.10 | 123.38 | 110.60 |
| 6 | T | 394 | ASP | C-N-CA | -7.09 | 103.97 | 121.70 |
| 4 | R | 132 | ASP | N-CA-CB | -7.08 | 97.86 | 110.60 |
| 4 | R | 398 | LYS | CB-CA-C | -7.08 | 96.24 | 110.40 |
| 6 | T | 387 | LYS | CA-C-N | -7.08 | 101.63 | 117.20 |
| 4 | X | 398 | LYS | CB-CA-C | -7.07 | 96.25 | 110.40 |
| 6 | H | 381 | LYS | CA-C-N | 7.07 | 132.75 | 117.20 |
| 6 | T | 407 | LEU | CB-CA-C | -7.07 | 96.77 | 110.20 |
| 4 | X | 132 | ASP | N-CA-CB | -7.07 | 97.88 | 110.60 |
| 4 | F | 399 | SER | CB-CA-C | -7.07 | 96.68 | 110.10 |
| 4 | F | 427 | PHE | O-C-N | 7.06 | 134.00 | 122.70 |
| 4 | R | 427 | PHE | O-C-N | 7.06 | 134.00 | 122.70 |
| 4 | L | 132 | ASP | N-CA-CB | -7.06 | 97.89 | 110.60 |
| 4 | L | 399 | SER | CB-CA-C | -7.06 | 96.69 | 110.10 |
| 4 | R | 399 | SER | CB-CA-C | -7.06 | 96.69 | 110.10 |
| 6 | Z | 381 | LYS | CA-C-N | 7.06 | 132.73 | 117.20 |
| 6 | Z | 414 | VAL | CA-C-N | 7.06 | 132.72 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 399 | SER | CB-CA-C | -7.05 | 96.70 | 110.10 |
| 6 | Z | 387 | LYS | CA-C-N | -7.05 | 101.68 | 117.20 |
| 4 | F | 132 | ASP | N-CA-CB | -7.05 | 97.91 | 110.60 |
| 6 | Z | 471 | LEU | CA-C-O | 7.05 | 134.90 | 120.10 |
| 6 | N | 414 | VAL | CA-C-N | 7.05 | 132.71 | 117.20 |
| 6 | T | 414 | VAL | CA-C-N | 7.04 | 132.70 | 117.20 |
| 5 | Y | 274 | ARG | O-C-N | -7.04 | 111.43 | 122.70 |
| 6 | H | 387 | LYS | CA-C-N | -7.04 | 101.72 | 117.20 |
| 6 | N | 381 | LYS | CA-C-N | 7.04 | 132.68 | 117.20 |
| 6 | N | 471 | LEU | CA-C-O | 7.04 | 134.88 | 120.10 |
| 6 | H | 414 | VAL | CA-C-N | 7.03 | 132.67 | 117.20 |
| 6 | N | 387 | LYS | CA-C-N | -7.03 | 101.74 | 117.20 |
| 6 | T | 381 | LYS | CA-C-N | 7.02 | 132.65 | 117.20 |
| 4 | X | 427 | PHE | O-C-N | 7.02 | 133.93 | 122.70 |
| 6 | H | 471 | LEU | CA-C-O | 7.02 | 134.84 | 120.10 |
| 3 | P | 1512 | TRP | O-C-N | 7.02 | 133.93 | 122.70 |
| 6 | T | 471 | LEU | CA-C-O | 7.01 | 134.83 | 120.10 |
| 4 | F | 299 | ASN | N-CA-C | -7.00 | 92.09 | 111.00 |
| 6 | T | 377 | ARG | CA-C-N | -7.00 | 101.79 | 117.20 |
| 4 | L | 299 | ASN | N-CA-C | -7.00 | 92.10 | 111.00 |
| 5 | S | 274 | ARG | O-C-N | -7.00 | 111.50 | 122.70 |
| 5 | G | 274 | ARG | O-C-N | -6.99 | 111.51 | 122.70 |
| 2 | I | 3 | THR | CA-C-N | -6.99 | 101.82 | 117.20 |
| 2 | O | 3 | THR | CA-C-N | -6.99 | 101.82 | 117.20 |
| 4 | R | 299 | ASN | N-CA-C | -6.99 | 92.13 | 111.00 |
| 4 | X | 299 | ASN | N-CA-C | -6.99 | 92.12 | 111.00 |
| 2 | C | 3 | THR | CA-C-N | -6.99 | 101.83 | 117.20 |
| 3 | D | 1543 | GLN | C-N-CA | -6.99 | 92.66 | 122.00 |
| 6 | N | 377 | ARG | CA-C-N | -6.99 | 101.83 | 117.20 |
| 4 | R | 433 | GLU | N-CA-C | -6.99 | 92.14 | 111.00 |
| 3 | D | 1512 | TRP | O-C-N | 6.98 | 133.87 | 122.70 |
| 6 | H | 377 | ARG | CA-C-N | -6.98 | 101.84 | 117.20 |
| 4 | X | 433 | GLU | N-CA-C | -6.98 | 92.15 | 111.00 |
| 5 | M | 274 | ARG | O-C-N | -6.98 | 111.53 | 122.70 |
| 6 | Z | 377 | ARG | CA-C-N | -6.98 | 101.84 | 117.20 |
| 3 | P | 1543 | GLN | C-N-CA | -6.97 | 92.71 | 122.00 |
| 4 | L | 433 | GLU | N-CA-C | -6.97 | 92.17 | 111.00 |
| 2 | U | 3 | THR | CA-C-N | -6.97 | 101.86 | 117.20 |
| 4 | F | 433 | GLU | N-CA-C | -6.97 | 92.18 | 111.00 |
| 4 | X | 455 | ILE | CB-CA-C | -6.95 | 97.70 | 111.60 |
| 4 | R | 455 | ILE | CB-CA-C | -6.94 | 97.72 | 111.60 |
| 2 | O | 484 | ARG | N-CA-CB | -6.93 | 98.13 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 484 | ARG | N-CA-CB | -6.92 | 98.14 | 110.60 |
| 4 | F | 455 | ILE | CB-CA-C | -6.92 | 97.77 | 111.60 |
| 4 | L | 455 | ILE | CB-CA-C | -6.92 | 97.77 | 111.60 |
| 2 | I | 484 | ARG | N-CA-CB | -6.91 | 98.16 | 110.60 |
| 4 | R | 211 | GLU | CB-CA-C | 6.91 | 124.22 | 110.40 |
| 2 | U | 484 | ARG | N-CA-CB | -6.91 | 98.16 | 110.60 |
| 4 | F | 211 | GLU | CB-CA-C | 6.91 | 124.21 | 110.40 |
| 4 | L | 211 | GLU | CB-CA-C | 6.90 | 124.20 | 110.40 |
| 4 | X | 211 | GLU | CB-CA-C | 6.89 | 124.18 | 110.40 |
| 5 | G | 392 | ILE | C-N-CA | -6.89 | 104.47 | 121.70 |
| 5 | S | 392 | ILE | C-N-CA | -6.89 | 104.48 | 121.70 |
| 3 | P | 879 | LEU | N-CA-C | 6.89 | 129.60 | 111.00 |
| 5 | Y | 392 | ILE | C-N-CA | -6.89 | 104.48 | 121.70 |
| 5 | M | 392 | ILE | C-N-CA | -6.89 | 104.48 | 121.70 |
| 5 | Y | 372 | ALA | N-CA-CB | 6.88 | 119.73 | 110.10 |
| 3 | D | 879 | LEU | N-CA-C | 6.88 | 129.58 | 111.00 |
| 5 | Y | 331 | THR | CA-C-N | -6.88 | 97.83 | 117.10 |
| 4 | R | 451 | GLU | C-N-CA | -6.87 | 104.52 | 121.70 |
| 5 | M | 331 | THR | CA-C-N | -6.87 | 97.86 | 117.10 |
| 5 | M | 372 | ALA | N-CA-CB | 6.86 | 119.71 | 110.10 |
| 5 | G | 331 | THR | CA-C-N | -6.86 | 97.89 | 117.10 |
| 4 | L | 451 | GLU | C-N-CA | -6.86 | 104.55 | 121.70 |
| 4 | X | 451 | GLU | C-N-CA | -6.86 | 104.55 | 121.70 |
| 6 | N | 413 | LEU | N-CA-CB | 6.86 | 124.12 | 110.40 |
| 4 | F | 451 | GLU | C-N-CA | -6.85 | 104.57 | 121.70 |
| 5 | S | 331 | THR | CA-C-N | -6.85 | 97.91 | 117.10 |
| 2 | O | 481 | ARG | N-CA-C | 6.85 | 129.50 | 111.00 |
| 5 | G | 372 | ALA | N-CA-CB | 6.85 | 119.69 | 110.10 |
| 6 | H | 413 | LEU | N-CA-CB | 6.85 | 124.09 | 110.40 |
| 3 | D | 1517 | SER | O-C-N | 6.84 | 133.65 | 122.70 |
| 5 | S | 372 | ALA | N-CA-CB | 6.84 | 119.68 | 110.10 |
| 2 | C | 481 | ARG | N-CA-C | 6.84 | 129.47 | 111.00 |
| 6 | T | 413 | LEU | N-CA-CB | 6.84 | 124.08 | 110.40 |
| 2 | U | 481 | ARG | N-CA-C | 6.84 | 129.47 | 111.00 |
| 2 | I | 481 | ARG | N-CA-C | 6.84 | 129.46 | 111.00 |
| 6 | Z | 413 | LEU | N-CA-CB | 6.83 | 124.06 | 110.40 |
| 4 | X | 461 | ARG | O-C-N | -6.83 | 111.77 | 122.70 |
| 3 | P | 1517 | SER | O-C-N | 6.83 | 133.63 | 122.70 |
| 6 | T | 481 | HIS | CB-CA-C | -6.83 | 96.74 | 110.40 |
| 5 | S | 378 | SER | CA-C-O | -6.82 | 105.77 | 120.10 |
| 6 | H | 481 | HIS | CB-CA-C | -6.82 | 96.76 | 110.40 |
| 6 | N | 481 | HIS | CB-CA-C | -6.82 | 96.76 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 461 | ARG | O-C-N | -6.82 | 111.79 | 122.70 |
| 5 | M | 378 | SER | CA-C-O | -6.82 | 105.78 | 120.10 |
| 4 | R | 465 | GLN | CA-C-N | 6.82 | 132.20 | 117.20 |
| 5 | Y | 378 | SER | CA-C-O | -6.82 | 105.78 | 120.10 |
| 5 | G | 378 | SER | CA-C-O | -6.81 | 105.79 | 120.10 |
| 4 | X | 465 | GLN | CA-C-N | 6.81 | 132.18 | 117.20 |
| 4 | F | 465 | GLN | CA-C-N | 6.80 | 132.16 | 117.20 |
| 4 | L | 461 | ARG | O-C-N | -6.80 | 111.83 | 122.70 |
| 5 | M | 381 | THR | N-CA-C | 6.79 | 129.35 | 111.00 |
| 6 | Z | 481 | HIS | CB-CA-C | -6.79 | 96.81 | 110.40 |
| 5 | Y | 381 | THR | N-CA-C | 6.79 | 129.33 | 111.00 |
| 4 | R | 461 | ARG | O-C-N | -6.79 | 111.84 | 122.70 |
| 4 | L | 465 | GLN | CA-C-N | 6.78 | 132.11 | 117.20 |
| 5 | S | 381 | THR | N-CA-C | 6.78 | 129.30 | 111.00 |
| 4 | L | 492 | GLU | CB-CA-C | -6.77 | 96.86 | 110.40 |
| 3 | P | 1508 | LYS | O-C-N | 6.77 | 133.53 | 122.70 |
| 3 | P | 328 | THR | CB-CA-C | -6.77 | 93.33 | 111.60 |
| 3 | D | 328 | THR | CB-CA-C | -6.76 | 93.34 | 111.60 |
| 4 | F | 492 | GLU | CB-CA-C | -6.76 | 96.88 | 110.40 |
| 5 | G | 381 | THR | N-CA-C | 6.76 | 129.25 | 111.00 |
| 4 | R | 492 | GLU | CB-CA-C | -6.76 | 96.89 | 110.40 |
| 4 | X | 492 | GLU | CB-CA-C | -6.75 | 96.91 | 110.40 |
| 4 | R | 428 | LYS | O-C-N | 6.75 | 134.67 | 123.20 |
| 3 | P | 1493 | ARG | CA-C-N | -6.74 | 102.37 | 117.20 |
| 3 | D | 1459 | PHE | N-CA-CB | 6.74 | 122.73 | 110.60 |
| 4 | F | 428 | LYS | O-C-N | 6.72 | 134.63 | 123.20 |
| 3 | D | 1493 | ARG | CA-C-N | -6.72 | 102.41 | 117.20 |
| 3 | D | 1508 | LYS | O-C-N | 6.72 | 133.45 | 122.70 |
| 3 | P | 1459 | PHE | N-CA-CB | 6.72 | 122.69 | 110.60 |
| 6 | Z | 485 | LEU | CB-CA-C | -6.71 | 97.44 | 110.20 |
| 4 | L | 221 | GLN | CA-C-N | 6.71 | 131.96 | 117.20 |
| 4 | X | 453 | TYR | CB-CA-C | -6.71 | 96.98 | 110.40 |
| 4 | X | 428 | LYS | O-C-N | 6.70 | 134.60 | 123.20 |
| 4 | R | 453 | TYR | CB-CA-C | -6.70 | 97.00 | 110.40 |
| 4 | X | 404 | GLN | N-CA-CB | 6.70 | 122.66 | 110.60 |
| 3 | P | 1507 | ASP | C-N-CA | 6.70 | 138.44 | 121.70 |
| 6 | T | 485 | LEU | CB-CA-C | -6.70 | 97.48 | 110.20 |
| 5 | Y | 253 | GLN | N-CA-C | -6.70 | 92.92 | 111.00 |
| 5 | G | 253 | GLN | N-CA-C | -6.69 | 92.93 | 111.00 |
| 6 | H | 485 | LEU | CB-CA-C | -6.69 | 97.48 | 110.20 |
| 4 | F | 221 | GLN | CA-C-N | 6.69 | 131.92 | 117.20 |
| 4 | F | 453 | TYR | CB-CA-C | -6.69 | 97.02 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 1507 | ASP | C-N-CA | 6.69 | 138.42 | 121.70 |
| 5 | S | 253 | GLN | N-CA-C | -6.68 | 92.95 | 111.00 |
| 4 | X | 221 | GLN | CA-C-N | 6.68 | 131.90 | 117.20 |
| 4 | L | 453 | TYR | CB-CA-C | -6.68 | 97.04 | 110.40 |
| 6 | N | 485 | LEU | CB-CA-C | -6.68 | 97.51 | 110.20 |
| 4 | R | 215 | LYS | N-CA-CB | -6.68 | 98.58 | 110.60 |
| 4 | L | 215 | LYS | N-CA-CB | -6.68 | 98.58 | 110.60 |
| 4 | L | 428 | LYS | O-C-N | 6.67 | 134.54 | 123.20 |
| 4 | R | 404 | GLN | N-CA-CB | 6.67 | 122.61 | 110.60 |
| 5 | Y | 346 | PHE | N-CA-CB | 6.67 | 122.61 | 110.60 |
| 5 | M | 253 | GLN | N-CA-C | -6.67 | 93.00 | 111.00 |
| 4 | R | 221 | GLN | CA-C-N | 6.66 | 131.84 | 117.20 |
| 4 | L | 404 | GLN | N-CA-CB | 6.66 | 122.58 | 110.60 |
| 4 | X | 215 | LYS | N-CA-CB | -6.65 | 98.63 | 110.60 |
| 4 | F | 215 | LYS | N-CA-CB | -6.65 | 98.64 | 110.60 |
| 6 | Z | 349 | ARG | CB-CA-C | -6.65 | 97.11 | 110.40 |
| 5 | G | 346 | PHE | N-CA-CB | 6.64 | 122.56 | 110.60 |
| 6 | T | 349 | ARG | CB-CA-C | -6.64 | 97.11 | 110.40 |
| 6 | N | 349 | ARG | CB-CA-C | -6.64 | 97.12 | 110.40 |
| 4 | X | 311 | GLN | N-CA-C | -6.64 | 93.07 | 111.00 |
| 4 | R | 311 | GLN | N-CA-C | -6.64 | 93.07 | 111.00 |
| 6 | T | 370 | GLU | N-CA-CB | 6.64 | 122.55 | 110.60 |
| 4 | F | 404 | GLN | N-CA-CB | 6.64 | 122.55 | 110.60 |
| 5 | S | 346 | PHE | N-CA-CB | 6.64 | 122.55 | 110.60 |
| 6 | H | 349 | ARG | CB-CA-C | -6.63 | 97.13 | 110.40 |
| 6 | H | 370 | GLU | N-CA-CB | 6.63 | 122.54 | 110.60 |
| 3 | P | 1448 | MET | CA-C-O | -6.63 | 106.17 | 120.10 |
| 5 | Y | 393 | TYR | N-CA-C | -6.63 | 93.09 | 111.00 |
| 4 | F | 311 | GLN | N-CA-C | -6.63 | 93.11 | 111.00 |
| 6 | N | 370 | GLU | N-CA-CB | 6.62 | 122.52 | 110.60 |
| 6 | Z | 370 | GLU | N-CA-CB | 6.62 | 122.52 | 110.60 |
| 6 | Z | 405 | ASP | O-C-N | 6.62 | 133.29 | 122.70 |
| 4 | L | 311 | GLN | N-CA-C | -6.62 | 93.13 | 111.00 |
| 5 | M | 346 | PHE | N-CA-CB | 6.62 | 122.51 | 110.60 |
| 5 | S | 393 | TYR | N-CA-C | -6.62 | 93.13 | 111.00 |
| 3 | D | 1448 | MET | CA-C-O | -6.62 | 106.21 | 120.10 |
| 5 | G | 393 | TYR | N-CA-C | -6.62 | 93.14 | 111.00 |
| 4 | F | 484 | ASP | CA-C-N | -6.59 | 102.69 | 117.20 |
| 5 | M | 393 | TYR | N-CA-C | -6.59 | 93.20 | 111.00 |
| 6 | N | 407 | LEU | N-CA-CB | 6.59 | 123.58 | 110.40 |
| 6 | Z | 407 | LEU | N-CA-CB | 6.59 | 123.58 | 110.40 |
| 4 | L | 419 | GLY | CA-C-N | 6.58 | 131.68 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | N | 405 | ASP | O-C-N | 6.58 | 133.23 | 122.70 |
| 4 | X | 484 | ASP | CA-C-N | -6.58 | 102.72 | 117.20 |
| 4 | L | 484 | ASP | CA-C-N | -6.57 | 102.74 | 117.20 |
| 6 | T | 407 | LEU | N-CA-CB | 6.57 | 123.54 | 110.40 |
| 4 | X | 419 | GLY | CA-C-N | 6.57 | 131.65 | 117.20 |
| 6 | N | 405 | ASP | N-CA-CB | 6.57 | 122.42 | 110.60 |
| 6 | T | 405 | ASP | N-CA-CB | 6.57 | 122.42 | 110.60 |
| 4 | R | 425 | THR | C-N-CA | -6.56 | 105.30 | 121.70 |
| 6 | Z | 405 | ASP | N-CA-CB | 6.56 | 122.41 | 110.60 |
| 6 | H | 405 | ASP | N-CA-CB | 6.56 | 122.40 | 110.60 |
| 6 | H | 405 | ASP | O-C-N | 6.55 | 133.18 | 122.70 |
| 4 | L | 425 | THR | C-N-CA | -6.55 | 105.32 | 121.70 |
| 6 | T | 405 | ASP | O-C-N | 6.55 | 133.18 | 122.70 |
| 6 | H | 407 | LEU | N-CA-CB | 6.55 | 123.50 | 110.40 |
| 2 | I | 7 | GLY | CA-C-N | 6.55 | 131.60 | 117.20 |
| 3 | P | 1503 | ILE | O-C-N | 6.54 | 133.17 | 122.70 |
| 4 | R | 484 | ASP | CA-C-N | -6.54 | 102.81 | 117.20 |
| 6 | Z | 406 | LEU | CA-C-N | 6.54 | 131.59 | 117.20 |
| 4 | R | 419 | GLY | CA-C-N | 6.54 | 131.59 | 117.20 |
| 2 | U | 7 | GLY | CA-C-N | 6.54 | 131.58 | 117.20 |
| 4 | F | 425 | THR | C-N-CA | -6.54 | 105.36 | 121.70 |
| 2 | C | 8 | GLU | O-C-N | 6.53 | 133.15 | 122.70 |
| 2 | O | 7 | GLY | CA-C-N | 6.53 | 131.57 | 117.20 |
| 3 | D | 1503 | ILE | O-C-N | 6.53 | 133.15 | 122.70 |
| 7 | J | 156 | VAL | C-N-CA | 6.53 | 138.03 | 121.70 |
| 2 | C | 7 | GLY | CA-C-N | 6.53 | 131.56 | 117.20 |
| 4 | X | 425 | THR | C-N-CA | -6.53 | 105.38 | 121.70 |
| 6 | H | 406 | LEU | CA-C-N | 6.52 | 131.55 | 117.20 |
| 6 | Z | 501 | GLU | CA-C-N | -6.52 | 102.85 | 117.20 |
| 4 | F | 419 | GLY | CA-C-N | 6.52 | 131.54 | 117.20 |
| 5 | M | 344 | ASP | CA-C-O | 6.52 | 133.78 | 120.10 |
| 3 | D | 1451 | ARG | CA-C-N | -6.51 | 102.87 | 117.20 |
| 4 | L | 452 | ARG | C-N-CA | 6.51 | 137.98 | 121.70 |
| 5 | Y | 344 | ASP | CA-C-O | 6.51 | 133.78 | 120.10 |
| 7 | V | 156 | VAL | C-N-CA | 6.51 | 137.98 | 121.70 |
| 6 | N | 501 | GLU | CA-C-N | -6.51 | 102.88 | 117.20 |
| 6 | N | 498 | LYS | N-CA-CB | 6.50 | 122.31 | 110.60 |
| 4 | X | 452 | ARG | C-N-CA | 6.50 | 137.95 | 121.70 |
| 2 | U | 8 | GLU | O-C-N | 6.50 | 133.10 | 122.70 |
| 2 | I | 8 | GLU | O-C-N | 6.50 | 133.10 | 122.70 |
| 6 | T | 501 | GLU | CA-C-N | -6.50 | 102.90 | 117.20 |
| 3 | D | 446 | ILE | CB-CA-C | -6.50 | 98.61 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 452 | ARG | C-N-CA | 6.50 | 137.94 | 121.70 |
| 2 | O | 8 | GLU | O-C-N | 6.50 | 133.09 | 122.70 |
| 3 | P | 1451 | ARG | CA-C-N | -6.50 | 102.91 | 117.20 |
| 3 | P | 1484 | ASP | CA-C-O | -6.50 | 106.46 | 120.10 |
| 6 | T | 406 | LEU | CA-C-N | 6.50 | 131.49 | 117.20 |
| 3 | D | 1484 | ASP | CA-C-O | -6.49 | 106.46 | 120.10 |
| 6 | N | 406 | LEU | CA-C-N | 6.49 | 131.49 | 117.20 |
| 3 | P | 446 | ILE | CB-CA-C | -6.49 | 98.61 | 111.60 |
| 6 | H | 501 | GLU | CA-C-N | -6.49 | 102.92 | 117.20 |
| 6 | Z | 498 | LYS | N-CA-CB | 6.49 | 122.28 | 110.60 |
| 5 | G | 344 | ASP | CA-C-O | 6.49 | 133.73 | 120.10 |
| 4 | R | 452 | ARG | C-N-CA | 6.49 | 137.93 | 121.70 |
| 5 | S | 344 | ASP | CA-C-O | 6.47 | 133.69 | 120.10 |
| 1 | E | 395 | GLY | N-CA-C | -6.47 | 96.93 | 113.10 |
| 6 | H | 391 | GLN | C-N-CA | 6.47 | 137.87 | 121.70 |
| 6 | H | 498 | LYS | N-CA-CB | 6.47 | 122.25 | 110.60 |
| 6 | N | 391 | GLN | C-N-CA | 6.47 | 137.87 | 121.70 |
| 6 | T | 498 | LYS | N-CA-CB | 6.47 | 122.24 | 110.60 |
| 4 | F | 328 | VAL | CA-C-O | -6.47 | 106.52 | 120.10 |
| 1 | A | 395 | GLY | N-CA-C | -6.46 | 96.95 | 113.10 |
| 1 | W | 395 | GLY | N-CA-C | -6.46 | 96.96 | 113.10 |
| 6 | Z | 405 | ASP | CA-C-N | -6.46 | 103.00 | 117.20 |
| 6 | N | 406 | LEU | CB-CA-C | -6.45 | 97.94 | 110.20 |
| 1 | B | 395 | GLY | N-CA-C | -6.45 | 96.97 | 113.10 |
| 6 | H | 405 | ASP | CA-C-N | -6.45 | 103.01 | 117.20 |
| 4 | L | 320 | GLU | N-CA-CB | 6.45 | 122.21 | 110.60 |
| 1 | Q | 395 | GLY | N-CA-C | -6.45 | 96.97 | 113.10 |
| 4 | R | 328 | VAL | CA-C-O | -6.45 | 106.56 | 120.10 |
| 6 | N | 408 | SER | O-C-N | 6.44 | 133.34 | 121.10 |
| 1 | K | 395 | GLY | N-CA-C | -6.44 | 97.00 | 113.10 |
| 6 | T | 405 | ASP | CA-C-N | -6.44 | 103.04 | 117.20 |
| 4 | L | 328 | VAL | CA-C-O | -6.43 | 106.59 | 120.10 |
| 6 | T | 391 | GLN | C-N-CA | 6.43 | 137.79 | 121.70 |
| 6 | Z | 408 | SER | O-C-N | 6.43 | 133.32 | 121.10 |
| 6 | N | 405 | ASP | CA-C-N | -6.43 | 103.05 | 117.20 |
| 6 | T | 406 | LEU | CB-CA-C | -6.43 | 97.99 | 110.20 |
| 6 | Z | 406 | LEU | CB-CA-C | -6.43 | 97.99 | 110.20 |
| 6 | H | 406 | LEU | CB-CA-C | -6.42 | 97.99 | 110.20 |
| 4 | X | 328 | VAL | CA-C-O | -6.42 | 106.61 | 120.10 |
| 5 | M | 313 | ILE | N-CA-C | -6.42 | 93.66 | 111.00 |
| 6 | Z | 391 | GLN | C-N-CA | 6.42 | 137.75 | 121.70 |
| 4 | L | 398 | LYS | CA-C-N | 6.41 | 131.31 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | S | 338 | GLU | CB-CA-C | 6.41 | 123.22 | 110.40 |
| 6 | H | 408 | SER | O-C-N | 6.41 | 133.28 | 121.10 |
| 4 | R | 398 | LYS | CA-C-N | 6.41 | 131.30 | 117.20 |
| 5 | S | 352 | GLN | CB-CA-C | -6.41 | 97.58 | 110.40 |
| 5 | M | 352 | GLN | CB-CA-C | -6.41 | 97.59 | 110.40 |
| 6 | T | 408 | SER | O-C-N | 6.41 | 133.27 | 121.10 |
| 4 | X | 398 | LYS | CA-C-N | 6.41 | 131.29 | 117.20 |
| 4 | F | 320 | GLU | N-CA-CB | 6.40 | 122.12 | 110.60 |
| 5 | S | 313 | ILE | N-CA-C | -6.40 | 93.71 | 111.00 |
| 5 | Y | 313 | ILE | N-CA-C | -6.40 | 93.71 | 111.00 |
| 5 | G | 313 | ILE | N-CA-C | -6.40 | 93.72 | 111.00 |
| 5 | G | 352 | GLN | CB-CA-C | -6.40 | 97.60 | 110.40 |
| 4 | X | 305 | ASP | CA-C-N | -6.40 | 99.19 | 117.10 |
| 4 | F | 236 | ASP | N-CA-CB | 6.39 | 122.11 | 110.60 |
| 5 | Y | 352 | GLN | CB-CA-C | -6.39 | 97.62 | 110.40 |
| 4 | F | 305 | ASP | CA-C-N | -6.39 | 99.20 | 117.10 |
| 4 | F | 398 | LYS | CA-C-N | 6.39 | 131.26 | 117.20 |
| 5 | M | 338 | GLU | CB-CA-C | 6.38 | 123.17 | 110.40 |
| 4 | R | 236 | ASP | N-CA-CB | 6.38 | 122.09 | 110.60 |
| 4 | R | 305 | ASP | CA-C-N | -6.38 | 99.23 | 117.10 |
| 4 | X | 320 | GLU | N-CA-CB | 6.38 | 122.09 | 110.60 |
| 4 | L | 305 | ASP | CA-C-N | -6.38 | 99.24 | 117.10 |
| 4 | F | 299 | ASN | O-C-N | -6.38 | 108.98 | 121.10 |
| 4 | L | 299 | ASN | O-C-N | -6.38 | 108.98 | 121.10 |
| 4 | X | 236 | ASP | N-CA-CB | 6.38 | 122.08 | 110.60 |
| 5 | G | 338 | GLU | CB-CA-C | 6.38 | 123.15 | 110.40 |
| 4 | L | 236 | ASP | N-CA-CB | 6.38 | 122.08 | 110.60 |
| 5 | Y | 373 | THR | N-CA-CB | 6.37 | 122.41 | 110.30 |
| 4 | R | 320 | GLU | N-CA-CB | 6.37 | 122.07 | 110.60 |
| 5 | Y | 338 | GLU | CB-CA-C | 6.37 | 123.14 | 110.40 |
| 4 | F | 301 | PRO | C-N-CA | 6.37 | 137.62 | 121.70 |
| 4 | L | 301 | PRO | C-N-CA | 6.37 | 137.62 | 121.70 |
| 5 | S | 373 | THR | N-CA-CB | 6.37 | 122.40 | 110.30 |
| 4 | R | 299 | ASN | O-C-N | -6.36 | 109.01 | 121.10 |
| 4 | X | 301 | PRO | C-N-CA | 6.36 | 137.60 | 121.70 |
| 4 | X | 299 | ASN | O-C-N | -6.36 | 109.02 | 121.10 |
| 5 | M | 373 | THR | N-CA-CB | 6.35 | 122.37 | 110.30 |
| 4 | R | 301 | PRO | C-N-CA | 6.35 | 137.57 | 121.70 |
| 3 | D | 1518 | ASN | O-C-N | 6.34 | 132.85 | 122.70 |
| 5 | G | 373 | THR | N-CA-CB | 6.34 | 122.34 | 110.30 |
| 7 | V | 161 | CYS | C-N-CA | 6.33 | 137.53 | 121.70 |
| 3 | P | 1518 | ASN | O-C-N | 6.33 | 132.83 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 414 | SER | C-N-CA | 6.33 | 137.51 | 121.70 |
| 1 | K | 414 | SER | C-N-CA | 6.33 | 137.51 | 121.70 |
| 1 | E | 414 | SER | C-N-CA | 6.32 | 137.49 | 121.70 |
| 1 | K | 415 | LYS | N-CA-CB | 6.32 | 121.97 | 110.60 |
| 1 | A | 415 | LYS | N-CA-CB | 6.31 | 121.96 | 110.60 |
| 1 | A | 414 | SER | C-N-CA | 6.31 | 137.48 | 121.70 |
| 7 | J | 161 | CYS | C-N-CA | 6.31 | 137.47 | 121.70 |
| 1 | Q | 415 | LYS | N-CA-CB | 6.31 | 121.95 | 110.60 |
| 4 | F | 221 | GLN | N-CA-CB | -6.31 | 99.25 | 110.60 |
| 5 | Y | 329 | GLN | N-CA-CB | 6.31 | 121.95 | 110.60 |
| 1 | Q | 414 | SER | C-N-CA | 6.31 | 137.47 | 121.70 |
| 1 | W | 414 | SER | C-N-CA | 6.30 | 137.45 | 121.70 |
| 1 | W | 415 | LYS | N-CA-CB | 6.30 | 121.94 | 110.60 |
| 1 | E | 415 | LYS | N-CA-CB | 6.30 | 121.94 | 110.60 |
| 3 | D | 1516 | LEU | O-C-N | 6.30 | 132.77 | 122.70 |
| 5 | M | 329 | GLN | N-CA-CB | 6.29 | 121.92 | 110.60 |
| 3 | P | 1522 | LEU | C-N-CA | -6.29 | 105.97 | 121.70 |
| 6 | N | 407 | LEU | N-CA-C | -6.29 | 94.03 | 111.00 |
| 6 | H | 407 | LEU | N-CA-C | -6.29 | 94.03 | 111.00 |
| 4 | L | 419 | GLY | N-CA-C | -6.29 | 97.39 | 113.10 |
| 4 | X | 221 | GLN | N-CA-CB | -6.29 | 99.28 | 110.60 |
| 4 | X | 419 | GLY | N-CA-C | -6.29 | 97.38 | 113.10 |
| 3 | D | 1522 | LEU | C-N-CA | -6.28 | 105.99 | 121.70 |
| 5 | G | 329 | GLN | N-CA-CB | 6.28 | 121.91 | 110.60 |
| 6 | N | 415 | LYS | N-CA-CB | 6.28 | 121.91 | 110.60 |
| 4 | R | 221 | GLN | N-CA-CB | -6.28 | 99.29 | 110.60 |
| 6 | Z | 407 | LEU | N-CA-C | -6.28 | 94.05 | 111.00 |
| 1 | B | 415 | LYS | N-CA-CB | 6.28 | 121.90 | 110.60 |
| 5 | S | 329 | GLN | N-CA-CB | 6.28 | 121.90 | 110.60 |
| 6 | T | 407 | LEU | N-CA-C | -6.28 | 94.06 | 111.00 |
| 3 | P | 1516 | LEU | O-C-N | 6.27 | 132.74 | 122.70 |
| 3 | D | 1538 | SER | CA-C-O | -6.27 | 106.93 | 120.10 |
| 6 | H | 415 | LYS | N-CA-CB | 6.27 | 121.89 | 110.60 |
| 4 | R | 455 | ILE | O-C-N | -6.27 | 112.67 | 122.70 |
| 5 | Y | 344 | ASP | N-CA-CB | 6.27 | 121.88 | 110.60 |
| 6 | H | 413 | LEU | O-C-N | -6.26 | 112.67 | 122.70 |
| 4 | R | 419 | GLY | N-CA-C | -6.26 | 97.44 | 113.10 |
| 4 | L | 221 | GLN | N-CA-CB | -6.26 | 99.33 | 110.60 |
| 3 | P | 1538 | SER | CA-C-O | -6.26 | 106.95 | 120.10 |
| 6 | T | 415 | LYS | N-CA-CB | 6.26 | 121.87 | 110.60 |
| 4 | X | 211 | GLU | CA-C-O | 6.26 | 133.24 | 120.10 |
| 4 | F | 419 | GLY | N-CA-C | -6.26 | 97.46 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | F | 455 | ILE | O-C-N | -6.25 | 112.69 | 122.70 |
| 4 | L | 211 | GLU | CA-C-O | 6.25 | 133.23 | 120.10 |
| 4 | R | 251 | GLY | C-N-CA | 6.25 | 137.33 | 121.70 |
| 4 | F | 211 | GLU | CA-C-O | 6.25 | 133.22 | 120.10 |
| 4 | L | 251 | GLY | C-N-CA | 6.25 | 137.31 | 121.70 |
| 4 | L | 290 | PRO | N-CA-C | 6.25 | 128.34 | 112.10 |
| 7 | V | 1466 | TRP | N-CA-C | 6.25 | 127.86 | 111.00 |
| 6 | Z | 415 | LYS | N-CA-CB | 6.25 | 121.84 | 110.60 |
| 6 | T | 413 | LEU | O-C-N | -6.24 | 112.71 | 122.70 |
| 4 | X | 290 | PRO | N-CA-C | 6.24 | 128.32 | 112.10 |
| 5 | S | 344 | ASP | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 5 | Y | 379 | HIS | N-CA-C | 6.24 | 127.84 | 111.00 |
| 4 | F | 290 | PRO | N-CA-C | 6.23 | 128.31 | 112.10 |
| 6 | Z | 413 | LEU | O-C-N | -6.23 | 112.72 | 122.70 |
| 5 | G | 379 | HIS | N-CA-C | 6.23 | 127.83 | 111.00 |
| 7 | J | 1466 | TRP | N-CA-C | 6.23 | 127.83 | 111.00 |
| 4 | X | 251 | GLY | C-N-CA | 6.23 | 137.27 | 121.70 |
| 4 | R | 290 | PRO | N-CA-C | 6.23 | 128.29 | 112.10 |
| 5 | Y | 341 | ALA | N-CA-C | -6.23 | 94.18 | 111.00 |
| 5 | S | 379 | HIS | N-CA-C | 6.23 | 127.81 | 111.00 |
| 4 | X | 455 | ILE | O-C-N | -6.23 | 112.74 | 122.70 |
| 4 | F | 251 | GLY | C-N-CA | 6.22 | 137.26 | 121.70 |
| 5 | G | 344 | ASP | N-CA-CB | 6.22 | 121.80 | 110.60 |
| 5 | S | 341 | ALA | N-CA-C | -6.22 | 94.20 | 111.00 |
| 5 | Y | 330 | LYS | CA-C-O | 6.22 | 133.16 | 120.10 |
| 5 | G | 341 | ALA | N-CA-C | -6.22 | 94.21 | 111.00 |
| 5 | M | 379 | HIS | N-CA-C | 6.22 | 127.79 | 111.00 |
| 3 | P | 1667 | ALA | CB-CA-C | -6.22 | 100.77 | 110.10 |
| 4 | L | 247 | ARG | C-N-CA | -6.22 | 106.15 | 121.70 |
| 5 | G | 330 | LYS | CA-C-O | 6.22 | 133.15 | 120.10 |
| 6 | N | 413 | LEU | O-C-N | -6.22 | 112.75 | 122.70 |
| 4 | F | 247 | ARG | C-N-CA | -6.21 | 106.16 | 121.70 |
| 5 | M | 341 | ALA | N-CA-C | -6.21 | 94.23 | 111.00 |
| 4 | X | 247 | ARG | C-N-CA | -6.21 | 106.17 | 121.70 |
| 3 | D | 1667 | ALA | CB-CA-C | -6.21 | 100.79 | 110.10 |
| 7 | J | 1466 | TRP | C-N-CA | -6.20 | 106.19 | 121.70 |
| 4 | R | 247 | ARG | C-N-CA | -6.20 | 106.20 | 121.70 |
| 4 | L | 455 | ILE | O-C-N | -6.20 | 112.78 | 122.70 |
| 6 | H | 412 | GLU | N-CA-CB | 6.20 | 121.75 | 110.60 |
| 4 | R | 211 | GLU | CA-C-O | 6.20 | 133.11 | 120.10 |
| 5 | M | 330 | LYS | CA-C-O | 6.19 | 133.10 | 120.10 |
| 5 | M | 344 | ASP | N-CA-CB | 6.19 | 121.74 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | V | 1466 | TRP | C-N-CA | -6.19 | 106.22 | 121.70 |
| 5 | S | 330 | LYS | CA-C-O | 6.18 | 133.09 | 120.10 |
| 6 | N | 412 | GLU | N-CA-CB | 6.17 | 121.72 | 110.60 |
| 3 | P | 1519 | SER | O-C-N | 6.17 | 133.69 | 123.20 |
| 4 | R | 469 | GLN | C-N-CA | -6.17 | 106.27 | 121.70 |
| 6 | T | 412 | GLU | N-CA-CB | 6.17 | 121.70 | 110.60 |
| 4 | X | 469 | GLN | C-N-CA | -6.17 | 106.29 | 121.70 |
| 4 | L | 469 | GLN | C-N-CA | -6.17 | 106.29 | 121.70 |
| 6 | N | 414 | VAL | O-C-N | -6.16 | 112.84 | 122.70 |
| 6 | T | 414 | VAL | O-C-N | -6.16 | 112.84 | 122.70 |
| 6 | Z | 414 | VAL | O-C-N | -6.16 | 112.85 | 122.70 |
| 3 | D | 1519 | SER | O-C-N | 6.15 | 133.66 | 123.20 |
| 4 | F | 343 | MET | CB-CA-C | -6.15 | 98.09 | 110.40 |
| 4 | F | 469 | GLN | C-N-CA | -6.15 | 106.32 | 121.70 |
| 4 | L | 343 | MET | CB-CA-C | -6.15 | 98.10 | 110.40 |
| 6 | Z | 340 | TRP | C-N-CA | 6.15 | 137.08 | 121.70 |
| 5 | S | 264 | GLU | CB-CA-C | 6.15 | 122.69 | 110.40 |
| 6 | T | 340 | TRP | C-N-CA | 6.15 | 137.07 | 121.70 |
| 6 | H | 340 | TRP | C-N-CA | 6.15 | 137.06 | 121.70 |
| 2 | U | 28 | HIS | N-CA-CB | -6.14 | 99.54 | 110.60 |
| 6 | H | 414 | VAL | O-C-N | -6.14 | 112.88 | 122.70 |
| 4 | R | 343 | MET | CB-CA-C | -6.13 | 98.13 | 110.40 |
| 6 | Z | 412 | GLU | N-CA-CB | 6.13 | 121.64 | 110.60 |
| 2 | O | 28 | HIS | N-CA-CB | -6.13 | 99.56 | 110.60 |
| 5 | Y | 264 | GLU | CB-CA-C | 6.13 | 122.66 | 110.40 |
| 7 | J | 1482 | GLY | N-CA-C | 6.13 | 128.42 | 113.10 |
| 4 | F | 311 | GLN | CB-CA-C | -6.12 | 98.15 | 110.40 |
| 4 | X | 343 | MET | CB-CA-C | -6.12 | 98.16 | 110.40 |
| 7 | V | 1482 | GLY | N-CA-C | 6.12 | 128.39 | 113.10 |
| 5 | M | 264 | GLU | CB-CA-C | 6.11 | 122.63 | 110.40 |
| 6 | N | 340 | TRP | C-N-CA | 6.11 | 136.97 | 121.70 |
| 5 | G | 264 | GLU | CB-CA-C | 6.10 | 122.61 | 110.40 |
| 2 | I | 28 | HIS | N-CA-CB | -6.10 | 99.61 | 110.60 |
| 4 | R | 311 | GLN | CB-CA-C | -6.10 | 98.19 | 110.40 |
| 5 | G | 330 | LYS | C-N-CA | 6.10 | 136.95 | 121.70 |
| 5 | S | 330 | LYS | C-N-CA | 6.10 | 136.95 | 121.70 |
| 4 | X | 311 | GLN | CB-CA-C | -6.10 | 98.20 | 110.40 |
| 6 | T | 388 | ARG | N-CA-C | 6.09 | 127.45 | 111.00 |
| 2 | C | 28 | HIS | N-CA-CB | -6.09 | 99.64 | 110.60 |
| 5 | M | 330 | LYS | C-N-CA | 6.08 | 136.90 | 121.70 |
| 3 | P | 1531 | GLU | C-N-CA | 6.08 | 136.90 | 121.70 |
| 5 | Y | 330 | LYS | C-N-CA | 6.08 | 136.91 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | N | 384 | LEU | CB-CA-C | -6.08 | 98.65 | 110.20 |
| 3 | D | 1531 | GLU | C-N-CA | 6.08 | 136.89 | 121.70 |
| 5 | S | 348 | ILE | CB-CA-C | 6.08 | 123.75 | 111.60 |
| 6 | T | 384 | LEU | CB-CA-C | -6.08 | 98.66 | 110.20 |
| 6 | H | 388 | ARG | N-CA-C | 6.07 | 127.40 | 111.00 |
| 6 | Z | 384 | LEU | CB-CA-C | -6.07 | 98.66 | 110.20 |
| 4 | L | 311 | GLN | CB-CA-C | -6.07 | 98.26 | 110.40 |
| 4 | L | 489 | LYS | C-N-CA | -6.07 | 106.53 | 121.70 |
| 4 | F | 202 | ILE | N-CA-C | 6.07 | 127.38 | 111.00 |
| 6 | H | 384 | LEU | CB-CA-C | -6.07 | 98.68 | 110.20 |
| 4 | L | 202 | ILE | N-CA-C | 6.06 | 127.37 | 111.00 |
| 4 | R | 489 | LYS | C-N-CA | -6.06 | 106.55 | 121.70 |
| 5 | M | 348 | ILE | CB-CA-C | 6.06 | 123.71 | 111.60 |
| 4 | F | 489 | LYS | C-N-CA | -6.05 | 106.56 | 121.70 |
| 4 | L | 468 | LYS | O-C-N | 6.05 | 132.38 | 122.70 |
| 6 | Z | 388 | ARG | N-CA-C | 6.05 | 127.33 | 111.00 |
| 4 | X | 489 | LYS | C-N-CA | -6.05 | 106.58 | 121.70 |
| 5 | G | 348 | ILE | CB-CA-C | 6.04 | 123.69 | 111.60 |
| 6 | N | 388 | ARG | N-CA-C | 6.04 | 127.32 | 111.00 |
| 4 | X | 202 | ILE | N-CA-C | 6.04 | 127.32 | 111.00 |
| 5 | Y | 398 | ALA | CB-CA-C | -6.04 | 101.04 | 110.10 |
| 5 | Y | 348 | ILE | CB-CA-C | 6.03 | 123.67 | 111.60 |
| 2 | O | 308 | LEU | C-N-CA | 6.03 | 136.78 | 121.70 |
| 5 | S | 398 | ALA | CB-CA-C | -6.03 | 101.06 | 110.10 |
| 5 | Y | 251 | ILE | C-N-CA | -6.03 | 106.62 | 121.70 |
| 3 | D | 1536 | LEU | O-C-N | -6.03 | 113.06 | 122.70 |
| 3 | P | 1472 | SER | CA-C-O | 6.03 | 132.75 | 120.10 |
| 5 | M | 251 | ILE | C-N-CA | -6.02 | 106.64 | 121.70 |
| 2 | U | 308 | LEU | C-N-CA | 6.02 | 136.76 | 121.70 |
| 4 | R | 468 | LYS | O-C-N | 6.02 | 132.34 | 122.70 |
| 3 | D | 1472 | SER | CA-C-O | 6.02 | 132.74 | 120.10 |
| 4 | R | 202 | ILE | N-CA-C | 6.02 | 127.25 | 111.00 |
| 4 | L | 236 | ASP | C-N-CA | -6.02 | 106.66 | 121.70 |
| 4 | R | 236 | ASP | C-N-CA | -6.02 | 106.65 | 121.70 |
| 4 | X | 448 | ARG | C-N-CA | -6.01 | 106.66 | 121.70 |
| 4 | F | 236 | ASP | C-N-CA | -6.01 | 106.67 | 121.70 |
| 2 | I | 308 | LEU | C-N-CA | 6.01 | 136.73 | 121.70 |
| 3 | P | 1536 | LEU | O-C-N | -6.01 | 113.08 | 122.70 |
| 5 | G | 398 | ALA | CB-CA-C | -6.00 | 101.09 | 110.10 |
| 5 | M | 398 | ALA | CB-CA-C | -6.00 | 101.09 | 110.10 |
| 5 | S | 251 | ILE | C-N-CA | -6.00 | 106.69 | 121.70 |
| 4 | X | 468 | LYS | O-C-N | 6.00 | 132.30 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 1448 | MET | C-N-CA | 5.99 | 136.69 | 121.70 |
| 4 | L | 448 | ARG | C-N-CA | -5.99 | 106.72 | 121.70 |
| 4 | X | 236 | ASP | C-N-CA | -5.99 | 106.72 | 121.70 |
| 2 | C | 308 | LEU | C-N-CA | 5.99 | 136.68 | 121.70 |
| 4 | F | 468 | LYS | O-C-N | 5.99 | 132.28 | 122.70 |
| 4 | F | 199 | GLU | CA-C-O | 5.99 | 132.67 | 120.10 |
| 4 | R | 448 | ARG | C-N-CA | -5.99 | 106.73 | 121.70 |
| 5 | G | 327 | ARG | N-CA-C | 5.99 | 127.16 | 111.00 |
| 5 | G | 251 | ILE | C-N-CA | -5.98 | 106.74 | 121.70 |
| 3 | P | 1448 | MET | C-N-CA | 5.98 | 136.65 | 121.70 |
| 4 | R | 199 | GLU | CA-C-O | 5.98 | 132.66 | 120.10 |
| 4 | F | 491 | VAL | CA-C-O | 5.98 | 132.66 | 120.10 |
| 4 | R | 222 | THR | N-CA-CB | 5.98 | 121.66 | 110.30 |
| 4 | X | 199 | GLU | CA-C-O | 5.98 | 132.66 | 120.10 |
| 4 | X | 491 | VAL | CA-C-O | 5.98 | 132.65 | 120.10 |
| 4 | F | 448 | ARG | C-N-CA | -5.97 | 106.76 | 121.70 |
| 4 | R | 207 | GLN | O-C-N | 5.97 | 132.26 | 122.70 |
| 4 | R | 491 | VAL | CA-C-O | 5.97 | 132.64 | 120.10 |
| 5 | Y | 327 | ARG | N-CA-C | 5.97 | 127.12 | 111.00 |
| 5 | S | 327 | ARG | N-CA-C | 5.97 | 127.11 | 111.00 |
| 4 | L | 207 | GLN | O-C-N | 5.96 | 132.24 | 122.70 |
| 5 | M | 327 | ARG | N-CA-C | 5.96 | 127.08 | 111.00 |
| 4 | L | 394 | GLU | C-N-CA | -5.95 | 106.82 | 121.70 |
| 4 | X | 207 | GLN | O-C-N | 5.95 | 132.22 | 122.70 |
| 4 | F | 222 | THR | N-CA-CB | 5.95 | 121.60 | 110.30 |
| 7 | J | 157 | GLU | N-CA-C | -5.95 | 94.94 | 111.00 |
| 4 | X | 394 | GLU | C-N-CA | -5.95 | 106.83 | 121.70 |
| 4 | L | 222 | THR | N-CA-CB | 5.95 | 121.59 | 110.30 |
| 4 | F | 207 | GLN | O-C-N | 5.94 | 132.21 | 122.70 |
| 4 | L | 491 | VAL | CA-C-O | 5.94 | 132.57 | 120.10 |
| 4 | R | 394 | GLU | C-N-CA | -5.94 | 106.85 | 121.70 |
| 7 | V | 157 | GLU | N-CA-C | -5.94 | 94.96 | 111.00 |
| 4 | L | 199 | GLU | CA-C-O | 5.94 | 132.57 | 120.10 |
| 4 | F | 394 | GLU | C-N-CA | -5.94 | 106.86 | 121.70 |
| 4 | F | 461 | ARG | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 4 | X | 222 | THR | N-CA-CB | 5.93 | 121.58 | 110.30 |
| 4 | R | 253 | SER | CB-CA-C | 5.93 | 121.37 | 110.10 |
| 4 | X | 461 | ARG | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 4 | F | 253 | SER | CB-CA-C | 5.93 | 121.37 | 110.10 |
| 4 | L | 461 | ARG | N-CA-CB | 5.93 | 121.27 | 110.60 |
| 4 | L | 253 | SER | CB-CA-C | 5.92 | 121.35 | 110.10 |
| 3 | D | 1503 | ILE | C-N-CA | 5.92 | 136.50 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 463 | ILE | N-CA-C | -5.92 | 95.03 | 111.00 |
| 6 | Z | 394 | ASP | CA-C-N | -5.91 | 104.19 | 117.20 |
| 3 | P | 1503 | ILE | C-N-CA | 5.91 | 136.48 | 121.70 |
| 6 | H | 394 | ASP | CA-C-N | -5.91 | 104.20 | 117.20 |
| 6 | T | 501 | GLU | N-CA-CB | 5.91 | 121.24 | 110.60 |
| 4 | L | 463 | ILE | N-CA-C | -5.91 | 95.05 | 111.00 |
| 4 | R | 461 | ARG | N-CA-CB | 5.91 | 121.23 | 110.60 |
| 4 | X | 463 | ILE | N-CA-C | -5.91 | 95.05 | 111.00 |
| 4 | X | 253 | SER | CB-CA-C | 5.91 | 121.32 | 110.10 |
| 6 | Z | 501 | GLU | N-CA-CB | 5.90 | 121.22 | 110.60 |
| 6 | N | 394 | ASP | CA-C-N | -5.90 | 104.22 | 117.20 |
| 5 | Y | 345 | TYR | O-C-N | -5.90 | 113.26 | 122.70 |
| 4 | F | 463 | ILE | N-CA-C | -5.90 | 95.08 | 111.00 |
| 5 | Y | 361 | ARG | N-CA-C | -5.89 | 95.09 | 111.00 |
| 4 | X | 306 | PRO | CA-C-N | 5.89 | 130.16 | 117.20 |
| 6 | N | 352 | LEU | CB-CA-C | 5.89 | 121.39 | 110.20 |
| 4 | F | 306 | PRO | CA-C-N | 5.89 | 130.15 | 117.20 |
| 4 | L | 453 | TYR | N-CA-CB | 5.88 | 121.19 | 110.60 |
| 5 | M | 345 | TYR | O-C-N | -5.88 | 113.28 | 122.70 |
| 5 | M | 342 | PRO | N-CA-C | 5.88 | 127.39 | 112.10 |
| 4 | R | 453 | TYR | N-CA-CB | 5.88 | 121.19 | 110.60 |
| 6 | Z | 352 | LEU | CB-CA-C | 5.88 | 121.38 | 110.20 |
| 4 | F | 453 | TYR | N-CA-CB | 5.88 | 121.18 | 110.60 |
| 6 | H | 501 | GLU | N-CA-CB | 5.88 | 121.18 | 110.60 |
| 4 | X | 446 | ALA | N-CA-CB | 5.88 | 118.33 | 110.10 |
| 5 | S | 361 | ARG | N-CA-C | -5.88 | 95.13 | 111.00 |
| 5 | Y | 342 | PRO | N-CA-C | 5.88 | 127.38 | 112.10 |
| 4 | R | 306 | PRO | CA-C-N | 5.87 | 130.12 | 117.20 |
| 6 | T | 352 | LEU | CB-CA-C | 5.87 | 121.36 | 110.20 |
| 5 | G | 361 | ARG | N-CA-C | -5.87 | 95.15 | 111.00 |
| 5 | G | 345 | TYR | O-C-N | -5.87 | 113.31 | 122.70 |
| 5 | S | 342 | PRO | N-CA-C | 5.87 | 127.36 | 112.10 |
| 4 | X | 453 | TYR | N-CA-CB | 5.87 | 121.17 | 110.60 |
| 5 | S | 345 | TYR | O-C-N | -5.87 | 113.31 | 122.70 |
| 4 | L | 306 | PRO | CA-C-N | 5.87 | 130.10 | 117.20 |
| 5 | G | 342 | PRO | N-CA-C | 5.86 | 127.35 | 112.10 |
| 5 | M | 361 | ARG | N-CA-C | -5.86 | 95.17 | 111.00 |
| 6 | N | 501 | GLU | N-CA-CB | 5.86 | 121.15 | 110.60 |
| 6 | T | 394 | ASP | CA-C-N | -5.86 | 104.30 | 117.20 |
| 4 | L | 446 | ALA | N-CA-CB | 5.85 | 118.29 | 110.10 |
| 4 | L | 457 | ALA | C-N-CA | -5.84 | 107.10 | 121.70 |
| 6 | H | 352 | LEU | CB-CA-C | 5.84 | 121.30 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 457 | ALA | C-N-CA | -5.84 | 107.10 | 121.70 |
| 6 | Z | 410 | LEU | C-N-CA | 5.84 | 136.30 | 121.70 |
| 4 | R | 457 | ALA | C-N-CA | -5.84 | 107.11 | 121.70 |
| 4 | F | 457 | ALA | C-N-CA | -5.83 | 107.13 | 121.70 |
| 6 | T | 470 | PRO | O-C-N | -5.83 | 113.38 | 122.70 |
| 4 | F | 488 | ILE | N-CA-C | 5.83 | 126.73 | 111.00 |
| 6 | T | 415 | LYS | C-N-CA | -5.83 | 107.14 | 121.70 |
| 6 | Z | 473 | GLN | N-CA-CB | 5.82 | 121.08 | 110.60 |
| 6 | T | 473 | GLN | N-CA-CB | 5.82 | 121.07 | 110.60 |
| 6 | N | 410 | LEU | C-N-CA | 5.82 | 136.24 | 121.70 |
| 6 | N | 470 | PRO | O-C-N | -5.82 | 113.39 | 122.70 |
| 4 | R | 343 | MET | CA-C-O | 5.82 | 132.31 | 120.10 |
| 2 | O | 6 | PHE | C-N-CA | 5.81 | 134.51 | 122.30 |
| 7 | J | 161 | CYS | CB-CA-C | -5.81 | 98.78 | 110.40 |
| 4 | R | 488 | ILE | N-CA-C | 5.81 | 126.69 | 111.00 |
| 2 | C | 6 | PHE | C-N-CA | 5.81 | 134.50 | 122.30 |
| 6 | N | 415 | LYS | C-N-CA | -5.81 | 107.18 | 121.70 |
| 6 | T | 410 | LEU | C-N-CA | 5.81 | 136.22 | 121.70 |
| 4 | X | 490 | LEU | CA-C-O | 5.81 | 132.29 | 120.10 |
| 5 | Y | 312 | LYS | CA-C-N | -5.81 | 104.42 | 117.20 |
| 4 | L | 488 | ILE | N-CA-C | 5.81 | 126.68 | 111.00 |
| 4 | F | 446 | ALA | N-CA-CB | 5.80 | 118.23 | 110.10 |
| 6 | H | 410 | LEU | C-N-CA | 5.80 | 136.21 | 121.70 |
| 6 | N | 473 | GLN | N-CA-CB | 5.80 | 121.05 | 110.60 |
| 6 | Z | 415 | LYS | C-N-CA | -5.80 | 107.19 | 121.70 |
| 4 | X | 343 | MET | CA-C-O | 5.80 | 132.29 | 120.10 |
| 6 | Z | 470 | PRO | O-C-N | -5.80 | 113.42 | 122.70 |
| 4 | F | 343 | MET | CA-C-O | 5.80 | 132.28 | 120.10 |
| 5 | M | 312 | LYS | CA-C-N | -5.80 | 104.44 | 117.20 |
| 2 | U | 6 | PHE | C-N-CA | 5.80 | 134.48 | 122.30 |
| 5 | G | 312 | LYS | CA-C-N | -5.80 | 104.44 | 117.20 |
| 4 | X | 488 | ILE | N-CA-C | 5.80 | 126.65 | 111.00 |
| 2 | C | 14 | GLU | C-N-CA | 5.79 | 136.18 | 121.70 |
| 2 | O | 14 | GLU | C-N-CA | 5.79 | 136.18 | 121.70 |
| 7 | V | 161 | CYS | CB-CA-C | -5.79 | 98.82 | 110.40 |
| 2 | I | 14 | GLU | C-N-CA | 5.79 | 136.17 | 121.70 |
| 4 | R | 446 | ALA | N-CA-CB | 5.79 | 118.21 | 110.10 |
| 4 | L | 343 | MET | CA-C-O | 5.79 | 132.25 | 120.10 |
| 5 | S | 312 | LYS | CA-C-N | -5.78 | 104.47 | 117.20 |
| 5 | G | 343 | ALA | C-N-CA | 5.78 | 136.16 | 121.70 |
| 6 | H | 473 | GLN | N-CA-CB | 5.78 | 121.01 | 110.60 |
| 4 | R | 490 | LEU | CA-C-O | 5.78 | 132.24 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | V | 1440 | VAL | C-N-CA | -5.78 | 107.25 | 121.70 |
| 7 | J | 1440 | VAL | C-N-CA | -5.78 | 107.25 | 121.70 |
| 4 | L | 490 | LEU | CA-C-O | 5.78 | 132.23 | 120.10 |
| 5 | S | 343 | ALA | C-N-CA | 5.78 | 136.14 | 121.70 |
| 6 | H | 415 | LYS | C-N-CA | -5.78 | 107.26 | 121.70 |
| 2 | I | 6 | PHE | C-N-CA | 5.78 | 134.43 | 122.30 |
| 2 | C | 8 | GLU | N-CA-CB | 5.77 | 120.99 | 110.60 |
| 6 | H | 470 | PRO | O-C-N | -5.77 | 113.47 | 122.70 |
| 4 | L | 454 | TYR | CB-CA-C | 5.77 | 121.93 | 110.40 |
| 5 | Y | 343 | ALA | C-N-CA | 5.77 | 136.11 | 121.70 |
| 5 | S | 338 | GLU | N-CA-CB | 5.76 | 120.97 | 110.60 |
| 5 | M | 343 | ALA | C-N-CA | 5.76 | 136.10 | 121.70 |
| 2 | U | 14 | GLU | C-N-CA | 5.76 | 136.10 | 121.70 |
| 2 | C | 484 | ARG | CA-C-N | -5.76 | 104.53 | 117.20 |
| 2 | O | 8 | GLU | N-CA-CB | 5.76 | 120.97 | 110.60 |
| 4 | F | 397 | ARG | CB-CA-C | -5.76 | 98.88 | 110.40 |
| 4 | R | 397 | ARG | CB-CA-C | -5.76 | 98.89 | 110.40 |
| 4 | X | 397 | ARG | CB-CA-C | -5.76 | 98.89 | 110.40 |
| 4 | X | 454 | TYR | CB-CA-C | 5.76 | 121.92 | 110.40 |
| 3 | D | 1540 | LEU | C-N-CA | -5.75 | 107.31 | 121.70 |
| 4 | F | 454 | TYR | CB-CA-C | 5.75 | 121.91 | 110.40 |
| 2 | I | 8 | GLU | N-CA-CB | 5.75 | 120.95 | 110.60 |
| 2 | I | 484 | ARG | CA-C-N | -5.75 | 104.54 | 117.20 |
| 3 | P | 1540 | LEU | C-N-CA | -5.75 | 107.31 | 121.70 |
| 2 | U | 8 | GLU | N-CA-CB | 5.75 | 120.96 | 110.60 |
| 5 | Y | 338 | GLU | N-CA-CB | 5.75 | 120.96 | 110.60 |
| 4 | F | 490 | LEU | CA-C-O | 5.75 | 132.18 | 120.10 |
| 5 | G | 338 | GLU | N-CA-CB | 5.75 | 120.95 | 110.60 |
| 5 | G | 393 | TYR | CA-C-N | 5.75 | 129.85 | 117.20 |
| 4 | L | 397 | ARG | CB-CA-C | -5.75 | 98.90 | 110.40 |
| 5 | Y | 393 | TYR | CA-C-N | 5.75 | 129.84 | 117.20 |
| 5 | Y | 378 | SER | O-C-N | -5.74 | 113.51 | 122.70 |
| 4 | R | 454 | TYR | CB-CA-C | 5.74 | 121.88 | 110.40 |
| 2 | U | 6 | PHE | N-CA-CB | -5.74 | 100.27 | 110.60 |
| 2 | U | 484 | ARG | CA-C-N | -5.74 | 104.57 | 117.20 |
| 5 | M | 338 | GLU | N-CA-CB | 5.74 | 120.93 | 110.60 |
| 5 | S | 393 | TYR | CA-C-N | 5.74 | 129.83 | 117.20 |
| 2 | O | 15 | GLN | N-CA-C | -5.73 | 95.53 | 111.00 |
| 2 | O | 484 | ARG | CA-C-N | -5.73 | 104.59 | 117.20 |
| 2 | C | 6 | PHE | N-CA-CB | -5.73 | 100.29 | 110.60 |
| 2 | C | 15 | GLN | N-CA-C | -5.73 | 95.53 | 111.00 |
| 2 | I | 15 | GLN | N-CA-C | -5.73 | 95.53 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 344 | ASP | O-C-N | -5.73 | 113.53 | 122.70 |
| 5 | M | 378 | SER | O-C-N | -5.73 | 113.53 | 122.70 |
| 5 | G | 378 | SER | O-C-N | -5.73 | 113.53 | 122.70 |
| 4 | L | 269 | ASN | N-CA-C | -5.73 | 95.54 | 111.00 |
| 2 | U | 15 | GLN | N-CA-C | -5.72 | 95.55 | 111.00 |
| 5 | S | 378 | SER | O-C-N | -5.72 | 113.55 | 122.70 |
| 4 | F | 269 | ASN | N-CA-C | -5.72 | 95.56 | 111.00 |
| 5 | M | 393 | TYR | CA-C-N | 5.71 | 129.77 | 117.20 |
| 1 | W | 395 | GLY | C-N-CA | 5.71 | 135.98 | 121.70 |
| 5 | S | 341 | ALA | N-CA-CB | 5.71 | 118.10 | 110.10 |
| 2 | I | 6 | PHE | N-CA-CB | -5.71 | 100.33 | 110.60 |
| 6 | N | 493 | ALA | CA-C-N | 5.71 | 129.75 | 117.20 |
| 1 | B | 395 | GLY | C-N-CA | 5.70 | 135.96 | 121.70 |
| 2 | O | 6 | PHE | N-CA-CB | -5.70 | 100.34 | 110.60 |
| 4 | X | 269 | ASN | N-CA-C | -5.70 | 95.61 | 111.00 |
| 1 | E | 395 | GLY | C-N-CA | 5.70 | 135.95 | 121.70 |
| 4 | R | 269 | ASN | N-CA-C | -5.70 | 95.61 | 111.00 |
| 5 | Y | 344 | ASP | O-C-N | -5.70 | 113.58 | 122.70 |
| 1 | Q | 395 | GLY | C-N-CA | 5.70 | 135.94 | 121.70 |
| 6 | Z | 493 | ALA | CA-C-N | 5.70 | 129.73 | 117.20 |
| 5 | G | 344 | ASP | O-C-N | -5.69 | 113.59 | 122.70 |
| 4 | F | 200 | THR | N-CA-C | 5.69 | 126.37 | 111.00 |
| 5 | M | 312 | LYS | O-C-N | 5.69 | 131.81 | 122.70 |
| 4 | F | 453 | TYR | C-N-CA | -5.69 | 107.48 | 121.70 |
| 1 | K | 395 | GLY | C-N-CA | 5.69 | 135.92 | 121.70 |
| 5 | S | 344 | ASP | O-C-N | -5.69 | 113.60 | 122.70 |
| 4 | F | 486 | GLU | CB-CA-C | 5.68 | 121.76 | 110.40 |
| 4 | L | 200 | THR | N-CA-C | 5.68 | 126.34 | 111.00 |
| 3 | P | 1485 | ALA | N-CA-C | -5.68 | 95.67 | 111.00 |
| 3 | D | 1485 | ALA | N-CA-C | -5.68 | 95.67 | 111.00 |
| 4 | L | 486 | GLU | CB-CA-C | 5.68 | 121.76 | 110.40 |
| 4 | R | 200 | THR | N-CA-C | 5.68 | 126.33 | 111.00 |
| 4 | X | 486 | GLU | CB-CA-C | 5.68 | 121.76 | 110.40 |
| 3 | P | 1537 | GLN | CA-C-O | 5.68 | 132.02 | 120.10 |
| 4 | X | 200 | THR | N-CA-C | 5.67 | 126.32 | 111.00 |
| 1 | A | 395 | GLY | C-N-CA | 5.67 | 135.88 | 121.70 |
| 3 | P | 1491 | ILE | CB-CA-C | -5.67 | 100.26 | 111.60 |
| 5 | G | 312 | LYS | O-C-N | 5.67 | 131.77 | 122.70 |
| 4 | X | 453 | TYR | C-N-CA | -5.67 | 107.53 | 121.70 |
| 5 | M | 341 | ALA | N-CA-CB | 5.67 | 118.03 | 110.10 |
| 4 | R | 453 | TYR | C-N-CA | -5.67 | 107.54 | 121.70 |
| 4 | R | 486 | GLU | CB-CA-C | 5.67 | 121.73 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | G | 253 | GLN | O-C-N | 5.66 | 131.76 | 122.70 |
| 6 | H | 493 | ALA | CA-C-N | 5.66 | 129.66 | 117.20 |
| 4 | L | 453 | TYR | C-N-CA | -5.66 | 107.54 | 121.70 |
| 5 | S | 253 | GLN | O-C-N | 5.66 | 131.76 | 122.70 |
| 6 | T | 493 | ALA | CA-C-N | 5.66 | 129.66 | 117.20 |
| 5 | Y | 312 | LYS | O-C-N | 5.66 | 131.76 | 122.70 |
| 3 | P | 878 | PRO | N-CA-C | 5.66 | 126.82 | 112.10 |
| 3 | D | 1491 | ILE | CB-CA-C | -5.66 | 100.28 | 111.60 |
| 5 | G | 341 | ALA | N-CA-CB | 5.66 | 118.03 | 110.10 |
| 5 | Y | 341 | ALA | N-CA-CB | 5.66 | 118.02 | 110.10 |
| 3 | D | 1537 | GLN | CA-C-O | 5.66 | 131.98 | 120.10 |
| 4 | X | 403 | ILE | CA-C-O | 5.65 | 131.97 | 120.10 |
| 4 | X | 472 | GLU | N-CA-C | -5.65 | 95.74 | 111.00 |
| 3 | D | 878 | PRO | N-CA-C | 5.65 | 126.78 | 112.10 |
| 3 | D | 1517 | SER | CA-C-N | -5.65 | 104.78 | 117.20 |
| 5 | Y | 253 | GLN | O-C-N | 5.64 | 131.72 | 122.70 |
| 4 | F | 232 | THR | CA-C-O | -5.63 | 108.27 | 120.10 |
| 4 | L | 401 | TYR | CA-C-O | 5.63 | 131.92 | 120.10 |
| 3 | P | 1517 | SER | CA-C-N | -5.63 | 104.81 | 117.20 |
| 4 | L | 472 | GLU | N-CA-C | -5.63 | 95.80 | 111.00 |
| 4 | X | 367 | THR | CA-C-O | -5.63 | 108.28 | 120.10 |
| 6 | Z | 385 | ASP | C-N-CA | -5.62 | 107.64 | 121.70 |
| 4 | F | 403 | ILE | CA-C-O | 5.62 | 131.90 | 120.10 |
| 4 | L | 367 | THR | CA-C-O | -5.62 | 108.30 | 120.10 |
| 4 | R | 403 | ILE | CA-C-O | 5.62 | 131.91 | 120.10 |
| 4 | R | 472 | GLU | N-CA-C | -5.62 | 95.82 | 111.00 |
| 6 | N | 385 | ASP | C-N-CA | -5.62 | 107.65 | 121.70 |
| 4 | F | 367 | THR | O-C-N | -5.62 | 113.71 | 122.70 |
| 4 | X | 403 | ILE | N-CA-C | 5.62 | 126.17 | 111.00 |
| 4 | F | 472 | GLU | N-CA-C | -5.62 | 95.83 | 111.00 |
| 4 | F | 403 | ILE | N-CA-C | 5.62 | 126.16 | 111.00 |
| 4 | L | 403 | ILE | CA-C-O | 5.62 | 131.89 | 120.10 |
| 5 | M | 253 | GLN | O-C-N | 5.62 | 131.69 | 122.70 |
| 4 | R | 403 | ILE | N-CA-C | 5.62 | 126.16 | 111.00 |
| 4 | R | 367 | THR | CA-C-O | -5.61 | 108.31 | 120.10 |
| 7 | V | 1474 | MET | N-CA-C | 5.61 | 126.15 | 111.00 |
| 5 | S | 312 | LYS | O-C-N | 5.61 | 131.68 | 122.70 |
| 3 | D | 1505 | SER | C-N-CA | -5.61 | 107.68 | 121.70 |
| 4 | R | 232 | THR | CA-C-O | -5.61 | 108.33 | 120.10 |
| 7 | J | 1474 | MET | N-CA-C | 5.60 | 126.13 | 111.00 |
| 4 | R | 401 | TYR | CA-C-O | 5.60 | 131.87 | 120.10 |
| 4 | R | 463 | ILE | CA-C-O | -5.60 | 108.33 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 232 | THR | CA-C-O | -5.60 | 108.33 | 120.10 |
| 5 | Y | 384 | ASP | CB-CA-C | -5.60 | 99.20 | 110.40 |
| 3 | D | 1448 | MET | O-C-N | 5.60 | 131.66 | 122.70 |
| 4 | F | 367 | THR | CA-C-O | -5.60 | 108.35 | 120.10 |
| 3 | P | 1448 | MET | O-C-N | 5.60 | 131.66 | 122.70 |
| 3 | P | 1505 | SER | C-N-CA | -5.60 | 107.71 | 121.70 |
| 4 | L | 403 | ILE | N-CA-C | 5.59 | 126.11 | 111.00 |
| 4 | L | 464 | LYS | CA-C-N | -5.59 | 104.89 | 117.20 |
| 6 | N | 353 | GLN | CB-CA-C | -5.59 | 99.21 | 110.40 |
| 6 | H | 385 | ASP | C-N-CA | -5.59 | 107.72 | 121.70 |
| 4 | L | 367 | THR | O-C-N | -5.59 | 113.75 | 122.70 |
| 5 | G | 384 | ASP | CB-CA-C | -5.59 | 99.22 | 110.40 |
| 4 | X | 401 | TYR | CA-C-O | 5.59 | 131.84 | 120.10 |
| 5 | M | 384 | ASP | CB-CA-C | -5.59 | 99.22 | 110.40 |
| 4 | F | 343 | MET | CA-C-N | -5.59 | 104.91 | 117.20 |
| 4 | F | 401 | TYR | CA-C-O | 5.58 | 131.83 | 120.10 |
| 5 | S | 384 | ASP | CB-CA-C | -5.58 | 99.23 | 110.40 |
| 6 | T | 385 | ASP | C-N-CA | -5.58 | 107.74 | 121.70 |
| 4 | X | 232 | THR | CA-C-O | -5.58 | 108.37 | 120.10 |
| 4 | L | 343 | MET | CA-C-N | -5.58 | 104.93 | 117.20 |
| 6 | H | 353 | GLN | CB-CA-C | -5.58 | 99.25 | 110.40 |
| 6 | T | 353 | GLN | CB-CA-C | -5.58 | 99.25 | 110.40 |
| 4 | X | 367 | THR | O-C-N | -5.58 | 113.78 | 122.70 |
| 4 | L | 463 | ILE | CA-C-O | -5.57 | 108.40 | 120.10 |
| 7 | V | 292 | GLU | CB-CA-C | -5.57 | 99.26 | 110.40 |
| 6 | Z | 353 | GLN | CB-CA-C | -5.57 | 99.26 | 110.40 |
| 5 | G | 302 | GLN | N-CA-CB | 5.57 | 120.62 | 110.60 |
| 4 | R | 367 | THR | O-C-N | -5.57 | 113.79 | 122.70 |
| 4 | R | 464 | LYS | CA-C-N | -5.57 | 104.95 | 117.20 |
| 4 | X | 464 | LYS | CA-C-N | -5.56 | 104.96 | 117.20 |
| 7 | J | 292 | GLU | CB-CA-C | -5.56 | 99.27 | 110.40 |
| 4 | R | 343 | MET | CA-C-N | -5.56 | 104.96 | 117.20 |
| 4 | X | 463 | ILE | CA-C-O | -5.56 | 108.42 | 120.10 |
| 2 | I | 252 | MET | N-CA-CB | 5.56 | 120.60 | 110.60 |
| 4 | X | 343 | MET | CA-C-N | -5.56 | 104.98 | 117.20 |
| 4 | F | 464 | LYS | CA-C-N | -5.55 | 104.98 | 117.20 |
| 4 | F | 463 | ILE | CA-C-O | -5.55 | 108.44 | 120.10 |
| 5 | S | 302 | GLN | N-CA-CB | 5.55 | 120.59 | 110.60 |
| 5 | M | 302 | GLN | N-CA-CB | 5.55 | 120.59 | 110.60 |
| 2 | C | 252 | MET | N-CA-CB | 5.54 | 120.58 | 110.60 |
| 3 | D | 1517 | SER | N-CA-CB | 5.54 | 118.82 | 110.50 |
| 2 | U | 252 | MET | N-CA-CB | 5.54 | 120.58 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | Z | 490 | GLN | CA-C-N | -5.54 | 105.00 | 117.20 |
| 1 | E | 442 | GLN | C-N-CA | 5.54 | 135.55 | 121.70 |
| 6 | N | 490 | GLN | CA-C-N | -5.54 | 105.02 | 117.20 |
| 6 | T | 490 | GLN | CA-C-N | -5.54 | 105.02 | 117.20 |
| 6 | H | 490 | GLN | CA-C-N | -5.54 | 105.02 | 117.20 |
| 2 | O | 252 | MET | N-CA-CB | 5.54 | 120.56 | 110.60 |
| 4 | F | 397 | ARG | CA-C-O | 5.53 | 131.72 | 120.10 |
| 6 | H | 428 | GLU | C-N-CA | -5.53 | 107.87 | 121.70 |
| 1 | Q | 442 | GLN | C-N-CA | 5.53 | 135.53 | 121.70 |
| 1 | W | 442 | GLN | C-N-CA | 5.53 | 135.53 | 121.70 |
| 1 | B | 442 | GLN | C-N-CA | 5.53 | 135.53 | 121.70 |
| 5 | Y | 302 | GLN | N-CA-CB | 5.53 | 120.55 | 110.60 |
| 1 | K | 442 | GLN | C-N-CA | 5.52 | 135.51 | 121.70 |
| 1 | A | 442 | GLN | C-N-CA | 5.52 | 135.50 | 121.70 |
| 4 | L | 397 | ARG | CA-C-O | 5.52 | 131.70 | 120.10 |
| 3 | P | 1667 | ALA | N-CA-CB | 5.52 | 117.83 | 110.10 |
| 4 | L | 443 | HIS | CB-CA-C | 5.52 | 121.44 | 110.40 |
| 3 | P | 1489 | HIS | CA-C-N | 5.52 | 129.35 | 117.20 |
| 6 | Z | 428 | GLU | C-N-CA | -5.52 | 107.90 | 121.70 |
| 4 | R | 415 | ASP | O-C-N | 5.52 | 131.53 | 122.70 |
| 3 | D | 1489 | HIS | CA-C-N | 5.51 | 129.33 | 117.20 |
| 4 | F | 443 | HIS | CB-CA-C | 5.51 | 121.43 | 110.40 |
| 4 | R | 443 | HIS | CB-CA-C | 5.51 | 121.43 | 110.40 |
| 3 | P | 1517 | SER | N-CA-CB | 5.51 | 118.77 | 110.50 |
| 4 | X | 443 | HIS | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 4 | X | 397 | ARG | CA-C-O | 5.51 | 131.67 | 120.10 |
| 3 | D | 1489 | HIS | N-CA-C | -5.51 | 96.13 | 111.00 |
| 6 | T | 428 | GLU | C-N-CA | -5.51 | 107.93 | 121.70 |
| 6 | Z | 377 | ARG | C-N-CA | -5.51 | 107.93 | 121.70 |
| 3 | P | 1489 | HIS | N-CA-C | -5.50 | 96.14 | 111.00 |
| 2 | U | 1 | MET | CB-CA-C | -5.50 | 99.39 | 110.40 |
| 5 | G | 352 | GLN | N-CA-C | 5.50 | 125.86 | 111.00 |
| 5 | S | 264 | GLU | N-CA-C | -5.50 | 96.14 | 111.00 |
| 4 | X | 415 | ASP | O-C-N | 5.50 | 131.50 | 122.70 |
| 5 | M | 264 | GLU | N-CA-C | -5.50 | 96.15 | 111.00 |
| 6 | N | 428 | GLU | C-N-CA | -5.50 | 107.95 | 121.70 |
| 4 | R | 397 | ARG | CA-C-O | 5.50 | 131.65 | 120.10 |
| 6 | T | 377 | ARG | C-N-CA | -5.50 | 107.96 | 121.70 |
| 7 | V | 708 | MET | N-CA-CB | 5.50 | 120.49 | 110.60 |
| 2 | I | 1 | MET | CB-CA-C | -5.49 | 99.41 | 110.40 |
| 3 | P | 1538 | SER | O-C-N | 5.49 | 131.48 | 122.70 |
| 4 | R | 207 | GLN | N-CA-CB | -5.49 | 100.72 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | N | 408 | SER | CA-C-O | -5.49 | 108.57 | 120.10 |
| 5 | M | 352 | GLN | N-CA-C | 5.49 | 125.82 | 111.00 |
| 7 | J | 708 | MET | N-CA-CB | 5.49 | 120.47 | 110.60 |
| 6 | N | 377 | ARG | C-N-CA | -5.49 | 107.98 | 121.70 |
| 5 | S | 322 | ALA | O-C-N | 5.48 | 131.47 | 122.70 |
| 3 | D | 1667 | ALA | N-CA-CB | 5.48 | 117.78 | 110.10 |
| 2 | O | 1 | MET | CB-CA-C | -5.48 | 99.43 | 110.40 |
| 5 | S | 352 | GLN | N-CA-C | 5.48 | 125.80 | 111.00 |
| 5 | G | 322 | ALA | O-C-N | 5.48 | 131.47 | 122.70 |
| 5 | Y | 352 | GLN | N-CA-C | 5.48 | 125.80 | 111.00 |
| 6 | T | 466 | ASP | CA-C-N | 5.48 | 129.25 | 117.20 |
| 6 | H | 377 | ARG | C-N-CA | -5.48 | 108.01 | 121.70 |
| 4 | X | 207 | GLN | N-CA-CB | -5.47 | 100.74 | 110.60 |
| 6 | Z | 408 | SER | CA-C-O | -5.47 | 108.61 | 120.10 |
| 5 | Y | 322 | ALA | O-C-N | 5.47 | 131.45 | 122.70 |
| 5 | M | 322 | ALA | O-C-N | 5.47 | 131.45 | 122.70 |
| 5 | Y | 264 | GLU | N-CA-C | -5.47 | 96.23 | 111.00 |
| 4 | L | 415 | ASP | O-C-N | 5.47 | 131.45 | 122.70 |
| 5 | M | 333 | PRO | O-C-N | -5.47 | 113.90 | 123.20 |
| 4 | L | 207 | GLN | N-CA-CB | -5.47 | 100.76 | 110.60 |
| 3 | P | 241 | LEU | N-CA-C | 5.46 | 125.75 | 111.00 |
| 6 | H | 408 | SER | CA-C-O | -5.46 | 108.64 | 120.10 |
| 6 | T | 408 | SER | CA-C-O | -5.46 | 108.64 | 120.10 |
| 3 | D | 241 | LEU | N-CA-C | 5.46 | 125.73 | 111.00 |
| 4 | R | 451 | GLU | O-C-N | 5.46 | 131.43 | 122.70 |
| 6 | T | 500 | GLU | C-N-CA | 5.46 | 135.34 | 121.70 |
| 5 | G | 264 | GLU | N-CA-C | -5.46 | 96.27 | 111.00 |
| 2 | O | 305 | LEU | CB-CA-C | 5.45 | 120.56 | 110.20 |
| 4 | F | 207 | GLN | N-CA-CB | -5.45 | 100.79 | 110.60 |
| 2 | C | 1 | MET | CB-CA-C | -5.45 | 99.51 | 110.40 |
| 3 | D | 1532 | ASP | C-N-CA | -5.45 | 108.09 | 121.70 |
| 3 | D | 1538 | SER | O-C-N | 5.45 | 131.41 | 122.70 |
| 5 | G | 380 | ILE | CA-C-N | 5.44 | 129.17 | 117.20 |
| 6 | Z | 466 | ASP | CA-C-N | 5.44 | 129.17 | 117.20 |
| 5 | G | 249 | PRO | CB-CA-C | 5.44 | 125.60 | 112.00 |
| 2 | U | 233 | VAL | N-CA-CB | 5.44 | 123.47 | 111.50 |
| 4 | F | 415 | ASP | O-C-N | 5.44 | 131.40 | 122.70 |
| 6 | H | 500 | GLU | C-N-CA | 5.44 | 135.30 | 121.70 |
| 6 | N | 500 | GLU | C-N-CA | 5.43 | 135.28 | 121.70 |
| 3 | P | 1483 | ARG | CA-C-N | -5.43 | 105.24 | 117.20 |
| 3 | P | 1532 | ASP | C-N-CA | -5.43 | 108.12 | 121.70 |
| 5 | Y | 380 | ILE | CA-C-N | 5.43 | 129.15 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 1474 | GLY | N-CA-C | 5.43 | 126.67 | 113.10 |
| 6 | H | 466 | ASP | CA-C-N | 5.43 | 129.15 | 117.20 |
| 4 | X | 451 | GLU | O-C-N | 5.43 | 131.39 | 122.70 |
| 6 | Z | 500 | GLU | C-N-CA | 5.43 | 135.27 | 121.70 |
| 4 | F | 451 | GLU | O-C-N | 5.43 | 131.38 | 122.70 |
| 4 | R | 306 | PRO | N-CA-CB | 5.43 | 109.81 | 103.30 |
| 2 | I | 233 | VAL | N-CA-CB | 5.43 | 123.44 | 111.50 |
| 7 | V | 868 | PRO | N-CA-C | 5.43 | 126.21 | 112.10 |
| 6 | N | 466 | ASP | CA-C-N | 5.42 | 129.14 | 117.20 |
| 2 | U | 28 | HIS | CA-C-N | -5.42 | 105.27 | 117.20 |
| 4 | X | 306 | PRO | N-CA-CB | 5.42 | 109.81 | 103.30 |
| 5 | M | 249 | PRO | CB-CA-C | 5.42 | 125.56 | 112.00 |
| 4 | F | 458 | ASP | CB-CA-C | -5.42 | 99.56 | 110.40 |
| 3 | P | 1515 | TYR | CA-C-N | -5.42 | 105.27 | 117.20 |
| 5 | G | 369 | ASN | N-CA-CB | -5.42 | 100.84 | 110.60 |
| 5 | M | 380 | ILE | CA-C-N | 5.42 | 129.12 | 117.20 |
| 2 | O | 233 | VAL | N-CA-CB | 5.42 | 123.42 | 111.50 |
| 2 | I | 305 | LEU | CB-CA-C | 5.42 | 120.49 | 110.20 |
| 2 | U | 305 | LEU | CB-CA-C | 5.42 | 120.50 | 110.20 |
| 7 | J | 868 | PRO | N-CA-C | 5.42 | 126.18 | 112.10 |
| 5 | M | 369 | ASN | N-CA-CB | -5.42 | 100.85 | 110.60 |
| 5 | Y | 333 | PRO | O-C-N | -5.42 | 113.99 | 123.20 |
| 2 | O | 28 | HIS | CA-C-N | -5.42 | 105.29 | 117.20 |
| 2 | C | 305 | LEU | CB-CA-C | 5.41 | 120.48 | 110.20 |
| 2 | C | 233 | VAL | N-CA-CB | 5.41 | 123.41 | 111.50 |
| 3 | D | 1515 | TYR | CA-C-N | -5.41 | 105.29 | 117.20 |
| 4 | F | 306 | PRO | N-CA-CB | 5.41 | 109.79 | 103.30 |
| 3 | D | 1483 | ARG | CA-C-N | -5.41 | 105.30 | 117.20 |
| 4 | F | 398 | LYS | CA-C-O | 5.41 | 131.46 | 120.10 |
| 2 | I | 28 | HIS | CA-C-N | -5.41 | 105.30 | 117.20 |
| 4 | L | 306 | PRO | N-CA-CB | 5.41 | 109.79 | 103.30 |
| 4 | X | 392 | LYS | CB-CA-C | 5.41 | 121.22 | 110.40 |
| 5 | Y | 369 | ASN | N-CA-CB | -5.41 | 100.86 | 110.60 |
| 5 | G | 377 | ASN | N-CA-C | 5.41 | 125.60 | 111.00 |
| 4 | L | 458 | ASP | CB-CA-C | -5.41 | 99.59 | 110.40 |
| 4 | R | 342 | GLN | C-N-CA | 5.41 | 135.21 | 121.70 |
| 2 | O | 485 | LEU | N-CA-C | -5.40 | 96.41 | 111.00 |
| 4 | X | 342 | GLN | C-N-CA | 5.40 | 135.21 | 121.70 |
| 7 | J | 1465 | GLU | N-CA-CB | 5.40 | 120.33 | 110.60 |
| 4 | R | 458 | ASP | CB-CA-C | -5.40 | 99.59 | 110.40 |
| 2 | U | 485 | LEU | N-CA-C | -5.40 | 96.41 | 111.00 |
| 5 | Y | 249 | PRO | CB-CA-C | 5.40 | 125.51 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 392 | LYS | CB-CA-C | 5.40 | 121.20 | 110.40 |
| 5 | S | 369 | ASN | N-CA-CB | -5.40 | 100.88 | 110.60 |
| 4 | L | 392 | LYS | CB-CA-C | 5.40 | 121.19 | 110.40 |
| 4 | F | 392 | LYS | CB-CA-C | 5.40 | 121.19 | 110.40 |
| 5 | G | 333 | PRO | O-C-N | -5.40 | 114.03 | 123.20 |
| 5 | S | 380 | ILE | CA-C-N | 5.40 | 129.07 | 117.20 |
| 4 | R | 398 | LYS | CA-C-O | 5.39 | 131.43 | 120.10 |
| 2 | I | 485 | LEU | N-CA-C | -5.39 | 96.44 | 111.00 |
| 6 | N | 366 | ILE | CB-CA-C | -5.39 | 100.81 | 111.60 |
| 5 | S | 249 | PRO | CB-CA-C | 5.39 | 125.48 | 112.00 |
| 5 | S | 333 | PRO | O-C-N | -5.39 | 114.04 | 123.20 |
| 2 | C | 28 | HIS | CA-C-N | -5.39 | 105.34 | 117.20 |
| 2 | C | 485 | LEU | N-CA-C | -5.39 | 96.45 | 111.00 |
| 3 | P | 1474 | GLY | N-CA-C | 5.39 | 126.57 | 113.10 |
| 4 | X | 458 | ASP | CB-CA-C | -5.39 | 99.62 | 110.40 |
| 4 | L | 342 | GLN | C-N-CA | 5.39 | 135.17 | 121.70 |
| 5 | M | 377 | ASN | N-CA-C | 5.39 | 125.54 | 111.00 |
| 4 | X | 398 | LYS | CA-C-O | 5.39 | 131.41 | 120.10 |
| 4 | R | 266 | GLU | C-N-CA | -5.38 | 108.24 | 121.70 |
| 5 | S | 377 | ASN | N-CA-C | 5.38 | 125.54 | 111.00 |
| 4 | L | 451 | GLU | O-C-N | 5.38 | 131.31 | 122.70 |
| 3 | P | 400 | LEU | N-CA-CB | 5.38 | 121.16 | 110.40 |
| 3 | D | 240 | PRO | N-CA-C | -5.38 | 98.12 | 112.10 |
| 4 | L | 398 | LYS | CA-C-O | 5.38 | 131.40 | 120.10 |
| 3 | D | 400 | LEU | N-CA-CB | 5.38 | 121.15 | 110.40 |
| 6 | H | 366 | ILE | CB-CA-C | -5.38 | 100.85 | 111.60 |
| 1 | K | 443 | LYS | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 5 | Y | 331 | THR | N-CA-C | 5.38 | 125.52 | 111.00 |
| 5 | Y | 377 | ASN | N-CA-C | 5.38 | 125.51 | 111.00 |
| 4 | X | 407 | GLU | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 6 | T | 366 | ILE | CB-CA-C | -5.37 | 100.85 | 111.60 |
| 4 | L | 266 | GLU | C-N-CA | -5.37 | 108.27 | 121.70 |
| 4 | L | 436 | SER | CA-C-N | -5.37 | 105.39 | 117.20 |
| 2 | U | 250 | VAL | CB-CA-C | 5.37 | 121.60 | 111.40 |
| 4 | X | 208 | GLN | CA-C-N | -5.37 | 105.39 | 117.20 |
| 3 | P | 240 | PRO | N-CA-C | -5.37 | 98.15 | 112.10 |
| 3 | P | 1502 | ARG | CA-C-N | -5.37 | 105.39 | 117.20 |
| 4 | F | 342 | GLN | C-N-CA | 5.36 | 135.11 | 121.70 |
| 4 | R | 436 | SER | CA-C-N | -5.36 | 105.40 | 117.20 |
| 4 | X | 436 | SER | CA-C-N | -5.36 | 105.40 | 117.20 |
| 4 | F | 407 | GLU | N-CA-CB | 5.36 | 120.25 | 110.60 |
| 5 | G | 322 | ALA | CA-C-O | -5.36 | 108.84 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 266 | GLU | C-N-CA | -5.36 | 108.30 | 121.70 |
| 1 | E | 443 | LYS | N-CA-CB | 5.36 | 120.25 | 110.60 |
| 1 | B | 443 | LYS | N-CA-CB | 5.36 | 120.24 | 110.60 |
| 2 | O | 3 | THR | CA-C-O | 5.36 | 131.35 | 120.10 |
| 7 | V | 1465 | GLU | N-CA-CB | 5.36 | 120.24 | 110.60 |
| 4 | L | 407 | GLU | N-CA-CB | 5.36 | 120.24 | 110.60 |
| 5 | M | 322 | ALA | CA-C-O | -5.36 | 108.86 | 120.10 |
| 5 | M | 331 | THR | N-CA-C | 5.36 | 125.46 | 111.00 |
| 1 | Q | 443 | LYS | N-CA-CB | 5.36 | 120.24 | 110.60 |
| 1 | W | 443 | LYS | N-CA-CB | 5.36 | 120.24 | 110.60 |
| 5 | Y | 322 | ALA | CA-C-O | -5.36 | 108.85 | 120.10 |
| 2 | O | 250 | VAL | CB-CA-C | 5.35 | 121.57 | 111.40 |
| 1 | A | 443 | LYS | N-CA-CB | 5.35 | 120.24 | 110.60 |
| 2 | C | 250 | VAL | CB-CA-C | 5.35 | 121.57 | 111.40 |
| 2 | C | 3 | THR | CA-C-O | 5.35 | 131.34 | 120.10 |
| 2 | I | 250 | VAL | CB-CA-C | 5.35 | 121.57 | 111.40 |
| 4 | R | 407 | GLU | N-CA-CB | 5.35 | 120.23 | 110.60 |
| 5 | S | 331 | THR | N-CA-C | 5.35 | 125.44 | 111.00 |
| 4 | F | 266 | GLU | C-N-CA | -5.35 | 108.33 | 121.70 |
| 3 | D | 1502 | ARG | CA-C-N | -5.34 | 105.44 | 117.20 |
| 4 | F | 208 | GLN | CA-C-N | -5.34 | 105.45 | 117.20 |
| 4 | F | 436 | SER | CA-C-N | -5.34 | 105.45 | 117.20 |
| 3 | P | 1470 | ILE | CA-C-O | -5.34 | 108.88 | 120.10 |
| 4 | X | 462 | GLU | O-C-N | -5.34 | 114.15 | 122.70 |
| 6 | Z | 405 | ASP | C-N-CA | -5.34 | 108.34 | 121.70 |
| 3 | D | 1470 | ILE | CA-C-O | -5.34 | 108.89 | 120.10 |
| 4 | F | 465 | GLN | CA-C-O | -5.34 | 108.89 | 120.10 |
| 5 | G | 352 | GLN | CA-C-N | -5.34 | 105.45 | 117.20 |
| 4 | L | 208 | GLN | CA-C-N | -5.34 | 105.45 | 117.20 |
| 4 | L | 462 | GLU | O-C-N | -5.34 | 114.16 | 122.70 |
| 2 | O | 484 | ARG | CB-CA-C | -5.34 | 99.72 | 110.40 |
| 3 | P | 1491 | ILE | CA-C-O | 5.34 | 131.31 | 120.10 |
| 5 | G | 331 | THR | N-CA-C | 5.34 | 125.41 | 111.00 |
| 6 | N | 405 | ASP | C-N-CA | -5.34 | 108.36 | 121.70 |
| 5 | S | 322 | ALA | CA-C-O | -5.34 | 108.89 | 120.10 |
| 2 | C | 484 | ARG | CB-CA-C | -5.33 | 99.73 | 110.40 |
| 2 | I | 484 | ARG | CB-CA-C | -5.33 | 99.73 | 110.40 |
| 6 | Z | 366 | ILE | CB-CA-C | -5.33 | 100.93 | 111.60 |
| 4 | R | 465 | GLN | CA-C-O | -5.33 | 108.91 | 120.10 |
| 6 | H | 405 | ASP | C-N-CA | -5.33 | 108.38 | 121.70 |
| 6 | T | 405 | ASP | C-N-CA | -5.33 | 108.39 | 121.70 |
| 2 | U | 484 | ARG | CB-CA-C | -5.33 | 99.75 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 406 | LEU | C-N-CA | -5.32 | 108.39 | 121.70 |
| 2 | I | 3 | THR | CA-C-O | 5.32 | 131.28 | 120.10 |
| 5 | M | 352 | GLN | CA-C-N | -5.32 | 105.50 | 117.20 |
| 6 | Z | 501 | GLU | CA-C-O | 5.32 | 131.26 | 120.10 |
| 3 | D | 1491 | ILE | CA-C-O | 5.32 | 131.26 | 120.10 |
| 4 | X | 367 | THR | N-CA-C | -5.32 | 96.65 | 111.00 |
| 4 | L | 465 | GLN | CA-C-O | -5.31 | 108.94 | 120.10 |
| 4 | L | 367 | THR | N-CA-C | -5.31 | 96.66 | 111.00 |
| 4 | R | 462 | GLU | O-C-N | -5.31 | 114.20 | 122.70 |
| 5 | S | 352 | GLN | CA-C-N | -5.31 | 105.51 | 117.20 |
| 6 | T | 406 | LEU | C-N-CA | -5.31 | 108.42 | 121.70 |
| 5 | Y | 352 | GLN | CA-C-N | -5.31 | 105.51 | 117.20 |
| 4 | R | 208 | GLN | CA-C-N | -5.31 | 105.52 | 117.20 |
| 4 | F | 367 | THR | N-CA-C | -5.31 | 96.67 | 111.00 |
| 4 | F | 462 | GLU | O-C-N | -5.31 | 114.21 | 122.70 |
| 2 | U | 3 | THR | CA-C-O | 5.30 | 131.24 | 120.10 |
| 6 | N | 406 | LEU | C-N-CA | -5.30 | 108.45 | 121.70 |
| 5 | S | 332 | PRO | CB-CA-C | 5.30 | 125.25 | 112.00 |
| 3 | D | 1521 | TYR | O-C-N | 5.30 | 131.18 | 122.70 |
| 4 | X | 465 | GLN | CA-C-O | -5.30 | 108.97 | 120.10 |
| 5 | G | 332 | PRO | CB-CA-C | 5.30 | 125.24 | 112.00 |
| 5 | Y | 332 | PRO | CB-CA-C | 5.30 | 125.24 | 112.00 |
| 6 | H | 501 | GLU | CA-C-O | 5.29 | 131.22 | 120.10 |
| 4 | R | 367 | THR | N-CA-C | -5.29 | 96.71 | 111.00 |
| 5 | S | 330 | LYS | N-CA-C | -5.29 | 96.71 | 111.00 |
| 7 | J | 708 | MET | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 6 | T | 501 | GLU | CA-C-O | 5.29 | 131.21 | 120.10 |
| 6 | Z | 406 | LEU | C-N-CA | -5.29 | 108.49 | 121.70 |
| 5 | M | 332 | PRO | CB-CA-C | 5.28 | 125.19 | 112.00 |
| 6 | N | 501 | GLU | CA-C-O | 5.28 | 131.18 | 120.10 |
| 2 | I | 233 | VAL | CA-C-N | -5.27 | 105.60 | 117.20 |
| 7 | V | 708 | MET | CB-CA-C | -5.27 | 99.86 | 110.40 |
| 5 | Y | 330 | LYS | N-CA-C | -5.27 | 96.77 | 111.00 |
| 2 | O | 233 | VAL | CA-C-N | -5.27 | 105.61 | 117.20 |
| 4 | L | 220 | ASN | N-CA-CB | 5.26 | 120.07 | 110.60 |
| 4 | L | 253 | SER | O-C-N | 5.26 | 131.12 | 122.70 |
| 4 | R | 460 | LEU | CA-C-N | 5.26 | 128.78 | 117.20 |
| 5 | G | 330 | LYS | N-CA-C | -5.26 | 96.80 | 111.00 |
| 5 | M | 330 | LYS | N-CA-C | -5.26 | 96.80 | 111.00 |
| 5 | M | 337 | HIS | CA-C-N | 5.26 | 128.77 | 117.20 |
| 4 | F | 491 | VAL | CA-C-N | -5.26 | 105.64 | 117.20 |
| 3 | P | 1521 | TYR | O-C-N | 5.26 | 131.11 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | X | 491 | VAL | CA-C-N | -5.26 | 105.64 | 117.20 |
| 6 | H | 495 | LEU | CB-CA-C | -5.25 | 100.22 | 110.20 |
| 4 | R | 447 | VAL | CA-C-N | -5.25 | 105.64 | 117.20 |
| 3 | D | 717 | SER | CA-C-N | 5.25 | 128.75 | 117.20 |
| 5 | S | 337 | HIS | CA-C-N | 5.25 | 128.75 | 117.20 |
| 2 | U | 233 | VAL | CA-C-N | -5.25 | 105.65 | 117.20 |
| 4 | X | 460 | LEU | CA-C-N | 5.25 | 128.75 | 117.20 |
| 2 | C | 233 | VAL | CA-C-N | -5.25 | 105.65 | 117.20 |
| 4 | F | 253 | SER | O-C-N | 5.25 | 131.09 | 122.70 |
| 4 | F | 460 | LEU | CA-C-N | 5.24 | 128.74 | 117.20 |
| 5 | Y | 337 | HIS | CA-C-N | 5.24 | 128.74 | 117.20 |
| 4 | F | 220 | ASN | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 4 | F | 253 | SER | N-CA-CB | 5.24 | 118.36 | 110.50 |
| 5 | S | 328 | THR | N-CA-C | -5.24 | 96.85 | 111.00 |
| 4 | X | 447 | VAL | CA-C-N | -5.24 | 105.67 | 117.20 |
| 5 | Y | 328 | THR | N-CA-C | -5.24 | 96.85 | 111.00 |
| 3 | D | 1504 | VAL | N-CA-CB | 5.24 | 123.03 | 111.50 |
| 4 | L | 447 | VAL | CA-C-N | -5.24 | 105.68 | 117.20 |
| 4 | L | 460 | LEU | CA-C-N | 5.24 | 128.72 | 117.20 |
| 4 | R | 491 | VAL | CA-C-N | -5.24 | 105.67 | 117.20 |
| 5 | G | 328 | THR | N-CA-C | -5.24 | 96.86 | 111.00 |
| 4 | R | 253 | SER | O-C-N | 5.24 | 131.08 | 122.70 |
| 4 | F | 447 | VAL | CA-C-N | -5.24 | 105.68 | 117.20 |
| 4 | L | 491 | VAL | CA-C-N | -5.23 | 105.69 | 117.20 |
| 5 | M | 338 | GLU | C-N-CA | -5.23 | 108.62 | 121.70 |
| 5 | G | 337 | HIS | CA-C-N | 5.23 | 128.70 | 117.20 |
| 6 | N | 495 | LEU | CB-CA-C | -5.23 | 100.27 | 110.20 |
| 3 | P | 717 | SER | CA-C-N | 5.23 | 128.70 | 117.20 |
| 4 | R | 253 | SER | N-CA-CB | 5.23 | 118.34 | 110.50 |
| 4 | X | 220 | ASN | N-CA-CB | 5.23 | 120.01 | 110.60 |
| 4 | F | 484 | ASP | N-CA-CB | -5.23 | 101.19 | 110.60 |
| 4 | R | 220 | ASN | N-CA-CB | 5.22 | 120.00 | 110.60 |
| 6 | T | 495 | LEU | CB-CA-C | -5.22 | 100.27 | 110.20 |
| 6 | Z | 495 | LEU | CB-CA-C | -5.22 | 100.28 | 110.20 |
| 4 | X | 458 | ASP | O-C-N | -5.22 | 114.34 | 122.70 |
| 5 | Y | 319 | LEU | CA-C-N | -5.22 | 105.71 | 117.20 |
| 4 | X | 253 | SER | N-CA-CB | 5.22 | 118.33 | 110.50 |
| 4 | X | 484 | ASP | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 4 | R | 484 | ASP | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 7 | J | 1465 | GLU | CB-CA-C | -5.22 | 99.96 | 110.40 |
| 3 | P | 1504 | VAL | N-CA-CB | 5.22 | 122.98 | 111.50 |
| 4 | X | 253 | SER | O-C-N | 5.22 | 131.05 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 484 | ASP | N-CA-CB | -5.22 | 101.21 | 110.60 |
| 5 | Y | 338 | GLU | C-N-CA | -5.22 | 108.66 | 121.70 |
| 5 | G | 338 | GLU | C-N-CA | -5.21 | 108.66 | 121.70 |
| 5 | M | 328 | THR | N-CA-C | -5.21 | 96.92 | 111.00 |
| 7 | V | 1465 | GLU | CB-CA-C | -5.21 | 99.97 | 110.40 |
| 4 | R | 267 | GLN | N-CA-CB | -5.21 | 101.22 | 110.60 |
| 3 | D | 1490 | GLU | CA-C-O | 5.21 | 131.03 | 120.10 |
| 5 | S | 319 | LEU | CA-C-N | -5.21 | 105.75 | 117.20 |
| 4 | L | 253 | SER | N-CA-CB | 5.20 | 118.30 | 110.50 |
| 3 | P | 1490 | GLU | CA-C-O | 5.20 | 131.02 | 120.10 |
| 5 | S | 338 | GLU | C-N-CA | -5.20 | 108.70 | 121.70 |
| 3 | D | 494 | LEU | CB-CA-C | -5.19 | 100.33 | 110.20 |
| 4 | X | 234 | PRO | N-CA-C | 5.19 | 125.60 | 112.10 |
| 5 | G | 319 | LEU | CA-C-N | -5.19 | 105.78 | 117.20 |
| 3 | D | 1516 | LEU | CA-C-O | -5.19 | 109.20 | 120.10 |
| 3 | P | 494 | LEU | CB-CA-C | -5.19 | 100.34 | 110.20 |
| 7 | J | 1467 | HIS | N-CA-CB | 5.19 | 119.94 | 110.60 |
| 4 | L | 468 | LYS | CA-C-O | -5.18 | 109.21 | 120.10 |
| 3 | P | 1516 | LEU | CA-C-O | -5.18 | 109.21 | 120.10 |
| 4 | R | 234 | PRO | N-CA-C | 5.18 | 125.57 | 112.10 |
| 7 | V | 1467 | HIS | N-CA-CB | 5.18 | 119.92 | 110.60 |
| 4 | X | 267 | GLN | N-CA-CB | -5.18 | 101.28 | 110.60 |
| 4 | X | 408 | GLU | N-CA-C | 5.18 | 124.98 | 111.00 |
| 5 | M | 319 | LEU | CA-C-N | -5.17 | 105.82 | 117.20 |
| 4 | X | 348 | GLN | C-N-CA | -5.17 | 108.77 | 121.70 |
| 4 | R | 408 | GLU | N-CA-C | 5.17 | 124.97 | 111.00 |
| 4 | R | 458 | ASP | O-C-N | -5.17 | 114.43 | 122.70 |
| 6 | N | 391 | GLN | CA-C-N | 5.17 | 128.56 | 117.20 |
| 4 | R | 467 | LEU | CB-CA-C | -5.17 | 100.39 | 110.20 |
| 2 | U | 10 | LEU | O-C-N | 5.17 | 130.96 | 122.70 |
| 4 | X | 468 | LYS | CA-C-O | -5.17 | 109.25 | 120.10 |
| 2 | C | 10 | LEU | O-C-N | 5.16 | 130.96 | 122.70 |
| 2 | O | 10 | LEU | O-C-N | 5.16 | 130.96 | 122.70 |
| 7 | V | 425 | PRO | C-N-CA | 5.16 | 134.61 | 121.70 |
| 4 | L | 408 | GLU | N-CA-C | 5.16 | 124.94 | 111.00 |
| 4 | F | 234 | PRO | N-CA-C | 5.16 | 125.52 | 112.10 |
| 4 | L | 234 | PRO | N-CA-C | 5.16 | 125.52 | 112.10 |
| 4 | X | 428 | LYS | C-N-CA | -5.16 | 111.46 | 122.30 |
| 4 | F | 408 | GLU | N-CA-C | 5.16 | 124.93 | 111.00 |
| 4 | R | 428 | LYS | C-N-CA | -5.16 | 111.47 | 122.30 |
| 4 | F | 458 | ASP | O-C-N | -5.16 | 114.45 | 122.70 |
| 4 | L | 267 | GLN | N-CA-CB | -5.15 | 101.32 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | L | 458 | ASP | O-C-N | -5.15 | 114.45 | 122.70 |
| 4 | F | 468 | LYS | CA-C-O | -5.15 | 109.28 | 120.10 |
| 4 | R | 348 | GLN | C-N-CA | -5.15 | 108.82 | 121.70 |
| 5 | S | 277 | SER | N-CA-C | 5.15 | 124.91 | 111.00 |
| 3 | D | 1486 | CYS | CA-C-N | -5.15 | 105.87 | 117.20 |
| 4 | R | 468 | LYS | CA-C-O | -5.15 | 109.29 | 120.10 |
| 3 | P | 1486 | CYS | CA-C-N | -5.15 | 105.88 | 117.20 |
| 6 | H | 391 | GLN | CA-C-N | 5.14 | 128.52 | 117.20 |
| 4 | F | 428 | LYS | C-N-CA | -5.14 | 111.50 | 122.30 |
| 4 | L | 428 | LYS | C-N-CA | -5.14 | 111.50 | 122.30 |
| 4 | F | 267 | GLN | N-CA-CB | -5.14 | 101.35 | 110.60 |
| 4 | L | 348 | GLN | C-N-CA | -5.14 | 108.85 | 121.70 |
| 7 | J | 317 | PRO | N-CA-C | 5.14 | 125.47 | 112.10 |
| 7 | J | 425 | PRO | C-N-CA | 5.14 | 134.55 | 121.70 |
| 6 | T | 391 | GLN | CA-C-N | 5.14 | 128.51 | 117.20 |
| 4 | F | 467 | LEU | CB-CA-C | -5.14 | 100.44 | 110.20 |
| 4 | L | 319 | SER | CA-C-N | 5.14 | 128.50 | 117.20 |
| 4 | L | 467 | LEU | CB-CA-C | -5.14 | 100.44 | 110.20 |
| 2 | I | 10 | LEU | O-C-N | 5.13 | 130.91 | 122.70 |
| 4 | F | 319 | SER | CA-C-N | 5.13 | 128.48 | 117.20 |
| 6 | H | 391 | GLN | N-CA-CB | 5.13 | 119.83 | 110.60 |
| 7 | V | 317 | PRO | N-CA-C | 5.13 | 125.43 | 112.10 |
| 4 | F | 432 | ASN | CB-CA-C | -5.13 | 100.15 | 110.40 |
| 6 | Z | 373 | THR | C-N-CA | -5.13 | 108.88 | 121.70 |
| 6 | Z | 391 | GLN | CA-C-N | 5.12 | 128.47 | 117.20 |
| 5 | G | 323 | GLU | CB-CA-C | 5.12 | 120.65 | 110.40 |
| 7 | J | 159 | ALA | N-CA-C | -5.12 | 97.17 | 111.00 |
| 4 | F | 467 | LEU | CA-C-N | 5.12 | 128.47 | 117.20 |
| 4 | X | 428 | LYS | CA-C-N | -5.12 | 105.96 | 116.20 |
| 4 | F | 348 | GLN | C-N-CA | -5.12 | 108.90 | 121.70 |
| 2 | I | 455 | VAL | CB-CA-C | -5.12 | 101.68 | 111.40 |
| 6 | N | 373 | THR | C-N-CA | -5.12 | 108.91 | 121.70 |
| 5 | Y | 277 | SER | N-CA-C | 5.11 | 124.81 | 111.00 |
| 6 | H | 373 | THR | C-N-CA | -5.11 | 108.92 | 121.70 |
| 2 | I | 3 | THR | C-N-CA | -5.11 | 108.92 | 121.70 |
| 4 | R | 319 | SER | CA-C-N | 5.11 | 128.45 | 117.20 |
| 4 | R | 428 | LYS | CA-C-N | -5.11 | 105.98 | 116.20 |
| 7 | V | 159 | ALA | N-CA-C | -5.11 | 97.20 | 111.00 |
| 5 | M | 274 | ARG | N-CA-CB | 5.11 | 119.80 | 110.60 |
| 2 | C | 307 | GLY | C-N-CA | 5.11 | 134.47 | 121.70 |
| 4 | L | 207 | GLN | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 4 | L | 231 | LYS | C-N-CA | 5.11 | 134.47 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | O | 3 | THR | C-N-CA | -5.11 | 108.93 | 121.70 |
| 2 | O | 455 | VAL | CB-CA-C | -5.11 | 101.69 | 111.40 |
| 5 | S | 274 | ARG | N-CA-CB | 5.11 | 119.79 | 110.60 |
| 2 | U | 307 | GLY | C-N-CA | 5.11 | 134.47 | 121.70 |
| 4 | X | 319 | SER | CA-C-N | 5.11 | 128.44 | 117.20 |
| 4 | X | 432 | ASN | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 4 | R | 432 | ASN | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 6 | Z | 391 | GLN | N-CA-CB | 5.11 | 119.79 | 110.60 |
| 7 | V | 95 | CYS | C-N-CA | 5.10 | 134.46 | 121.70 |
| 2 | I | 307 | GLY | C-N-CA | 5.10 | 134.46 | 121.70 |
| 5 | M | 277 | SER | N-CA-C | 5.10 | 124.78 | 111.00 |
| 2 | U | 3 | THR | C-N-CA | -5.10 | 108.94 | 121.70 |
| 4 | X | 467 | LEU | CA-C-N | 5.10 | 128.43 | 117.20 |
| 5 | G | 277 | SER | N-CA-C | 5.10 | 124.77 | 111.00 |
| 4 | L | 432 | ASN | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 2 | O | 307 | GLY | C-N-CA | 5.10 | 134.45 | 121.70 |
| 5 | Y | 274 | ARG | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 6 | N | 391 | GLN | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 4 | L | 428 | LYS | CA-C-N | -5.10 | 106.00 | 116.20 |
| 4 | X | 467 | LEU | CB-CA-C | -5.10 | 100.51 | 110.20 |
| 4 | F | 428 | LYS | CA-C-N | -5.09 | 106.01 | 116.20 |
| 5 | G | 274 | ARG | N-CA-CB | 5.09 | 119.77 | 110.60 |
| 4 | R | 468 | LYS | C-N-CA | -5.09 | 108.97 | 121.70 |
| 4 | L | 467 | LEU | CA-C-N | 5.09 | 128.40 | 117.20 |
| 6 | T | 391 | GLN | N-CA-CB | 5.09 | 119.76 | 110.60 |
| 7 | J | 95 | CYS | C-N-CA | 5.09 | 134.42 | 121.70 |
| 5 | M | 323 | GLU | CB-CA-C | 5.09 | 120.57 | 110.40 |
| 2 | U | 455 | VAL | CB-CA-C | -5.09 | 101.74 | 111.40 |
| 2 | C | 3 | THR | C-N-CA | -5.08 | 108.99 | 121.70 |
| 2 | C | 455 | VAL | CB-CA-C | -5.08 | 101.74 | 111.40 |
| 2 | O | 654 | SER | C-N-CA | 5.08 | 134.41 | 121.70 |
| 2 | U | 654 | SER | C-N-CA | 5.08 | 134.41 | 121.70 |
| 5 | S | 323 | GLU | CB-CA-C | 5.08 | 120.56 | 110.40 |
| 2 | C | 654 | SER | C-N-CA | 5.08 | 134.40 | 121.70 |
| 6 | Z | 474 | ILE | N-CA-CB | 5.08 | 122.48 | 110.80 |
| 4 | R | 207 | GLN | CB-CA-C | -5.08 | 100.25 | 110.40 |
| 2 | I | 654 | SER | C-N-CA | 5.07 | 134.38 | 121.70 |
| 4 | R | 467 | LEU | CA-C-N | 5.07 | 128.36 | 117.20 |
| 7 | J | 1371 | GLN | CB-CA-C | -5.07 | 100.26 | 110.40 |
| 7 | J | 1465 | GLU | CA-C-O | -5.07 | 109.45 | 120.10 |
| 4 | L | 468 | LYS | C-N-CA | -5.07 | 109.02 | 121.70 |
| 6 | N | 474 | ILE | N-CA-CB | 5.07 | 122.46 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | R | 231 | LYS | C-N-CA | 5.07 | 134.37 | 121.70 |
| 6 | T | 474 | ILE | N-CA-CB | 5.07 | 122.46 | 110.80 |
| 7 | V | 1371 | GLN | CB-CA-C | -5.07 | 100.26 | 110.40 |
| 7 | V | 1465 | GLU | CA-C-O | -5.07 | 109.46 | 120.10 |
| 6 | H | 474 | ILE | N-CA-CB | 5.07 | 122.45 | 110.80 |
| 6 | T | 373 | THR | C-N-CA | -5.07 | 109.03 | 121.70 |
| 4 | X | 231 | LYS | C-N-CA | 5.07 | 134.36 | 121.70 |
| 4 | F | 231 | LYS | C-N-CA | 5.06 | 134.36 | 121.70 |
| 4 | X | 207 | GLN | CB-CA-C | -5.06 | 100.28 | 110.40 |
| 4 | F | 207 | GLN | CB-CA-C | -5.06 | 100.28 | 110.40 |
| 4 | X | 468 | LYS | C-N-CA | -5.06 | 109.06 | 121.70 |
| 4 | F | 447 | VAL | CA-C-O | 5.05 | 130.72 | 120.10 |
| 5 | Y | 323 | GLU | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 2 | C | 306 | PRO | N-CA-C | 5.05 | 125.22 | 112.10 |
| 4 | F | 468 | LYS | C-N-CA | -5.05 | 109.08 | 121.70 |
| 3 | D | 1491 | ILE | CA-C-N | -5.04 | 106.11 | 116.20 |
| 2 | O | 10 | LEU | CA-C-N | -5.04 | 106.11 | 117.20 |
| 3 | P | 1491 | ILE | CA-C-N | -5.04 | 106.12 | 116.20 |
| 4 | R | 401 | TYR | CB-CA-C | -5.04 | 100.33 | 110.40 |
| 4 | X | 391 | ILE | C-N-CA | -5.04 | 109.11 | 121.70 |
| 2 | C | 10 | LEU | CA-C-N | -5.03 | 106.12 | 117.20 |
| 2 | I | 306 | PRO | N-CA-C | 5.03 | 125.18 | 112.10 |
| 7 | J | 162 | VAL | N-CA-C | -5.03 | 97.41 | 111.00 |
| 2 | U | 10 | LEU | CA-C-N | -5.03 | 106.13 | 117.20 |
| 2 | U | 306 | PRO | N-CA-C | 5.03 | 125.18 | 112.10 |
| 4 | X | 447 | VAL | CA-C-O | 5.03 | 130.66 | 120.10 |
| 5 | G | 304 | ASN | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 5 | M | 304 | ASN | N-CA-CB | 5.03 | 119.65 | 110.60 |
| 2 | O | 306 | PRO | N-CA-C | 5.03 | 125.17 | 112.10 |
| 4 | L | 299 | ASN | CA-C-N | 5.03 | 131.18 | 117.10 |
| 4 | L | 447 | VAL | CA-C-O | 5.03 | 130.66 | 120.10 |
| 4 | R | 447 | VAL | CA-C-O | 5.03 | 130.66 | 120.10 |
| 6 | H | 446 | ARG | C-N-CA | 5.03 | 134.26 | 121.70 |
| 4 | L | 401 | TYR | CB-CA-C | -5.03 | 100.35 | 110.40 |
| 4 | X | 305 | ASP | O-C-N | 5.02 | 130.65 | 121.10 |
| 3 | P | 650 | LEU | CB-CA-C | -5.02 | 100.66 | 110.20 |
| 7 | V | 162 | VAL | N-CA-C | -5.02 | 97.44 | 111.00 |
| 4 | X | 299 | ASN | CA-C-N | 5.02 | 131.16 | 117.10 |
| 4 | X | 401 | TYR | CB-CA-C | -5.02 | 100.36 | 110.40 |
| 4 | F | 299 | ASN | CA-C-N | 5.02 | 131.15 | 117.10 |
| 2 | I | 10 | LEU | CA-C-N | -5.02 | 106.16 | 117.20 |
| 4 | R | 391 | ILE | C-N-CA | -5.02 | 109.16 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | S | 304 | ASN | N-CA-CB | 5.02 | 119.63 | 110.60 |
| 7 | V | 867 | LEU | N-CA-C | 5.02 | 124.54 | 111.00 |
| 3 | D | 1521 | TYR | C-N-CA | -5.01 | 109.17 | 121.70 |
| 4 | F | 401 | TYR | CB-CA-C | -5.01 | 100.38 | 110.40 |
| 4 | R | 299 | ASN | CA-C-N | 5.01 | 131.12 | 117.10 |
| 6 | Z | 446 | ARG | C-N-CA | 5.01 | 134.22 | 121.70 |
| 4 | L | 391 | ILE | C-N-CA | -5.01 | 109.18 | 121.70 |
| 6 | N | 446 | ARG | C-N-CA | 5.01 | 134.22 | 121.70 |
| 3 | D | 650 | LEU | CB-CA-C | -5.01 | 100.69 | 110.20 |
| 4 | F | 391 | ILE | C-N-CA | -5.00 | 109.19 | 121.70 |
| 7 | J | 867 | LEU | N-CA-C | 5.00 | 124.51 | 111.00 |

All (100) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 2 | C | 11 | GLN | CA |
| 4 | F | 200 | THR | CA |
| 4 | F | 210 | VAL | CA |
| 4 | F | 211 | GLU | CA |
| 4 | F | 305 | ASP | CA |
| 4 | F | 341 | ASP | CA |
| 4 | F | 423 | ALA | CA |
| 4 | F | 454 | TYR | CA |
| 4 | F | 459 | LEU | CA |
| 4 | F | 460 | LEU | CA |
| 4 | F | 486 | GLU | CA |
| 5 | G | 327 | ARG | CA |
| 5 | G | 330 | LYS | CA |
| 5 | G | 338 | GLU | CA |
| 5 | G | 339 | TYR | CA |
| 5 | G | 340 | ALA | CA |
| 5 | G | 341 | ALA | CA |
| 5 | G | 344 | ASP | CA |
| 5 | G | 373 | THR | CA |
| 5 | G | 405 | SER | CA |
| 6 | H | 352 | LEU | CA |
| 6 | H | 356 | THR | CA |
| 6 | H | 387 | LYS | CA |
| 6 | H | 446 | ARG | CA |
| 6 | H | 494 | LEU | CA |
| 2 | I | 11 | GLN | CA |
| 4 | L | 200 | THR | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 4 | L | 210 | VAL | CA |
| 4 | L | 211 | GLU | CA |
| 4 | L | 305 | ASP | CA |
| 4 | L | 341 | ASP | CA |
| 4 | L | 423 | ALA | CA |
| 4 | L | 454 | TYR | CA |
| 4 | L | 459 | LEU | CA |
| 4 | L | 460 | LEU | CA |
| 4 | L | 486 | GLU | CA |
| 5 | M | 327 | ARG | CA |
| 5 | M | 330 | LYS | CA |
| 5 | M | 338 | GLU | CA |
| 5 | M | 339 | TYR | CA |
| 5 | M | 340 | ALA | CA |
| 5 | M | 341 | ALA | CA |
| 5 | M | 344 | ASP | CA |
| 5 | M | 373 | THR | CA |
| 5 | M | 405 | SER | CA |
| 6 | N | 352 | LEU | CA |
| 6 | N | 356 | THR | CA |
| 6 | N | 387 | LYS | CA |
| 6 | N | 446 | ARG | CA |
| 6 | N | 494 | LEU | CA |
| 2 | O | 11 | GLN | CA |
| 4 | R | 200 | THR | CA |
| 4 | R | 210 | VAL | CA |
| 4 | R | 211 | GLU | CA |
| 4 | R | 305 | ASP | CA |
| 4 | R | 341 | ASP | CA |
| 4 | R | 423 | ALA | CA |
| 4 | R | 454 | TYR | CA |
| 4 | R | 459 | LEU | CA |
| 4 | R | 460 | LEU | CA |
| 4 | R | 486 | GLU | CA |
| 5 | S | 327 | ARG | CA |
| 5 | S | 330 | LYS | CA |
| 5 | S | 338 | GLU | CA |
| 5 | S | 339 | TYR | CA |
| 5 | S | 340 | ALA | CA |
| 5 | S | 341 | ALA | CA |
| 5 | S | 344 | ASP | CA |
| 5 | S | 373 | THR | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 5 | S | 405 | SER | CA |
| 6 | T | 352 | LEU | CA |
| 6 | T | 356 | THR | CA |
| 6 | T | 387 | LYS | CA |
| 6 | T | 446 | ARG | CA |
| 6 | T | 494 | LEU | CA |
| 2 | U | 11 | GLN | CA |
| 4 | X | 200 | THR | CA |
| 4 | X | 210 | VAL | CA |
| 4 | X | 211 | GLU | CA |
| 4 | X | 305 | ASP | CA |
| 4 | X | 341 | ASP | CA |
| 4 | X | 423 | ALA | CA |
| 4 | X | 454 | TYR | CA |
| 4 | X | 459 | LEU | CA |
| 4 | X | 460 | LEU | CA |
| 4 | X | 486 | GLU | CA |
| 5 | Y | 327 | ARG | CA |
| 5 | Y | 330 | LYS | CA |
| 5 | Y | 338 | GLU | CA |
| 5 | Y | 339 | TYR | CA |
| 5 | Y | 340 | ALA | CA |
| 5 | Y | 341 | ALA | CA |
| 5 | Y | 344 | ASP | CA |
| 5 | Y | 373 | THR | CA |
| 5 | Y | 405 | SER | CA |
| 6 | Z | 352 | LEU | CA |
| 6 | Z | 356 | THR | CA |
| 6 | Z | 387 | LYS | CA |
| 6 | Z | 446 | ARG | CA |
| 6 | Z | 494 | LEU | CA |

All (288) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 259 | SER | Mainchain |
| 1 | B | 259 | SER | Mainchain |
| 2 | C | 11 | GLN | Mainchain |
| 2 | C | 4 | GLU | Mainchain |
| 2 | C | 6 | PHE | Mainchain |
| 2 | C | 7 | GLY | Mainchain |
| 3 | D | 1448 | MET | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | D | 1449 | TRP | Peptide |
| 3 | D | 1450 | GLU | Peptide |
| 3 | D | 1484 | ASP | Mainchain |
| 3 | D | 1485 | ALA | Mainchain |
| 3 | D | 1486 | CYS | Mainchain |
| 3 | D | 1489 | HIS | Mainchain |
| 3 | D | 1503 | ILE | Mainchain |
| 3 | D | 1507 | ASP | Mainchain |
| 3 | D | 1508 | LYS | Mainchain,Peptide |
| 3 | D | 1509 | GLN | Mainchain |
| 3 | D | 1512 | TRP | Mainchain |
| 3 | D | 1516 | LEU | Mainchain |
| 3 | D | 1517 | SER | Mainchain,Peptide |
| 3 | D | 1518 | ASN | Mainchain |
| 3 | D | 1519 | SER | Peptide |
| 3 | D | 1538 | SER | Mainchain |
| 3 | D | 1541 | THR | Mainchain |
| 3 | D | 1542 | PRO | Mainchain |
| 1 | E | 259 | SER | Mainchain |
| 4 | F | 200 | THR | Mainchain |
| 4 | F | 208 | GLN | Mainchain |
| 4 | F | 210 | VAL | Mainchain |
| 4 | F | 221 | GLN | Mainchain,Peptide |
| 4 | F | 236 | ASP | Mainchain |
| 4 | F | 245 | VAL | Mainchain |
| 4 | F | 250 | ASN | Mainchain |
| 4 | F | 253 | SER | Mainchain |
| 4 | F | 393 | GLN | Mainchain |
| 4 | F | 397 | ARG | Mainchain |
| 4 | F | 398 | LYS | Mainchain,Peptide |
| 4 | F | 399 | SER | Peptide |
| 4 | F | 400 | GLY | Mainchain |
| 4 | F | 401 | TYR | Mainchain |
| 4 | F | 403 | ILE | Peptide |
| 4 | F | 419 | GLY | Mainchain |
| 4 | F | 420 | GLU | Mainchain |
| 4 | F | 421 | LEU | Mainchain |
| 4 | F | 422 | ASN | Mainchain,Peptide |
| 4 | F | 423 | ALA | Mainchain |
| 4 | F | 424 | PRO | Mainchain,Peptide |
| 4 | F | 425 | THR | Mainchain |
| 4 | F | 426 | GLN | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | F | 445 | GLY | Mainchain |
| 4 | F | 446 | ALA | Mainchain |
| 4 | F | 448 | ARG | Mainchain |
| 4 | F | 452 | ARG | Mainchain |
| 4 | F | 454 | TYR | Mainchain,Peptide |
| 4 | F | 456 | ASP | Mainchain |
| 4 | F | 457 | ALA | Mainchain |
| 4 | F | 459 | LEU | Mainchain |
| 4 | F | 462 | GLU | Mainchain |
| 4 | F | 463 | ILE | Peptide |
| 4 | F | 472 | GLU | Mainchain |
| 4 | F | 487 | ASP | Mainchain |
| 5 | G | 321 | ASN | Mainchain |
| 5 | G | 325 | ALA | Mainchain |
| 5 | G | 326 | LEU | Mainchain,Peptide |
| 5 | G | 329 | GLN | Mainchain |
| 5 | G | 330 | LYS | Mainchain |
| 5 | G | 340 | ALA | Mainchain,Peptide |
| 5 | G | 341 | ALA | Mainchain |
| 5 | G | 343 | ALA | Mainchain |
| 6 | H | 374 | SER | Mainchain |
| 6 | H | 407 | LEU | Mainchain |
| 6 | H | 408 | SER | Peptide |
| 6 | H | 493 | ALA | Peptide |
| 6 | H | 497 | ARG | Mainchain |
| 2 | I | 11 | GLN | Mainchain |
| 2 | I | 4 | GLU | Mainchain |
| 2 | I | 6 | PHE | Mainchain |
| 2 | I | 7 | GLY | Mainchain |
| 7 | J | 1386 | LYS | Peptide |
| 7 | J | 1387 | SER | Peptide |
| 7 | J | 1465 | GLU | Mainchain |
| 1 | K | 259 | SER | Mainchain |
| 4 | L | 200 | THR | Mainchain |
| 4 | L | 208 | GLN | Mainchain |
| 4 | L | 210 | VAL | Mainchain |
| 4 | L | 221 | GLN | Mainchain,Peptide |
| 4 | L | 236 | ASP | Mainchain |
| 4 | L | 245 | VAL | Mainchain |
| 4 | L | 250 | ASN | Mainchain |
| 4 | L | 253 | SER | Mainchain |
| 4 | L | 393 | GLN | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | L | 397 | ARG | Mainchain |
| 4 | L | 398 | LYS | Mainchain,Peptide |
| 4 | L | 399 | SER | Peptide |
| 4 | L | 400 | GLY | Mainchain |
| 4 | L | 401 | TYR | Mainchain |
| 4 | L | 403 | ILE | Peptide |
| 4 | L | 419 | GLY | Mainchain |
| 4 | L | 420 | GLU | Mainchain |
| 4 | L | 421 | LEU | Mainchain |
| 4 | L | 422 | ASN | Mainchain,Peptide |
| 4 | L | 423 | ALA | Mainchain |
| 4 | L | 424 | PRO | Mainchain,Peptide |
| 4 | L | 425 | THR | Mainchain |
| 4 | L | 426 | GLN | Mainchain |
| 4 | L | 445 | GLY | Mainchain |
| 4 | L | 446 | ALA | Mainchain |
| 4 | L | 448 | ARG | Mainchain |
| 4 | L | 452 | ARG | Mainchain |
| 4 | L | 454 | TYR | Mainchain,Peptide |
| 4 | L | 456 | ASP | Mainchain |
| 4 | L | 457 | ALA | Mainchain |
| 4 | L | 459 | LEU | Mainchain |
| 4 | L | 462 | GLU | Mainchain |
| 4 | L | 463 | ILE | Peptide |
| 4 | L | 472 | GLU | Mainchain |
| 4 | L | 487 | ASP | Mainchain |
| 5 | M | 321 | ASN | Mainchain |
| 5 | M | 325 | ALA | Mainchain |
| 5 | M | 326 | LEU | Mainchain,Peptide |
| 5 | M | 329 | GLN | Mainchain |
| 5 | M | 330 | LYS | Mainchain |
| 5 | M | 340 | ALA | Mainchain,Peptide |
| 5 | M | 341 | ALA | Mainchain |
| 5 | M | 343 | ALA | Mainchain |
| 6 | N | 374 | SER | Mainchain |
| 6 | N | 407 | LEU | Mainchain |
| 6 | N | 408 | SER | Peptide |
| 6 | N | 493 | ALA | Peptide |
| 6 | N | 497 | ARG | Mainchain |
| 2 | O | 11 | GLN | Mainchain |
| 2 | O | 4 | GLU | Mainchain |
| 2 | O | 6 | PHE | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | O | 7 | GLY | Mainchain |
| 3 | P | 1448 | MET | Mainchain |
| 3 | P | 1449 | TRP | Peptide |
| 3 | P | 1450 | GLU | Peptide |
| 3 | P | 1484 | ASP | Mainchain |
| 3 | P | 1485 | ALA | Mainchain |
| 3 | P | 1486 | CYS | Mainchain |
| 3 | P | 1489 | HIS | Mainchain |
| 3 | P | 1503 | ILE | Mainchain |
| 3 | P | 1507 | ASP | Mainchain |
| 3 | P | 1508 | LYS | Mainchain,Peptide |
| 3 | P | 1509 | GLN | Mainchain |
| 3 | P | 1516 | LEU | Mainchain |
| 3 | P | 1517 | SER | Mainchain,Peptide |
| 3 | P | 1518 | ASN | Mainchain |
| 3 | P | 1519 | SER | Peptide |
| 3 | P | 1538 | SER | Mainchain |
| 3 | P | 1541 | THR | Mainchain |
| 3 | P | 1542 | PRO | Mainchain |
| 1 | Q | 259 | SER | Mainchain |
| 4 | R | 200 | THR | Mainchain |
| 4 | R | 208 | GLN | Mainchain |
| 4 | R | 210 | VAL | Mainchain |
| 4 | R | 221 | GLN | Mainchain,Peptide |
| 4 | R | 236 | ASP | Mainchain |
| 4 | R | 245 | VAL | Mainchain |
| 4 | R | 250 | ASN | Mainchain |
| 4 | R | 253 | SER | Mainchain |
| 4 | R | 393 | GLN | Mainchain |
| 4 | R | 397 | ARG | Mainchain |
| 4 | R | 398 | LYS | Mainchain,Peptide |
| 4 | R | 399 | SER | Peptide |
| 4 | R | 400 | GLY | Mainchain |
| 4 | R | 401 | TYR | Mainchain |
| 4 | R | 403 | ILE | Peptide |
| 4 | R | 419 | GLY | Mainchain |
| 4 | R | 420 | GLU | Mainchain |
| 4 | R | 421 | LEU | Mainchain |
| 4 | R | 422 | ASN | Mainchain,Peptide |
| 4 | R | 423 | ALA | Mainchain |
| 4 | R | 424 | PRO | Mainchain,Peptide |
| 4 | R | 425 | THR | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | R | 426 | GLN | Mainchain |
| 4 | R | 445 | GLY | Mainchain |
| 4 | R | 446 | ALA | Mainchain |
| 4 | R | 448 | ARG | Mainchain |
| 4 | R | 452 | ARG | Mainchain |
| 4 | R | 454 | TYR | Mainchain,Peptide |
| 4 | R | 456 | ASP | Mainchain |
| 4 | R | 457 | ALA | Mainchain |
| 4 | R | 459 | LEU | Mainchain |
| 4 | R | 462 | GLU | Mainchain |
| 4 | R | 463 | ILE | Peptide |
| 4 | R | 472 | GLU | Mainchain |
| 4 | R | 487 | ASP | Mainchain |
| 5 | S | 321 | ASN | Mainchain |
| 5 | S | 325 | ALA | Mainchain |
| 5 | S | 326 | LEU | Mainchain,Peptide |
| 5 | S | 329 | GLN | Mainchain |
| 5 | S | 330 | LYS | Mainchain |
| 5 | S | 340 | ALA | Mainchain,Peptide |
| 5 | S | 341 | ALA | Mainchain |
| 5 | S | 343 | ALA | Mainchain |
| 6 | T | 374 | SER | Mainchain |
| 6 | T | 407 | LEU | Mainchain |
| 6 | T | 408 | SER | Peptide |
| 6 | T | 493 | ALA | Peptide |
| 2 | U | 11 | GLN | Mainchain |
| 2 | U | 4 | GLU | Mainchain |
| 2 | U | 6 | PHE | Mainchain |
| 2 | U | 7 | GLY | Mainchain |
| 7 | V | 1386 | LYS | Peptide |
| 7 | V | 1387 | SER | Peptide |
| 7 | V | 1465 | GLU | Mainchain |
| 1 | W | 259 | SER | Mainchain |
| 4 | X | 200 | THR | Mainchain |
| 4 | X | 208 | GLN | Mainchain |
| 4 | X | 210 | VAL | Mainchain |
| 4 | X | 221 | GLN | Mainchain,Peptide |
| 4 | X | 236 | ASP | Mainchain |
| 4 | X | 245 | VAL | Mainchain |
| 4 | X | 250 | ASN | Mainchain |
| 4 | X | 253 | SER | Mainchain |
| 4 | X | 393 | GLN | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | X | 397 | ARG | Mainchain |
| 4 | X | 398 | LYS | Mainchain,Peptide |
| 4 | X | 399 | SER | Peptide |
| 4 | X | 400 | GLY | Mainchain |
| 4 | X | 401 | TYR | Mainchain |
| 4 | X | 403 | ILE | Peptide |
| 4 | X | 419 | GLY | Mainchain |
| 4 | X | 420 | GLU | Mainchain |
| 4 | X | 421 | LEU | Mainchain |
| 4 | X | 422 | ASN | Mainchain,Peptide |
| 4 | X | 423 | ALA | Mainchain |
| 4 | X | 424 | PRO | Mainchain,Peptide |
| 4 | X | 425 | THR | Mainchain |
| 4 | X | 426 | GLN | Mainchain |
| 4 | X | 445 | GLY | Mainchain |
| 4 | X | 446 | ALA | Mainchain |
| 4 | X | 448 | ARG | Mainchain |
| 4 | X | 452 | ARG | Mainchain |
| 4 | X | 454 | TYR | Mainchain,Peptide |
| 4 | X | 456 | ASP | Mainchain |
| 4 | X | 457 | ALA | Mainchain |
| 4 | X | 459 | LEU | Mainchain |
| 4 | X | 462 | GLU | Mainchain |
| 4 | X | 463 | ILE | Peptide |
| 4 | X | 472 | GLU | Mainchain |
| 4 | X | 487 | ASP | Mainchain |
| 5 | Y | 321 | ASN | Mainchain |
| 5 | Y | 325 | ALA | Mainchain |
| 5 | Y | 326 | LEU | Mainchain,Peptide |
| 5 | Y | 329 | GLN | Mainchain |
| 5 | Y | 330 | LYS | Mainchain |
| 5 | Y | 340 | ALA | Mainchain,Peptide |
| 5 | Y | 341 | ALA | Mainchain |
| 5 | Y | 343 | ALA | Mainchain |
| 6 | Z | 374 | SER | Mainchain |
| 6 | Z | 407 | LEU | Mainchain |
| 6 | Z | 408 | SER | Peptide |
| 6 | Z | 493 | ALA | Peptide |
| 6 | Z | 497 | ARG | Mainchain |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3214 | 0 | 1424 | 23 | 0 |
| 1 | B | 3214 | 0 | 1424 | 23 | 0 |
| 1 | E | 5366 | 0 | 2364 | 58 | 0 |
| 1 | K | 5366 | 0 | 2360 | 73 | 0 |
| 1 | Q | 5366 | 0 | 2364 | 63 | 0 |
| 1 | W | 5366 | 0 | 2364 | 56 | 0 |
| 2 | C | 3152 | 0 | 1401 | 155 | 0 |
| 2 | I | 3152 | 0 | 1406 | 30 | 0 |
| 2 | O | 3152 | 0 | 1403 | 88 | 0 |
| 2 | U | 3152 | 0 | 1406 | 30 | 0 |
| 3 | D | 5094 | 0 | 2272 | 121 | 0 |
| 3 | P | 5094 | 0 | 2273 | 77 | 0 |
| 4 | F | 1658 | 0 | 715 | 168 | 0 |
| 4 | L | 1658 | 0 | 715 | 169 | 0 |
| 4 | R | 1658 | 0 | 714 | 169 | 0 |
| 4 | X | 1658 | 0 | 715 | 168 | 0 |
| 5 | G | 853 | 0 | 384 | 57 | 0 |
| 5 | M | 853 | 0 | 384 | 55 | 0 |
| 5 | S | 853 | 0 | 384 | 55 | 0 |
| 5 | Y | 853 | 0 | 384 | 57 | 0 |
| 6 | H | 842 | 0 | 365 | 36 | 0 |
| 6 | N | 842 | 0 | 365 | 39 | 0 |
| 6 | T | 842 | 0 | 365 | 38 | 0 |
| 6 | Z | 842 | 0 | 365 | 38 | 0 |
| 7 | J | 6213 | 0 | 2770 | 79 | 0 |
| 7 | V | 6213 | 0 | 2770 | 78 | 0 |
| All | All | 76526 | 0 | 33856 | 1791 | 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 16.

All (1791) 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) |
|---|---|---|---|
| 5:S:366:GLU:CA | 5:S:366:GLU:CB | 1.76 | 1.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:451:GLU:CA | 4:F:451:GLU:CB | 1.77 | 1.63 |
| 6:N:490:GLN:CA | 6:N:490:GLN:CB | 1.75 | 1.62 |
| 4:F:454:TYR:CA | 4:F:454:TYR:CB | 1.77 | 1.62 |
| 4:X:447:VAL:CA | 4:X:447:VAL:CB | 1.78 | 1.62 |
| 6:T:490:GLN:CA | 6:T:490:GLN:CB | 1.75 | 1.62 |
| 1:E:1165:TYR:CA | 1:K:727:PHE:HA | 1.19 | 1.61 |
| 6:H:490:GLN:CA | 6:H:490:GLN:CB | 1.75 | 1.61 |
| 2:O:783:SER:CB | 1:W:92:GLU:H | 1.05 | 1.61 |
| 4:X:454:TYR:CB | 4:X:454:TYR:CA | 1.77 | 1.60 |
| 2:O:783:SER:H | 1:W:92:GLU:CB | 1.13 | 1.60 |
| 4:X:451:GLU:CA | 4:X:451:GLU:CB | 1.77 | 1.60 |
| 2:C:678:GLY:H | 1:K:847:ARG:CB | 0.97 | 1.59 |
| 6:Z:490:GLN:CB | 6:Z:490:GLN:CA | 1.75 | 1.59 |
| 4:L:235:ASP:CA | 4:L:235:ASP:CB | 1.79 | 1.59 |
| 4:L:454:TYR:CA | 4:L:454:TYR:CB | 1.77 | 1.59 |
| 4:L:447:VAL:CA | 4:L:447:VAL:CB | 1.78 | 1.58 |
| 4:F:235:ASP:CB | 4:F:235:ASP:CA | 1.79 | 1.58 |
| 5:Y:366:GLU:CA | 5:Y:366:GLU:CB | 1.76 | 1.58 |
| 4:X:260:THR:CA | 4:X:260:THR:CB | 1.82 | 1.58 |
| 4:R:488:ILE:N | 4:R:488:ILE:CA | 1.67 | 1.58 |
| 4:X:457:ALA:CA | 4:X:457:ALA:CB | 1.83 | 1.57 |
| 4:X:488:ILE:N | 4:X:488:ILE:CA | 1.67 | 1.57 |
| 5:M:366:GLU:CB | 5:M:366:GLU:CA | 1.76 | 1.57 |
| 4:R:454:TYR:CA | 4:R:454:TYR:CB | 1.77 | 1.57 |
| 4:F:447:VAL:CB | 4:F:447:VAL:CA | 1.78 | 1.56 |
| 4:R:447:VAL:CA | 4:R:447:VAL:CB | 1.78 | 1.56 |
| 4:F:455:ILE:CA | 4:F:455:ILE:CB | 1.84 | 1.56 |
| 4:R:451:GLU:CA | 4:R:451:GLU:CB | 1.77 | 1.56 |
| 4:X:235:ASP:CA | 4:X:235:ASP:CB | 1.78 | 1.56 |
| 4:L:455:ILE:CA | 4:L:455:ILE:CB | 1.84 | 1.56 |
| 4:R:260:THR:CB | 4:R:260:THR:CA | 1.82 | 1.55 |
| 4:R:483:ASP:CA | 4:R:483:ASP:CB | 1.85 | 1.55 |
| 4:L:488:ILE:N | 4:L:488:ILE:CA | 1.67 | 1.55 |
| 2:C:303:ALA:HB1 | 1:Q:849:ASN:CA | 1.10 | 1.55 |
| 4:L:457:ALA:CB | 4:L:457:ALA:CA | 1.83 | 1.55 |
| 2:C:303:ALA:CB | 1:Q:849:ASN:CA | 1.75 | 1.54 |
| 5:G:366:GLU:CB | 5:G:366:GLU:CA | 1.76 | 1.54 |
| 4:R:455:ILE:CB | 4:R:455:ILE:CA | 1.84 | 1.54 |
| 6:T:497:ARG:CA | 6:T:497:ARG:N | 1.69 | 1.54 |
| 4:L:450:GLU:CA | 4:L:451:GLU:N | 1.70 | 1.54 |
| 4:L:260:THR:CA | 4:L:260:THR:CB | 1.82 | 1.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:455:ILE:CB | 4:X:455:ILE:CA | 1.84 | 1.54 |
| 4:L:328:VAL:CA | 4:L:328:VAL:C | 1.75 | 1.54 |
| 4:L:451:GLU:CB | 4:L:451:GLU:CA | 1.77 | 1.54 |
| 4:R:450:GLU:N | 4:R:450:GLU:CA | 1.71 | 1.54 |
| 6:H:497:ARG:N | 6:H:497:ARG:CA | 1.69 | 1.53 |
| 4:L:492:GLU:C | 4:L:492:GLU:CA | 1.75 | 1.53 |
| 4:X:328:VAL:C | 4:X:328:VAL:CA | 1.75 | 1.53 |
| 4:X:456:ASP:CA | 4:X:456:ASP:C | 1.76 | 1.53 |
| 4:X:483:ASP:CA | 4:X:483:ASP:CB | 1.85 | 1.53 |
| 4:R:235:ASP:CA | 4:R:235:ASP:CB | 1.79 | 1.53 |
| 4:X:450:GLU:CA | 4:X:451:GLU:N | 1.70 | 1.53 |
| 4:F:488:ILE:N | 4:F:488:ILE:CA | 1.67 | 1.53 |
| 4:L:483:ASP:CB | 4:L:483:ASP:CA | 1.85 | 1.53 |
| 4:F:328:VAL:CA | 4:F:328:VAL:C | 1.75 | 1.53 |
| 2:C:303:ALA:CA | 1:Q:849:ASN:HA | 1.29 | 1.52 |
| 6:H:381:LYS:N | 6:H:381:LYS:CA | 1.71 | 1.52 |
| 4:L:450:GLU:CA | 4:L:450:GLU:N | 1.71 | 1.52 |
| 4:L:456:ASP:C | 4:L:456:ASP:CA | 1.76 | 1.52 |
| 4:L:458:ASP:CA | 4:L:458:ASP:CB | 1.87 | 1.52 |
| 4:X:450:GLU:CA | 4:X:450:GLU:N | 1.71 | 1.52 |
| 4:F:329:GLY:N | 4:F:329:GLY:CA | 1.72 | 1.52 |
| 4:X:492:GLU:CA | 4:X:492:GLU:C | 1.75 | 1.52 |
| 5:Y:327:ARG:CB | 5:Y:327:ARG:CA | 1.87 | 1.52 |
| 5:S:327:ARG:CA | 5:S:327:ARG:CB | 1.87 | 1.52 |
| 4:R:450:GLU:CA | 4:R:451:GLU:N | 1.70 | 1.51 |
| 4:R:328:VAL:C | 4:R:328:VAL:CA | 1.75 | 1.51 |
| 2:C:303:ALA:C | 1:Q:849:ASN:HA | 1.22 | 1.51 |
| 4:R:492:GLU:C | 4:R:492:GLU:CA | 1.75 | 1.51 |
| 4:R:456:ASP:C | 4:R:456:ASP:CA | 1.76 | 1.51 |
| 5:Y:325:ALA:CA | 5:Y:325:ALA:C | 1.78 | 1.51 |
| 2:C:534:LEU:CB | 3:D:1667:ALA:H | 1.21 | 1.51 |
| 4:F:260:THR:CA | 4:F:260:THR:CB | 1.82 | 1.51 |
| 4:X:329:GLY:N | 4:X:329:GLY:CA | 1.71 | 1.51 |
| 5:Y:326:LEU:CA | 5:Y:326:LEU:C | 1.79 | 1.51 |
| 6:Z:463:ALA:N | 6:Z:463:ALA:CA | 1.74 | 1.51 |
| 2:C:303:ALA:CB | 1:Q:849:ASN:CB | 1.87 | 1.50 |
| 4:F:457:ALA:CA | 4:F:457:ALA:CB | 1.83 | 1.50 |
| 4:L:311:GLN:CA | 4:L:311:GLN:C | 1.77 | 1.50 |
| 4:R:329:GLY:N | 4:R:329:GLY:CA | 1.71 | 1.50 |
| 4:F:450:GLU:N | 4:F:450:GLU:CA | 1.71 | 1.50 |
| 4:F:456:ASP:CA | 4:F:456:ASP:C | 1.76 | 1.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:483:ASP:CA | 4:F:483:ASP:CB | 1.85 | 1.50 |
| 6:H:463:ALA:N | 6:H:463:ALA:CA | 1.74 | 1.50 |
| 6:N:463:ALA:N | 6:N:463:ALA:CA | 1.74 | 1.50 |
| 4:F:450:GLU:CA | 4:F:451:GLU:N | 1.70 | 1.50 |
| 4:R:311:GLN:CA | 4:R:311:GLN:C | 1.77 | 1.50 |
| 4:X:453:TYR:N | 4:X:453:TYR:CA | 1.75 | 1.50 |
| 2:O:783:SER:CB | 1:W:92:GLU:N | 1.72 | 1.50 |
| 4:R:457:ALA:CA | 4:R:457:ALA:CB | 1.83 | 1.50 |
| 6:T:381:LYS:N | 6:T:381:LYS:CA | 1.71 | 1.50 |
| 4:F:492:GLU:CA | 4:F:492:GLU:C | 1.75 | 1.50 |
| 6:Z:381:LYS:N | 6:Z:381:LYS:CA | 1.71 | 1.50 |
| 5:G:325:ALA:CA | 5:G:325:ALA:C | 1.78 | 1.49 |
| 5:G:327:ARG:CA | 5:G:327:ARG:CB | 1.87 | 1.49 |
| 2:C:306:PRO:HA | 1:Q:849:ASN:CB | 1.04 | 1.49 |
| 2:C:678:GLY:N | 1:K:847:ARG:CB | 1.74 | 1.49 |
| 5:G:326:LEU:CA | 5:G:326:LEU:C | 1.79 | 1.49 |
| 4:L:329:GLY:N | 4:L:329:GLY:CA | 1.71 | 1.49 |
| 5:S:326:LEU:C | 5:S:326:LEU:CA | 1.79 | 1.49 |
| 4:X:311:GLN:C | 4:X:311:GLN:CA | 1.77 | 1.49 |
| 4:F:458:ASP:CB | 4:F:458:ASP:CA | 1.87 | 1.49 |
| 4:F:472:GLU:N | 4:F:472:GLU:CA | 1.76 | 1.49 |
| 6:N:381:LYS:N | 6:N:381:LYS:CA | 1.71 | 1.49 |
| 4:L:453:TYR:N | 4:L:453:TYR:CA | 1.75 | 1.49 |
| 5:M:326:LEU:C | 5:M:326:LEU:CA | 1.79 | 1.49 |
| 1:E:1165:TYR:HA | 1:K:727:PHE:CA | 1.36 | 1.49 |
| 4:L:493:HIS:N | 4:L:493:HIS:CA | 1.76 | 1.49 |
| 5:S:325:ALA:C | 5:S:325:ALA:CA | 1.78 | 1.49 |
| 5:G:379:HIS:N | 5:G:379:HIS:CA | 1.76 | 1.48 |
| 6:Z:497:ARG:N | 6:Z:497:ARG:CA | 1.69 | 1.48 |
| 5:M:325:ALA:C | 5:M:325:ALA:CA | 1.77 | 1.48 |
| 6:N:497:ARG:N | 6:N:497:ARG:CA | 1.69 | 1.48 |
| 4:X:472:GLU:N | 4:X:472:GLU:CA | 1.76 | 1.48 |
| 4:F:311:GLN:C | 4:F:311:GLN:CA | 1.77 | 1.48 |
| 4:R:458:ASP:CA | 4:R:458:ASP:CB | 1.87 | 1.48 |
| 4:X:458:ASP:CA | 4:X:458:ASP:CB | 1.87 | 1.48 |
| 5:S:327:ARG:CA | 5:S:327:ARG:N | 1.77 | 1.48 |
| 5:S:379:HIS:N | 5:S:379:HIS:CA | 1.76 | 1.48 |
| 5:Y:379:HIS:N | 5:Y:379:HIS:CA | 1.76 | 1.48 |
| 6:T:463:ALA:N | 6:T:463:ALA:CA | 1.74 | 1.48 |
| 5:Y:276:SER:C | 5:Y:276:SER:CA | 1.82 | 1.48 |
| 5:G:276:SER:CA | 5:G:276:SER:C | 1.82 | 1.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:M:327:ARG:CA | 5:M:327:ARG:CB | 1.87 | 1.47 |
| 5:M:327:ARG:CA | 5:M:327:ARG:N | 1.77 | 1.47 |
| 4:F:493:HIS:N | 4:F:493:HIS:CA | 1.76 | 1.47 |
| 4:R:472:GLU:N | 4:R:472:GLU:CA | 1.76 | 1.47 |
| 5:G:327:ARG:CA | 5:G:327:ARG:N | 1.77 | 1.47 |
| 5:S:276:SER:C | 5:S:276:SER:CA | 1.82 | 1.47 |
| 4:X:400:GLY:N | 4:X:401:TYR:N | 1.63 | 1.47 |
| 4:R:454:TYR:CA | 4:R:454:TYR:C | 1.83 | 1.46 |
| 6:T:411:GLU:C | 6:T:412:GLU:N | 1.69 | 1.46 |
| 6:Z:411:GLU:C | 6:Z:412:GLU:N | 1.69 | 1.46 |
| 4:F:453:TYR:N | 4:F:453:TYR:CA | 1.75 | 1.46 |
| 5:M:276:SER:CA | 5:M:276:SER:C | 1.82 | 1.46 |
| 5:M:379:HIS:N | 5:M:379:HIS:CA | 1.76 | 1.46 |
| 6:N:411:GLU:C | 6:N:412:GLU:N | 1.69 | 1.46 |
| 4:R:453:TYR:N | 4:R:453:TYR:CA | 1.75 | 1.46 |
| 4:R:493:HIS:N | 4:R:493:HIS:CA | 1.76 | 1.46 |
| 4:X:493:HIS:N | 4:X:493:HIS:CA | 1.76 | 1.46 |
| 4:X:492:GLU:C | 4:X:493:HIS:N | 1.69 | 1.45 |
| 4:R:299:ASN:CA | 4:R:299:ASN:C | 1.84 | 1.45 |
| 4:R:367:THR:C | 4:R:367:THR:CA | 1.85 | 1.45 |
| 4:L:472:GLU:N | 4:L:472:GLU:CA | 1.76 | 1.45 |
| 4:R:492:GLU:C | 4:R:493:HIS:N | 1.69 | 1.45 |
| 4:F:299:ASN:C | 4:F:299:ASN:CA | 1.84 | 1.45 |
| 6:H:462:GLY:CA | 6:H:462:GLY:C | 1.85 | 1.45 |
| 4:L:299:ASN:CA | 4:L:299:ASN:C | 1.84 | 1.45 |
| 4:L:367:THR:C | 4:L:367:THR:CA | 1.85 | 1.45 |
| 5:M:326:LEU:CA | 5:M:326:LEU:N | 1.80 | 1.45 |
| 4:X:454:TYR:CA | 4:X:454:TYR:C | 1.83 | 1.45 |
| 4:F:454:TYR:CA | 4:F:454:TYR:C | 1.83 | 1.44 |
| 2:C:524:ARG:CB | 3:D:1609:ILE:C | 1.86 | 1.44 |
| 4:F:367:THR:CA | 4:F:367:THR:C | 1.85 | 1.44 |
| 4:F:454:TYR:C | 4:F:454:TYR:HA | 1.38 | 1.44 |
| 2:I:15:GLN:CA | 2:I:15:GLN:C | 1.84 | 1.44 |
| 5:S:326:LEU:CA | 5:S:326:LEU:N | 1.80 | 1.44 |
| 4:X:299:ASN:C | 4:X:299:ASN:CA | 1.84 | 1.44 |
| 4:L:454:TYR:CA | 4:L:454:TYR:C | 1.83 | 1.44 |
| 2:U:15:GLN:C | 2:U:15:GLN:CA | 1.84 | 1.44 |
| 2:C:15:GLN:C | 2:C:15:GLN:CA | 1.84 | 1.44 |
| 4:F:400:GLY:N | 4:F:401:TYR:N | 1.63 | 1.44 |
| 6:T:374:SER:CA | 6:T:374:SER:CB | 1.96 | 1.44 |
| 4:L:492:GLU:C | 4:L:493:HIS:N | 1.69 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Z:462:GLY:C | 6:Z:462:GLY:CA | 1.85 | 1.43 |
| 4:R:222:THR:C | 4:R:222:THR:CA | 1.87 | 1.43 |
| 6:T:462:GLY:C | 6:T:462:GLY:CA | 1.85 | 1.43 |
| 5:Y:327:ARG:CA | 5:Y:327:ARG:N | 1.77 | 1.43 |
| 6:H:411:GLU:C | 6:H:412:GLU:N | 1.69 | 1.43 |
| 4:L:400:GLY:N | 4:L:400:GLY:CA | 1.82 | 1.43 |
| 4:R:400:GLY:N | 4:R:400:GLY:CA | 1.82 | 1.43 |
| 5:G:326:LEU:CA | 5:G:326:LEU:N | 1.80 | 1.43 |
| 4:R:400:GLY:N | 4:R:401:TYR:N | 1.63 | 1.43 |
| 4:X:367:THR:CA | 4:X:367:THR:C | 1.85 | 1.43 |
| 5:Y:326:LEU:CA | 5:Y:326:LEU:N | 1.80 | 1.43 |
| 4:L:400:GLY:N | 4:L:401:TYR:N | 1.63 | 1.43 |
| 6:N:462:GLY:CA | 6:N:462:GLY:C | 1.85 | 1.43 |
| 6:Z:374:SER:CB | 6:Z:374:SER:CA | 1.96 | 1.43 |
| 2:C:303:ALA:CB | 1:Q:849:ASN:N | 1.75 | 1.42 |
| 4:F:492:GLU:C | 4:F:493:HIS:N | 1.69 | 1.42 |
| 6:H:409:PRO:CA | 6:H:409:PRO:C | 1.88 | 1.42 |
| 5:M:339:TYR:C | 5:M:340:ALA:N | 1.72 | 1.42 |
| 6:N:374:SER:CA | 6:N:374:SER:CB | 1.96 | 1.42 |
| 2:C:487:CYS:CB | 3:D:1661:ARG:CB | 1.95 | 1.42 |
| 4:F:453:TYR:CA | 4:F:453:TYR:CB | 1.97 | 1.42 |
| 2:O:15:GLN:CA | 2:O:15:GLN:C | 1.84 | 1.42 |
| 5:S:339:TYR:C | 5:S:340:ALA:N | 1.72 | 1.42 |
| 4:F:459:LEU:CA | 4:F:459:LEU:C | 1.86 | 1.42 |
| 5:M:378:SER:CA | 5:M:378:SER:C | 1.88 | 1.42 |
| 4:F:222:THR:CA | 4:F:222:THR:C | 1.87 | 1.41 |
| 4:L:459:LEU:CA | 4:L:459:LEU:C | 1.86 | 1.41 |
| 4:X:400:GLY:N | 4:X:400:GLY:CA | 1.82 | 1.41 |
| 4:X:459:LEU:C | 4:X:459:LEU:CA | 1.86 | 1.41 |
| 5:Y:378:SER:C | 5:Y:378:SER:CA | 1.88 | 1.41 |
| 4:L:222:THR:CA | 4:L:222:THR:C | 1.87 | 1.41 |
| 5:S:378:SER:CA | 5:S:378:SER:C | 1.89 | 1.41 |
| 6:T:409:PRO:CA | 6:T:409:PRO:C | 1.88 | 1.41 |
| 4:X:222:THR:CA | 4:X:222:THR:C | 1.87 | 1.41 |
| 5:G:339:TYR:C | 5:G:340:ALA:N | 1.72 | 1.41 |
| 6:H:374:SER:CA | 6:H:374:SER:CB | 1.96 | 1.41 |
| 5:Y:339:TYR:C | 5:Y:340:ALA:N | 1.72 | 1.41 |
| 4:F:400:GLY:N | 4:F:400:GLY:CA | 1.82 | 1.41 |
| 6:N:409:PRO:CA | 6:N:409:PRO:C | 1.88 | 1.41 |
| 6:Z:409:PRO:C | 6:Z:409:PRO:CA | 1.88 | 1.41 |
| 4:L:453:TYR:CA | 4:L:453:TYR:CB | 1.97 | 1.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:459:LEU:C | 4:R:459:LEU:CA | 1.87 | 1.40 |
| 4:X:453:TYR:CA | 4:X:453:TYR:CB | 1.97 | 1.40 |
| 5:G:378:SER:CA | 5:G:378:SER:C | 1.89 | 1.39 |
| 4:R:453:TYR:CA | 4:R:453:TYR:CB | 1.97 | 1.39 |
| 2:O:783:SER:CB | 1:W:91:PRO:N | 1.84 | 1.39 |
| 2:C:303:ALA:HB1 | 1:Q:849:ASN:N | 1.09 | 1.38 |
| 2:C:306:PRO:CA | 1:Q:849:ASN:CB | 2.00 | 1.38 |
| 2:C:674:TYR:CB | 1:K:849:ASN:HA | 1.47 | 1.36 |
| 4:L:454:TYR:C | 4:L:454:TYR:HA | 1.37 | 1.36 |
| 4:F:450:GLU:C | 4:F:450:GLU:O | 1.64 | 1.36 |
| 4:F:458:ASP:CA | 4:F:458:ASP:C | 1.94 | 1.36 |
| 4:R:450:GLU:C | 4:R:450:GLU:O | 1.64 | 1.35 |
| 4:F:401:TYR:N | 4:F:401:TYR:CA | 1.90 | 1.35 |
| 4:X:401:TYR:N | 4:X:401:TYR:CA | 1.90 | 1.35 |
| 2:C:483:GLU:CB | 3:D:1658:ALA:HA | 1.57 | 1.35 |
| 2:C:676:ALA:HB1 | 1:K:846:ILE:O | 1.23 | 1.35 |
| 4:X:450:GLU:O | 4:X:450:GLU:C | 1.64 | 1.35 |
| 4:L:401:TYR:N | 4:L:401:TYR:CA | 1.90 | 1.34 |
| 4:R:454:TYR:C | 4:R:454:TYR:HA | 1.37 | 1.34 |
| 4:R:458:ASP:CA | 4:R:458:ASP:C | 1.94 | 1.34 |
| 4:L:458:ASP:CA | 4:L:458:ASP:C | 1.94 | 1.34 |
| 4:L:450:GLU:C | 4:L:450:GLU:O | 1.64 | 1.34 |
| 4:R:401:TYR:N | 4:R:401:TYR:CA | 1.90 | 1.34 |
| 2:C:303:ALA:CA | 1:Q:849:ASN:CA | 2.00 | 1.33 |
| 4:X:458:ASP:CA | 4:X:458:ASP:C | 1.94 | 1.33 |
| 4:R:458:ASP:C | 4:R:459:LEU:N | 1.82 | 1.33 |
| 4:X:454:TYR:C | 4:X:454:TYR:HA | 1.37 | 1.32 |
| 4:F:458:ASP:C | 4:F:459:LEU:N | 1.82 | 1.32 |
| 2:O:654:SER:C | 3:P:1454:ALA:O | 1.67 | 1.32 |
| 4:X:458:ASP:C | 4:X:459:LEU:N | 1.82 | 1.32 |
| 4:L:458:ASP:C | 4:L:459:LEU:N | 1.82 | 1.31 |
| 2:O:589:ASN:O | 1:W:850:ALA:N | 1.63 | 1.31 |
| 2:C:534:LEU:CB | 3:D:1667:ALA:N | 1.92 | 1.30 |
| 2:C:303:ALA:HB1 | 1:Q:849:ASN:CB | 1.50 | 1.30 |
| 5:S:341:ALA:N | 5:S:341:ALA:CA | 1.94 | 1.30 |
| 5:G:341:ALA:N | 5:G:341:ALA:CA | 1.94 | 1.30 |
| 5:M:341:ALA:N | 5:M:341:ALA:CA | 1.93 | 1.29 |
| 2:C:530:ARG:O | 3:D:1664:ASP:CA | 1.77 | 1.29 |
| 5:Y:341:ALA:N | 5:Y:341:ALA:CA | 1.94 | 1.29 |
| 5:G:327:ARG:CA | 5:G:327:ARG:C | 2.02 | 1.28 |
| 4:L:451:GLU:CA | 4:L:451:GLU:C | 2.02 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:451:GLU:CA | 4:R:451:GLU:C | 2.02 | 1.28 |
| 4:X:451:GLU:CA | 4:X:451:GLU:C | 2.02 | 1.28 |
| 2:C:524:ARG:CB | 3:D:1609:ILE:CB | 2.11 | 1.28 |
| 4:F:451:GLU:CA | 4:F:451:GLU:C | 2.02 | 1.28 |
| 2:C:531:LEU:O | 3:D:1663:GLN:CB | 1.81 | 1.27 |
| 2:C:674:TYR:CB | 1:K:849:ASN:CA | 2.08 | 1.27 |
| 5:S:327:ARG:CA | 5:S:327:ARG:C | 2.02 | 1.26 |
| 5:Y:327:ARG:CA | 5:Y:327:ARG:C | 2.01 | 1.26 |
| 5:M:327:ARG:CA | 5:M:327:ARG:C | 2.02 | 1.26 |
| 4:R:399:SER:C | 4:R:400:GLY:CA | 2.04 | 1.25 |
| 4:X:399:SER:C | 4:X:400:GLY:CA | 2.04 | 1.25 |
| 4:R:222:THR:CA | 4:R:222:THR:N | 1.99 | 1.25 |
| 1:E:852:VAL:CB | 2:O:304:PRO:CB | 2.13 | 1.25 |
| 4:L:399:SER:C | 4:L:400:GLY:CA | 2.04 | 1.25 |
| 4:L:222:THR:CA | 4:L:222:THR:N | 1.99 | 1.25 |
| 4:F:399:SER:C | 4:F:400:GLY:CA | 2.04 | 1.25 |
| 4:X:222:THR:CA | 4:X:222:THR:N | 1.99 | 1.24 |
| 4:F:222:THR:CA | 4:F:222:THR:N | 1.99 | 1.24 |
| 4:L:402:ALA:HB3 | 4:L:403:ILE:N | 1.11 | 1.24 |
| 4:L:450:GLU:CB | 4:L:451:GLU:N | 2.00 | 1.24 |
| 4:F:402:ALA:HB3 | 4:F:403:ILE:N | 1.11 | 1.24 |
| 4:F:450:GLU:CB | 4:F:451:GLU:N | 2.00 | 1.24 |
| 4:X:450:GLU:CB | 4:X:451:GLU:N | 2.00 | 1.24 |
| 2:O:654:SER:O | 3:P:1455:PRO:HA | 1.06 | 1.23 |
| 4:R:450:GLU:CB | 4:R:451:GLU:N | 2.00 | 1.23 |
| 2:O:783:SER:N | 1:W:92:GLU:CB | 1.87 | 1.21 |
| 4:F:457:ALA:CB | 4:F:457:ALA:N | 2.05 | 1.20 |
| 2:O:654:SER:O | 3:P:1455:PRO:CA | 1.89 | 1.20 |
| 4:R:402:ALA:HB3 | 4:R:403:ILE:N | 1.12 | 1.20 |
| 4:R:457:ALA:CB | 4:R:457:ALA:N | 2.05 | 1.20 |
| 4:X:455:ILE:O | 4:X:457:ALA:N | 1.76 | 1.19 |
| 4:X:450:GLU:O | 4:X:451:GLU:HA | 1.38 | 1.19 |
| 4:R:450:GLU:O | 4:R:451:GLU:HA | 1.37 | 1.19 |
| 4:X:457:ALA:CB | 4:X:457:ALA:N | 2.05 | 1.19 |
| 4:L:450:GLU:O | 4:L:451:GLU:HA | 1.37 | 1.18 |
| 4:L:455:ILE:O | 4:L:457:ALA:N | 1.76 | 1.18 |
| 5:M:341:ALA:N | 5:M:342:PRO:N | 1.92 | 1.18 |
| 4:R:487:ASP:CA | 4:R:487:ASP:C | 2.13 | 1.18 |
| 4:F:456:ASP:C | 4:F:456:ASP:CB | 2.12 | 1.17 |
| 5:G:341:ALA:N | 5:G:342:PRO:N | 1.92 | 1.17 |
| 5:S:341:ALA:N | 5:S:342:PRO:N | 1.92 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:487:ASP:CA | 4:X:487:ASP:C | 2.13 | 1.17 |
| 4:F:487:ASP:C | 4:F:487:ASP:CA | 2.13 | 1.17 |
| 5:G:339:TYR:C | 5:G:340:ALA:CA | 2.13 | 1.17 |
| 4:L:457:ALA:CB | 4:L:457:ALA:N | 2.05 | 1.17 |
| 4:L:487:ASP:C | 4:L:487:ASP:CA | 2.13 | 1.17 |
| 2:C:524:ARG:O | 3:D:1610:PRO:N | 1.77 | 1.17 |
| 4:R:456:ASP:C | 4:R:456:ASP:CB | 2.12 | 1.17 |
| 5:M:379:HIS:C | 5:M:380:ILE:N | 1.99 | 1.16 |
| 4:R:455:ILE:O | 4:R:457:ALA:N | 1.76 | 1.16 |
| 5:Y:339:TYR:C | 5:Y:340:ALA:CA | 2.13 | 1.16 |
| 2:C:304:PRO:N | 1:Q:849:ASN:HA | 1.60 | 1.16 |
| 4:F:455:ILE:O | 4:F:457:ALA:N | 1.76 | 1.16 |
| 5:G:379:HIS:C | 5:G:380:ILE:N | 1.98 | 1.16 |
| 4:L:456:ASP:C | 4:L:456:ASP:CB | 2.12 | 1.16 |
| 2:C:531:LEU:O | 3:D:1664:ASP:N | 1.79 | 1.16 |
| 1:E:1165:TYR:CA | 1:K:727:PHE:CA | 2.04 | 1.16 |
| 5:M:327:ARG:N | 5:M:327:ARG:HA | 1.56 | 1.16 |
| 5:M:339:TYR:C | 5:M:340:ALA:CA | 2.13 | 1.16 |
| 5:S:339:TYR:C | 5:S:340:ALA:CA | 2.13 | 1.16 |
| 5:Y:327:ARG:N | 5:Y:327:ARG:HA | 1.56 | 1.16 |
| 1:E:1169:SER:CB | 1:K:575:ARG:CB | 2.24 | 1.15 |
| 5:Y:341:ALA:N | 5:Y:342:PRO:N | 1.92 | 1.15 |
| 4:X:456:ASP:C | 4:X:456:ASP:CB | 2.12 | 1.15 |
| 2:O:654:SER:CA | 3:P:1454:ALA:O | 1.95 | 1.15 |
| 5:S:379:HIS:C | 5:S:380:ILE:N | 1.98 | 1.15 |
| 5:Y:379:HIS:C | 5:Y:380:ILE:N | 1.99 | 1.15 |
| 4:F:493:HIS:CA | 4:F:493:HIS:CB | 2.25 | 1.15 |
| 4:X:493:HIS:CA | 4:X:493:HIS:CB | 2.25 | 1.15 |
| 4:R:493:HIS:CA | 4:R:493:HIS:CB | 2.25 | 1.14 |
| 1:E:1165:TYR:CB | 1:K:727:PHE:CA | 2.21 | 1.14 |
| 4:L:493:HIS:CA | 4:L:493:HIS:CB | 2.25 | 1.14 |
| 4:X:402:ALA:HB3 | 4:X:403:ILE:N | 1.11 | 1.13 |
| 4:R:450:GLU:CA | 4:R:450:GLU:C | 2.16 | 1.13 |
| 4:F:450:GLU:CA | 4:F:450:GLU:C | 2.16 | 1.13 |
| 4:L:402:ALA:CB | 4:L:403:ILE:N | 1.92 | 1.13 |
| 4:R:452:ARG:HA | 4:R:453:TYR:CA | 1.76 | 1.12 |
| 5:S:327:ARG:N | 5:S:327:ARG:HA | 1.56 | 1.12 |
| 2:O:779:GLU:CB | 1:W:136:TYR:CB | 2.27 | 1.12 |
| 2:C:530:ARG:O | 3:D:1664:ASP:HA | 0.95 | 1.11 |
| 4:L:450:GLU:CA | 4:L:450:GLU:C | 2.16 | 1.11 |
| 4:F:402:ALA:CB | 4:F:403:ILE:H | 1.56 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:450:GLU:O | 4:F:451:GLU:HA | 1.38 | 1.11 |
| 5:G:327:ARG:N | 5:G:327:ARG:HA | 1.56 | 1.11 |
| 5:M:326:LEU:C | 5:M:326:LEU:CB | 2.19 | 1.11 |
| 2:C:677:GLN:O | 1:K:852:VAL:CB | 1.97 | 1.11 |
| 5:G:326:LEU:C | 5:G:326:LEU:CB | 2.19 | 1.11 |
| 5:S:326:LEU:C | 5:S:326:LEU:CB | 2.19 | 1.11 |
| 4:X:450:GLU:CA | 4:X:450:GLU:C | 2.16 | 1.11 |
| 5:Y:326:LEU:C | 5:Y:326:LEU:CB | 2.19 | 1.10 |
| 2:C:303:ALA:C | 1:Q:849:ASN:CA | 2.12 | 1.10 |
| 2:C:674:TYR:CB | 1:K:849:ASN:CB | 2.29 | 1.10 |
| 1:E:848:ASP:HA | 2:O:303:ALA:HB1 | 1.34 | 1.10 |
| 2:C:483:GLU:CB | 3:D:1658:ALA:CA | 2.30 | 1.09 |
| 4:L:452:ARG:HA | 4:L:453:TYR:CA | 1.77 | 1.09 |
| 6:Z:490:GLN:CB | 6:Z:490:GLN:C | 2.21 | 1.09 |
| 4:F:454:TYR:HA | 4:F:455:ILE:N | 1.67 | 1.09 |
| 2:C:676:ALA:CB | 1:K:846:ILE:O | 1.99 | 1.08 |
| 6:H:408:SER:HA | 6:H:410:LEU:H | 1.18 | 1.08 |
| 4:L:402:ALA:CB | 4:L:403:ILE:H | 1.56 | 1.08 |
| 4:L:454:TYR:HA | 4:L:455:ILE:N | 1.67 | 1.08 |
| 6:T:490:GLN:CB | 6:T:490:GLN:C | 2.21 | 1.08 |
| 4:X:402:ALA:CB | 4:X:403:ILE:H | 1.56 | 1.08 |
| 2:C:538:LYS:CB | 3:D:1671:GLN:HA | 1.78 | 1.08 |
| 6:N:490:GLN:CB | 6:N:490:GLN:C | 2.21 | 1.08 |
| 2:O:783:SER:CB | 1:W:91:PRO:CA | 2.31 | 1.08 |
| 4:X:452:ARG:HA | 4:X:453:TYR:CA | 1.76 | 1.08 |
| 4:X:454:TYR:CB | 4:X:454:TYR:N | 2.17 | 1.08 |
| 4:F:452:ARG:HA | 4:F:453:TYR:CA | 1.77 | 1.07 |
| 2:O:654:SER:O | 3:P:1454:ALA:O | 1.64 | 1.07 |
| 6:T:408:SER:HA | 6:T:410:LEU:H | 1.18 | 1.07 |
| 4:F:454:TYR:CB | 4:F:454:TYR:N | 2.17 | 1.07 |
| 6:H:490:GLN:CB | 6:H:490:GLN:C | 2.21 | 1.07 |
| 2:C:303:ALA:HB2 | 1:Q:849:ASN:CB | 1.85 | 1.07 |
| 4:L:454:TYR:CB | 4:L:454:TYR:N | 2.17 | 1.07 |
| 4:R:454:TYR:HA | 4:R:455:ILE:N | 1.67 | 1.07 |
| 5:S:326:LEU:CA | 5:S:326:LEU:O | 2.03 | 1.07 |
| 7:V:846:ALA:HB3 | 7:V:852:ILE:H | 1.14 | 1.07 |
| 4:X:454:TYR:HA | 4:X:455:ILE:N | 1.66 | 1.07 |
| 7:J:846:ALA:HB3 | 7:J:852:ILE:H | 1.14 | 1.06 |
| 4:R:402:ALA:CB | 4:R:403:ILE:H | 1.56 | 1.06 |
| 5:Y:326:LEU:CA | 5:Y:326:LEU:O | 2.03 | 1.06 |
| 2:C:524:ARG:CB | 3:D:1609:ILE:O | 2.03 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:402:ALA:CB | 4:X:403:ILE:N | 1.92 | 1.06 |
| 5:M:326:LEU:CA | 5:M:326:LEU:O | 2.03 | 1.05 |
| 4:R:454:TYR:CB | 4:R:454:TYR:N | 2.17 | 1.05 |
| 6:Z:408:SER:HA | 6:Z:410:LEU:H | 1.18 | 1.05 |
| 4:F:402:ALA:CB | 4:F:403:ILE:N | 1.92 | 1.05 |
| 5:G:326:LEU:CA | 5:G:326:LEU:O | 2.03 | 1.04 |
| 3:D:1663:GLN:HA | 3:D:1667:ALA:HB2 | 1.39 | 1.04 |
| 6:H:411:GLU:C | 6:H:411:GLU:CA | 2.26 | 1.04 |
| 4:R:400:GLY:C | 4:R:401:TYR:CA | 2.26 | 1.04 |
| 6:T:411:GLU:C | 6:T:411:GLU:CA | 2.26 | 1.04 |
| 6:Z:411:GLU:C | 6:Z:411:GLU:CA | 2.26 | 1.04 |
| 3:P:1663:GLN:HA | 3:P:1667:ALA:HB2 | 1.39 | 1.03 |
| 4:L:400:GLY:C | 4:L:401:TYR:CA | 2.26 | 1.03 |
| 6:N:411:GLU:C | 6:N:411:GLU:CA | 2.26 | 1.03 |
| 4:F:400:GLY:C | 4:F:401:TYR:CA | 2.26 | 1.03 |
| 4:R:458:ASP:CB | 4:R:459:LEU:N | 2.22 | 1.03 |
| 4:L:458:ASP:CB | 4:L:459:LEU:N | 2.22 | 1.03 |
| 4:X:400:GLY:C | 4:X:401:TYR:CA | 2.26 | 1.03 |
| 4:L:458:ASP:O | 4:L:460:LEU:N | 1.92 | 1.03 |
| 4:R:458:ASP:O | 4:R:460:LEU:N | 1.92 | 1.02 |
| 4:X:458:ASP:O | 4:X:460:LEU:N | 1.92 | 1.02 |
| 4:L:451:GLU:C | 4:L:451:GLU:HA | 1.77 | 1.02 |
| 4:X:451:GLU:C | 4:X:451:GLU:HA | 1.78 | 1.02 |
| 5:M:380:ILE:N | 5:M:380:ILE:CA | 2.23 | 1.02 |
| 5:Y:380:ILE:N | 5:Y:380:ILE:CA | 2.23 | 1.02 |
| 4:F:458:ASP:CB | 4:F:459:LEU:N | 2.22 | 1.02 |
| 6:N:408:SER:HA | 6:N:410:LEU:H | 1.18 | 1.02 |
| 4:X:458:ASP:CB | 4:X:459:LEU:N | 2.22 | 1.02 |
| 4:F:458:ASP:O | 4:F:460:LEU:N | 1.92 | 1.01 |
| 5:G:380:ILE:N | 5:G:380:ILE:CA | 2.23 | 1.00 |
| 1:E:1165:TYR:CB | 1:K:727:PHE:HA | 1.89 | 1.00 |
| 2:C:524:ARG:CB | 3:D:1609:ILE:CA | 2.39 | 1.00 |
| 5:S:380:ILE:N | 5:S:380:ILE:CA | 2.23 | 0.99 |
| 1:E:847:ARG:O | 2:O:303:ALA:HB1 | 1.61 | 0.99 |
| 4:R:402:ALA:CB | 4:R:403:ILE:N | 1.92 | 0.99 |
| 4:F:451:GLU:C | 4:F:451:GLU:HA | 1.77 | 0.99 |
| 5:Y:366:GLU:CB | 5:Y:366:GLU:C | 2.31 | 0.99 |
| 2:O:783:SER:H | 1:W:92:GLU:CA | 1.75 | 0.99 |
| 2:C:538:LYS:CB | 3:D:1671:GLN:CA | 2.27 | 0.99 |
| 5:S:366:GLU:CB | 5:S:366:GLU:C | 2.31 | 0.99 |
| 4:R:451:GLU:C | 4:R:451:GLU:HA | 1.77 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1165:TYR:CB | 1:K:727:PHE:C | 2.32 | 0.98 |
| 5:M:366:GLU:CB | 5:M:366:GLU:C | 2.31 | 0.98 |
| 2:O:589:ASN:CB | 1:W:849:ASN:CB | 2.43 | 0.97 |
| 5:G:366:GLU:CB | 5:G:366:GLU:C | 2.31 | 0.97 |
| 4:L:453:TYR:O | 4:L:455:ILE:CB | 2.13 | 0.97 |
| 4:R:452:ARG:CA | 4:R:453:TYR:CA | 2.41 | 0.97 |
| 2:O:783:SER:CB | 1:W:91:PRO:C | 2.32 | 0.96 |
| 4:X:222:THR:C | 4:X:222:THR:CB | 2.34 | 0.96 |
| 4:R:222:THR:C | 4:R:222:THR:CB | 2.34 | 0.96 |
| 4:F:453:TYR:O | 4:F:455:ILE:CB | 2.13 | 0.96 |
| 4:L:222:THR:C | 4:L:222:THR:CB | 2.34 | 0.95 |
| 2:C:303:ALA:CA | 1:Q:849:ASN:CB | 2.34 | 0.95 |
| 4:X:453:TYR:O | 4:X:455:ILE:CB | 2.13 | 0.95 |
| 4:R:453:TYR:O | 4:R:455:ILE:CB | 2.13 | 0.95 |
| 4:R:311:GLN:C | 4:R:311:GLN:CB | 2.35 | 0.95 |
| 4:X:452:ARG:CA | 4:X:453:TYR:CA | 2.41 | 0.95 |
| 4:X:458:ASP:C | 4:X:459:LEU:CA | 2.35 | 0.95 |
| 4:F:222:THR:C | 4:F:222:THR:CB | 2.34 | 0.95 |
| 2:C:304:PRO:N | 1:Q:849:ASN:CA | 2.29 | 0.94 |
| 4:F:458:ASP:C | 4:F:459:LEU:CA | 2.35 | 0.94 |
| 4:L:458:ASP:C | 4:L:459:LEU:CA | 2.35 | 0.94 |
| 4:F:311:GLN:C | 4:F:311:GLN:CB | 2.35 | 0.94 |
| 4:L:452:ARG:CA | 4:L:453:TYR:CA | 2.41 | 0.94 |
| 4:X:455:ILE:O | 4:X:456:ASP:C | 2.02 | 0.94 |
| 4:L:311:GLN:C | 4:L:311:GLN:CB | 2.36 | 0.94 |
| 4:R:458:ASP:C | 4:R:459:LEU:CA | 2.35 | 0.94 |
| 2:C:523:LEU:H | 3:D:1613:VAL:CB | 1.81 | 0.94 |
| 2:C:303:ALA:CB | 1:Q:849:ASN:H | 1.81 | 0.94 |
| 4:X:311:GLN:C | 4:X:311:GLN:CB | 2.35 | 0.93 |
| 4:R:455:ILE:O | 4:R:456:ASP:C | 2.02 | 0.93 |
| 4:F:452:ARG:CA | 4:F:453:TYR:CA | 2.41 | 0.93 |
| 1:E:848:ASP:HA | 2:O:303:ALA:CB | 1.99 | 0.93 |
| 4:L:455:ILE:O | 4:L:456:ASP:C | 2.02 | 0.92 |
| 2:C:675:ARG:N | 1:K:849:ASN:CB | 2.26 | 0.92 |
| 6:T:409:PRO:C | 6:T:409:PRO:CB | 2.38 | 0.92 |
| 6:Z:409:PRO:C | 6:Z:409:PRO:CB | 2.38 | 0.92 |
| 2:C:303:ALA:HB3 | 1:Q:849:ASN:N | 1.81 | 0.92 |
| 2:C:523:LEU:CB | 3:D:1613:VAL:CB | 2.47 | 0.92 |
| 6:H:409:PRO:C | 6:H:409:PRO:CB | 2.37 | 0.92 |
| 2:C:15:GLN:C | 2:C:15:GLN:CB | 2.39 | 0.92 |
| 2:I:15:GLN:C | 2:I:15:GLN:CB | 2.39 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:N:409:PRO:C | 6:N:409:PRO:CB | 2.38 | 0.92 |
| 2:C:524:ARG:C | 3:D:1610:PRO:CA | 2.31 | 0.92 |
| 2:U:15:GLN:C | 2:U:15:GLN:CB | 2.38 | 0.91 |
| 4:L:450:GLU:O | 4:L:451:GLU:C | 2.09 | 0.91 |
| 2:C:483:GLU:CB | 3:D:1658:ALA:CB | 2.49 | 0.91 |
| 4:F:450:GLU:O | 4:F:451:GLU:C | 2.09 | 0.91 |
| 3:D:1663:GLN:CA | 3:D:1667:ALA:HB2 | 2.01 | 0.91 |
| 4:R:450:GLU:O | 4:R:451:GLU:C | 2.09 | 0.90 |
| 2:O:15:GLN:C | 2:O:15:GLN:CB | 2.39 | 0.90 |
| 3:D:751:ALA:HB3 | 3:D:754:ARG:CB | 2.02 | 0.90 |
| 2:O:654:SER:CB | 3:P:1454:ALA:O | 2.19 | 0.90 |
| 4:X:450:GLU:O | 4:X:451:GLU:C | 2.09 | 0.90 |
| 4:X:399:SER:C | 4:X:400:GLY:HA3 | 1.93 | 0.90 |
| 2:C:535:TYR:CA | 3:D:1663:GLN:HA | 2.02 | 0.90 |
| 3:P:1663:GLN:CA | 3:P:1667:ALA:HB2 | 2.01 | 0.90 |
| 3:P:751:ALA:HB3 | 3:P:754:ARG:CB | 2.02 | 0.89 |
| 4:F:451:GLU:CA | 4:F:452:ARG:N | 2.36 | 0.89 |
| 4:L:451:GLU:CA | 4:L:452:ARG:N | 2.36 | 0.89 |
| 4:F:399:SER:C | 4:F:400:GLY:HA3 | 1.93 | 0.89 |
| 2:C:303:ALA:HA | 1:Q:849:ASN:CB | 2.02 | 0.89 |
| 2:O:783:SER:CA | 1:W:92:GLU:H | 1.85 | 0.89 |
| 7:V:846:ALA:HB2 | 7:V:849:ASN:N | 1.88 | 0.89 |
| 4:R:451:GLU:CA | 4:R:452:ARG:N | 2.36 | 0.89 |
| 7:J:846:ALA:HB2 | 7:J:849:ASN:N | 1.88 | 0.88 |
| 4:L:399:SER:C | 4:L:400:GLY:HA3 | 1.93 | 0.88 |
| 2:C:355:TYR:HA | 2:C:362:ARG:CB | 2.04 | 0.88 |
| 2:O:355:TYR:HA | 2:O:362:ARG:CB | 2.04 | 0.88 |
| 2:O:589:ASN:C | 1:W:850:ALA:H | 1.76 | 0.88 |
| 4:X:472:GLU:N | 4:X:472:GLU:CB | 2.37 | 0.87 |
| 2:I:355:TYR:HA | 2:I:362:ARG:CB | 2.04 | 0.87 |
| 1:E:1170:SER:H | 1:K:576:TYR:CB | 1.86 | 0.87 |
| 5:Y:326:LEU:C | 5:Y:327:ARG:CA | 2.43 | 0.87 |
| 5:M:326:LEU:C | 5:M:327:ARG:CA | 2.43 | 0.87 |
| 5:S:326:LEU:C | 5:S:327:ARG:CA | 2.43 | 0.87 |
| 4:R:458:ASP:CA | 4:R:459:LEU:N | 2.38 | 0.87 |
| 2:C:303:ALA:HB1 | 1:Q:848:ASP:C | 1.95 | 0.87 |
| 2:U:355:TYR:HA | 2:U:362:ARG:CB | 2.04 | 0.87 |
| 2:C:534:LEU:CB | 3:D:1666:SER:N | 2.38 | 0.87 |
| 4:L:458:ASP:CA | 4:L:459:LEU:N | 2.38 | 0.87 |
| 4:F:458:ASP:CA | 4:F:459:LEU:N | 2.38 | 0.86 |
| 4:X:451:GLU:CA | 4:X:452:ARG:N | 2.36 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:458:ASP:CA | 4:X:459:LEU:N | 2.38 | 0.86 |
| 4:F:455:ILE:O | 4:F:456:ASP:C | 2.02 | 0.86 |
| 2:O:591:GLY:HA3 | 1:W:849:ASN:O | 1.66 | 0.86 |
| 2:C:303:ALA:HA | 1:Q:849:ASN:HA | 1.52 | 0.86 |
| 4:R:399:SER:C | 4:R:400:GLY:HA3 | 1.93 | 0.85 |
| 4:F:402:ALA:HB3 | 4:F:403:ILE:H | 1.04 | 0.85 |
| 5:G:326:LEU:C | 5:G:327:ARG:CA | 2.43 | 0.85 |
| 4:L:472:GLU:N | 4:L:472:GLU:CB | 2.37 | 0.85 |
| 2:C:522:CYS:CB | 3:D:1664:ASP:CB | 2.54 | 0.85 |
| 4:F:472:GLU:N | 4:F:472:GLU:CB | 2.37 | 0.85 |
| 5:S:326:LEU:CB | 5:S:327:ARG:N | 2.39 | 0.85 |
| 5:M:326:LEU:CB | 5:M:327:ARG:N | 2.39 | 0.84 |
| 2:C:306:PRO:HA | 1:Q:849:ASN:CA | 2.05 | 0.84 |
| 2:C:677:GLN:C | 1:K:852:VAL:CB | 2.45 | 0.84 |
| 6:T:411:GLU:O | 6:T:412:GLU:N | 2.11 | 0.84 |
| 5:G:326:LEU:CB | 5:G:327:ARG:N | 2.39 | 0.84 |
| 6:N:411:GLU:O | 6:N:412:GLU:N | 2.11 | 0.84 |
| 2:C:524:ARG:C | 3:D:1610:PRO:N | 2.30 | 0.84 |
| 4:R:472:GLU:N | 4:R:472:GLU:CB | 2.37 | 0.84 |
| 2:C:486:ARG:CB | 3:D:1661:ARG:C | 2.39 | 0.84 |
| 1:E:852:VAL:CB | 2:O:305:LEU:N | 2.41 | 0.84 |
| 4:X:402:ALA:HB3 | 4:X:403:ILE:H | 1.04 | 0.84 |
| 5:Y:326:LEU:CB | 5:Y:327:ARG:N | 2.39 | 0.84 |
| 2:C:535:TYR:CB | 3:D:1663:GLN:CB | 2.56 | 0.83 |
| 4:L:453:TYR:CA | 4:L:453:TYR:C | 2.47 | 0.83 |
| 1:E:1169:SER:CB | 1:K:572:ALA:HA | 2.07 | 0.83 |
| 4:X:453:TYR:CA | 4:X:453:TYR:C | 2.47 | 0.83 |
| 4:F:453:TYR:CA | 4:F:453:TYR:C | 2.47 | 0.83 |
| 2:C:679:ILE:O | 1:K:854:GLY:N | 1.98 | 0.83 |
| 4:R:402:ALA:HB3 | 4:R:403:ILE:H | 1.04 | 0.83 |
| 6:Z:411:GLU:O | 6:Z:412:GLU:N | 2.11 | 0.83 |
| 7:V:1512:SER:O | 7:V:1546:ALA:HB3 | 1.79 | 0.83 |
| 4:R:453:TYR:CA | 4:R:453:TYR:C | 2.47 | 0.83 |
| 4:R:456:ASP:CA | 4:R:457:ALA:N | 2.33 | 0.82 |
| 4:L:488:ILE:N | 4:L:488:ILE:HA | 1.94 | 0.82 |
| 7:J:1512:SER:O | 7:J:1546:ALA:HB3 | 1.79 | 0.82 |
| 2:C:535:TYR:CB | 3:D:1663:GLN:HA | 2.10 | 0.82 |
| 4:L:402:ALA:HB3 | 4:L:403:ILE:H | 1.04 | 0.82 |
| 6:H:374:SER:CB | 6:H:374:SER:N | 2.43 | 0.81 |
| 4:R:488:ILE:N | 4:R:488:ILE:HA | 1.94 | 0.81 |
| 7:J:1175:GLY:HA3 | 7:J:1197:GLN:H | 1.44 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:535:TYR:H | 3:D:1664:ASP:H | 1.28 | 0.81 |
| 6:Z:374:SER:CB | 6:Z:374:SER:N | 2.44 | 0.81 |
| 6:N:497:ARG:N | 6:N:497:ARG:CB | 2.43 | 0.81 |
| 5:S:379:HIS:CA | 5:S:379:HIS:C | 2.49 | 0.81 |
| 6:N:374:SER:CB | 6:N:374:SER:N | 2.44 | 0.81 |
| 7:V:1175:GLY:HA3 | 7:V:1197:GLN:H | 1.44 | 0.81 |
| 5:Y:379:HIS:CA | 5:Y:379:HIS:C | 2.49 | 0.81 |
| 6:Z:497:ARG:N | 6:Z:497:ARG:CB | 2.43 | 0.81 |
| 4:L:456:ASP:CA | 4:L:457:ALA:N | 2.33 | 0.81 |
| 5:G:379:HIS:CA | 5:G:379:HIS:C | 2.49 | 0.81 |
| 6:N:374:SER:CB | 6:N:374:SER:C | 2.50 | 0.81 |
| 6:H:411:GLU:O | 6:H:412:GLU:N | 2.11 | 0.80 |
| 4:R:158:ASN:HA | 4:R:322:LEU:HA | 1.62 | 0.80 |
| 6:T:374:SER:CB | 6:T:374:SER:N | 2.44 | 0.80 |
| 4:X:158:ASN:HA | 4:X:322:LEU:HA | 1.62 | 0.80 |
| 2:C:173:PRO:N | 3:D:1686:PRO:C | 2.19 | 0.80 |
| 4:F:158:ASN:HA | 4:F:322:LEU:HA | 1.62 | 0.80 |
| 2:C:524:ARG:CB | 3:D:1610:PRO:N | 2.44 | 0.80 |
| 3:D:286:GLN:CB | 3:D:304:LYS:HA | 2.11 | 0.80 |
| 4:F:455:ILE:CB | 4:F:455:ILE:C | 2.50 | 0.80 |
| 5:G:366:GLU:CB | 5:G:366:GLU:N | 2.45 | 0.80 |
| 4:X:455:ILE:CB | 4:X:455:ILE:C | 2.50 | 0.80 |
| 6:H:374:SER:CB | 6:H:374:SER:C | 2.50 | 0.80 |
| 3:P:286:GLN:CB | 3:P:304:LYS:HA | 2.11 | 0.80 |
| 5:S:366:GLU:CB | 5:S:366:GLU:N | 2.45 | 0.80 |
| 6:T:374:SER:CB | 6:T:374:SER:C | 2.50 | 0.80 |
| 4:L:158:ASN:HA | 4:L:322:LEU:HA | 1.62 | 0.80 |
| 5:M:379:HIS:CA | 5:M:379:HIS:C | 2.49 | 0.80 |
| 7:J:846:ALA:HB3 | 7:J:852:ILE:N | 1.96 | 0.80 |
| 2:C:303:ALA:HA | 1:Q:849:ASN:CA | 2.08 | 0.79 |
| 4:L:455:ILE:CB | 4:L:455:ILE:C | 2.50 | 0.79 |
| 4:R:457:ALA:CB | 4:R:457:ALA:H | 1.95 | 0.79 |
| 2:I:15:GLN:C | 2:I:15:GLN:N | 2.36 | 0.79 |
| 6:T:497:ARG:N | 6:T:497:ARG:CB | 2.43 | 0.79 |
| 5:Y:366:GLU:CB | 5:Y:366:GLU:N | 2.45 | 0.79 |
| 3:D:647:LEU:CB | 3:D:706:ALA:HB1 | 2.12 | 0.79 |
| 2:U:15:GLN:C | 2:U:15:GLN:N | 2.36 | 0.79 |
| 7:V:251:ARG:CB | 7:V:256:GLU:HA | 2.13 | 0.79 |
| 6:Z:374:SER:CB | 6:Z:374:SER:C | 2.50 | 0.79 |
| 4:R:455:ILE:CB | 4:R:455:ILE:C | 2.50 | 0.79 |
| 4:L:311:GLN:C | 4:L:311:GLN:N | 2.36 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:311:GLN:C | 4:R:311:GLN:N | 2.36 | 0.79 |
| 5:M:366:GLU:CB | 5:M:366:GLU:N | 2.45 | 0.79 |
| 3:P:647:LEU:CB | 3:P:706:ALA:HB1 | 2.12 | 0.78 |
| 3:P:1663:GLN:C | 3:P:1667:ALA:HB2 | 2.03 | 0.78 |
| 2:C:535:TYR:CB | 3:D:1663:GLN:CA | 2.62 | 0.78 |
| 3:D:1663:GLN:C | 3:D:1667:ALA:HB2 | 2.03 | 0.78 |
| 4:F:456:ASP:CA | 4:F:457:ALA:N | 2.33 | 0.78 |
| 2:O:15:GLN:C | 2:O:15:GLN:N | 2.36 | 0.78 |
| 4:F:457:ALA:CB | 4:F:457:ALA:H | 1.95 | 0.78 |
| 7:J:251:ARG:CB | 7:J:256:GLU:HA | 2.13 | 0.78 |
| 7:V:493:LEU:O | 7:V:520:GLN:HA | 1.84 | 0.78 |
| 7:V:846:ALA:HB3 | 7:V:852:ILE:N | 1.96 | 0.78 |
| 4:F:311:GLN:C | 4:F:311:GLN:N | 2.36 | 0.78 |
| 2:O:591:GLY:CA | 1:W:849:ASN:O | 2.32 | 0.78 |
| 4:X:311:GLN:C | 4:X:311:GLN:N | 2.36 | 0.78 |
| 4:R:235:ASP:CB | 4:R:235:ASP:N | 2.47 | 0.77 |
| 4:X:456:ASP:CA | 4:X:457:ALA:N | 2.34 | 0.77 |
| 7:J:493:LEU:O | 7:J:520:GLN:HA | 1.84 | 0.77 |
| 4:R:449:SER:C | 4:R:450:GLU:C | 2.43 | 0.77 |
| 4:X:235:ASP:CB | 4:X:235:ASP:N | 2.47 | 0.77 |
| 5:M:339:TYR:C | 5:M:340:ALA:CB | 2.53 | 0.77 |
| 2:C:15:GLN:C | 2:C:15:GLN:N | 2.36 | 0.77 |
| 6:T:408:SER:HA | 6:T:410:LEU:N | 1.97 | 0.77 |
| 4:L:235:ASP:CB | 4:L:235:ASP:N | 2.47 | 0.77 |
| 1:E:276:ASP:CB | 1:E:295:SER:CB | 2.63 | 0.77 |
| 1:W:276:ASP:CB | 1:W:295:SER:CB | 2.63 | 0.77 |
| 4:X:457:ALA:CB | 4:X:457:ALA:H | 1.95 | 0.77 |
| 4:R:456:ASP:O | 4:R:457:ALA:C | 2.18 | 0.77 |
| 2:C:523:LEU:N | 3:D:1613:VAL:CB | 2.48 | 0.77 |
| 6:H:497:ARG:N | 6:H:497:ARG:CB | 2.43 | 0.77 |
| 5:S:339:TYR:C | 5:S:340:ALA:CB | 2.53 | 0.77 |
| 1:K:276:ASP:CB | 1:K:295:SER:CB | 2.63 | 0.77 |
| 2:O:654:SER:O | 3:P:1454:ALA:C | 2.22 | 0.77 |
| 6:Z:408:SER:HA | 6:Z:410:LEU:N | 1.98 | 0.77 |
| 1:A:276:ASP:CB | 1:A:295:SER:CB | 2.63 | 0.76 |
| 5:G:339:TYR:C | 5:G:340:ALA:CB | 2.53 | 0.76 |
| 4:X:449:SER:C | 4:X:450:GLU:C | 2.43 | 0.76 |
| 4:R:487:ASP:C | 4:R:487:ASP:N | 2.39 | 0.76 |
| 2:C:531:LEU:O | 3:D:1663:GLN:C | 2.23 | 0.76 |
| 4:F:449:SER:C | 4:F:450:GLU:C | 2.43 | 0.76 |
| 5:Y:339:TYR:C | 5:Y:340:ALA:CB | 2.53 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:276:ASP:CB | 1:Q:295:SER:CB | 2.63 | 0.76 |
| 4:F:487:ASP:C | 4:F:487:ASP:N | 2.39 | 0.76 |
| 4:F:235:ASP:CB | 4:F:235:ASP:N | 2.47 | 0.76 |
| 4:L:449:SER:C | 4:L:450:GLU:C | 2.43 | 0.76 |
| 1:B:276:ASP:CB | 1:B:295:SER:CB | 2.63 | 0.76 |
| 4:F:456:ASP:O | 4:F:457:ALA:C | 2.18 | 0.76 |
| 6:H:408:SER:HA | 6:H:410:LEU:N | 1.98 | 0.76 |
| 1:E:1165:TYR:HA | 1:K:727:PHE:N | 2.00 | 0.75 |
| 4:F:471:GLN:C | 4:F:472:GLU:CA | 2.54 | 0.75 |
| 4:L:492:GLU:C | 4:L:492:GLU:CB | 2.54 | 0.75 |
| 4:X:471:GLN:C | 4:X:472:GLU:CA | 2.55 | 0.75 |
| 1:Q:326:ALA:HB1 | 1:Q:387:LEU:CB | 2.17 | 0.75 |
| 4:X:487:ASP:C | 4:X:487:ASP:N | 2.39 | 0.75 |
| 4:F:488:ILE:N | 4:F:488:ILE:HA | 1.94 | 0.75 |
| 4:F:492:GLU:C | 4:F:492:GLU:CB | 2.55 | 0.75 |
| 4:L:487:ASP:C | 4:L:487:ASP:N | 2.39 | 0.75 |
| 2:C:530:ARG:C | 3:D:1664:ASP:HA | 2.02 | 0.75 |
| 1:K:326:ALA:HB1 | 1:K:387:LEU:CB | 2.17 | 0.75 |
| 4:X:492:GLU:C | 4:X:492:GLU:CB | 2.55 | 0.75 |
| 1:A:326:ALA:HB1 | 1:A:387:LEU:CB | 2.17 | 0.75 |
| 1:E:326:ALA:HB1 | 1:E:387:LEU:CB | 2.17 | 0.75 |
| 6:N:408:SER:HA | 6:N:410:LEU:N | 1.97 | 0.75 |
| 1:W:326:ALA:HB1 | 1:W:387:LEU:CB | 2.17 | 0.75 |
| 6:H:497:ARG:N | 6:H:497:ARG:C | 2.40 | 0.74 |
| 2:C:524:ARG:C | 3:D:1610:PRO:HA | 2.06 | 0.74 |
| 4:L:471:GLN:C | 4:L:472:GLU:CA | 2.55 | 0.74 |
| 2:O:589:ASN:O | 1:W:849:ASN:CB | 2.35 | 0.74 |
| 4:R:471:GLN:C | 4:R:472:GLU:CA | 2.55 | 0.74 |
| 4:R:492:GLU:C | 4:R:492:GLU:CB | 2.55 | 0.74 |
| 4:L:457:ALA:CB | 4:L:457:ALA:H | 1.95 | 0.74 |
| 1:B:326:ALA:HB1 | 1:B:387:LEU:CB | 2.17 | 0.74 |
| 2:O:783:SER:CB | 1:W:90:PRO:C | 2.56 | 0.74 |
| 4:L:456:ASP:O | 4:L:457:ALA:C | 2.18 | 0.73 |
| 6:H:381:LYS:N | 6:H:381:LYS:C | 2.42 | 0.73 |
| 4:F:399:SER:O | 4:F:400:GLY:CA | 2.36 | 0.73 |
| 4:R:299:ASN:C | 4:R:299:ASN:N | 2.42 | 0.73 |
| 6:T:497:ARG:N | 6:T:497:ARG:C | 2.40 | 0.73 |
| 4:R:140:LYS:HA | 4:R:149:GLY:H | 1.54 | 0.73 |
| 4:R:456:ASP:C | 4:R:456:ASP:N | 2.39 | 0.73 |
| 4:L:456:ASP:C | 4:L:456:ASP:N | 2.39 | 0.73 |
| 5:M:341:ALA:H | 5:M:342:PRO:N | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:534:LEU:CB | 3:D:1665:VAL:C | 2.52 | 0.73 |
| 4:R:399:SER:O | 4:R:400:GLY:CA | 2.36 | 0.73 |
| 4:X:299:ASN:C | 4:X:299:ASN:N | 2.42 | 0.73 |
| 4:F:140:LYS:HA | 4:F:149:GLY:H | 1.54 | 0.72 |
| 4:L:140:LYS:HA | 4:L:149:GLY:H | 1.54 | 0.72 |
| 4:F:299:ASN:C | 4:F:299:ASN:N | 2.42 | 0.72 |
| 4:X:399:SER:O | 4:X:400:GLY:CA | 2.36 | 0.72 |
| 3:D:1663:GLN:HA | 3:D:1667:ALA:CB | 2.18 | 0.72 |
| 4:R:446:ALA:O | 4:R:449:SER:CB | 2.38 | 0.72 |
| 7:V:1465:GLU:C | 7:V:1473:LEU:HA | 2.10 | 0.72 |
| 4:X:446:ALA:O | 4:X:449:SER:CB | 2.38 | 0.72 |
| 4:F:402:ALA:HB2 | 4:F:403:ILE:H | 1.53 | 0.72 |
| 4:F:446:ALA:O | 4:F:449:SER:CB | 2.38 | 0.72 |
| 4:L:446:ALA:O | 4:L:449:SER:CB | 2.38 | 0.72 |
| 4:X:488:ILE:N | 4:X:488:ILE:HA | 1.94 | 0.72 |
| 7:J:1467:HIS:CB | 7:J:1475:ARG:HA | 2.20 | 0.72 |
| 4:X:456:ASP:O | 4:X:457:ALA:C | 2.18 | 0.72 |
| 2:C:676:ALA:C | 1:K:846:ILE:O | 2.28 | 0.72 |
| 1:K:22:ALA:HB1 | 1:K:780:ALA:HA | 1.71 | 0.72 |
| 7:V:860:TYR:CB | 7:V:869:ARG:H | 2.02 | 0.72 |
| 6:Z:497:ARG:N | 6:Z:497:ARG:C | 2.40 | 0.72 |
| 1:B:22:ALA:HB1 | 1:B:780:ALA:HA | 1.71 | 0.72 |
| 7:J:860:TYR:CB | 7:J:869:ARG:H | 2.02 | 0.72 |
| 4:L:299:ASN:C | 4:L:299:ASN:N | 2.42 | 0.72 |
| 4:X:140:LYS:HA | 4:X:149:GLY:H | 1.54 | 0.72 |
| 6:N:497:ARG:N | 6:N:497:ARG:C | 2.40 | 0.71 |
| 2:C:304:PRO:N | 1:Q:849:ASN:C | 2.39 | 0.71 |
| 4:L:399:SER:O | 4:L:400:GLY:CA | 2.36 | 0.71 |
| 4:L:450:GLU:N | 4:L:450:GLU:C | 2.44 | 0.71 |
| 4:R:450:GLU:N | 4:R:450:GLU:C | 2.44 | 0.71 |
| 7:V:1467:HIS:CB | 7:V:1475:ARG:HA | 2.20 | 0.71 |
| 4:F:450:GLU:N | 4:F:450:GLU:C | 2.44 | 0.71 |
| 4:X:450:GLU:N | 4:X:450:GLU:C | 2.44 | 0.71 |
| 4:X:455:ILE:CB | 4:X:456:ASP:N | 2.54 | 0.71 |
| 1:E:22:ALA:HB1 | 1:E:780:ALA:HA | 1.71 | 0.71 |
| 4:F:456:ASP:C | 4:F:456:ASP:N | 2.39 | 0.71 |
| 4:R:455:ILE:CB | 4:R:456:ASP:N | 2.54 | 0.71 |
| 6:N:381:LYS:N | 6:N:381:LYS:C | 2.42 | 0.71 |
| 7:J:1465:GLU:C | 7:J:1473:LEU:HA | 2.10 | 0.71 |
| 1:Q:22:ALA:HB1 | 1:Q:780:ALA:HA | 1.71 | 0.71 |
| 4:R:454:TYR:HA | 4:R:455:ILE:CA | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:456:ASP:C | 4:X:456:ASP:N | 2.39 | 0.71 |
| 1:A:22:ALA:HB1 | 1:A:780:ALA:HA | 1.71 | 0.71 |
| 7:J:1520:ARG:HA | 7:J:1541:ALA:HB2 | 1.73 | 0.70 |
| 4:X:402:ALA:HB2 | 4:X:403:ILE:H | 1.52 | 0.70 |
| 4:L:454:TYR:HA | 4:L:455:ILE:CA | 2.20 | 0.70 |
| 1:E:1165:TYR:CB | 1:K:727:PHE:O | 2.37 | 0.70 |
| 4:R:252:THR:CB | 4:R:320:GLU:CB | 2.70 | 0.70 |
| 7:V:643:ALA:HB1 | 7:V:658:MET:O | 1.92 | 0.70 |
| 4:L:455:ILE:CB | 4:L:456:ASP:N | 2.54 | 0.70 |
| 4:X:454:TYR:HA | 4:X:455:ILE:CA | 2.20 | 0.70 |
| 6:N:408:SER:CA | 6:N:410:LEU:H | 2.01 | 0.70 |
| 4:R:455:ILE:C | 4:R:457:ALA:N | 2.45 | 0.70 |
| 6:Z:381:LYS:N | 6:Z:381:LYS:CB | 2.55 | 0.70 |
| 6:H:408:SER:CA | 6:H:410:LEU:H | 2.01 | 0.70 |
| 7:J:643:ALA:HB1 | 7:J:658:MET:O | 1.92 | 0.70 |
| 4:F:455:ILE:CB | 4:F:456:ASP:N | 2.54 | 0.70 |
| 6:T:381:LYS:N | 6:T:381:LYS:C | 2.42 | 0.70 |
| 4:X:455:ILE:C | 4:X:457:ALA:N | 2.45 | 0.70 |
| 2:C:679:ILE:O | 1:K:851:ALA:O | 2.08 | 0.70 |
| 6:T:381:LYS:N | 6:T:381:LYS:CB | 2.55 | 0.70 |
| 6:T:408:SER:CA | 6:T:410:LEU:H | 2.01 | 0.70 |
| 1:W:22:ALA:HB1 | 1:W:780:ALA:HA | 1.71 | 0.70 |
| 4:L:158:ASN:HA | 4:L:321:LYS:O | 1.92 | 0.69 |
| 4:L:455:ILE:C | 4:L:457:ALA:N | 2.45 | 0.69 |
| 6:N:381:LYS:N | 6:N:381:LYS:CB | 2.55 | 0.69 |
| 3:P:1663:GLN:HA | 3:P:1667:ALA:CB | 2.18 | 0.69 |
| 4:R:402:ALA:HB2 | 4:R:403:ILE:H | 1.52 | 0.69 |
| 4:R:451:GLU:CB | 4:R:451:GLU:N | 2.55 | 0.69 |
| 6:Z:381:LYS:N | 6:Z:381:LYS:C | 2.42 | 0.69 |
| 4:X:158:ASN:HA | 4:X:321:LYS:O | 1.93 | 0.69 |
| 5:Y:342:PRO:C | 5:Y:343:ALA:C | 2.49 | 0.69 |
| 4:X:260:THR:CB | 4:X:260:THR:C | 2.61 | 0.69 |
| 4:L:402:ALA:HB2 | 4:L:403:ILE:H | 1.52 | 0.69 |
| 4:R:399:SER:C | 4:R:401:TYR:N | 2.37 | 0.69 |
| 1:K:942:PRO:HA | 1:K:943:GLN:CB | 2.17 | 0.69 |
| 4:L:328:VAL:CA | 4:L:328:VAL:O | 2.40 | 0.69 |
| 2:O:522:CYS:N | 3:P:1662:CYS:C | 2.32 | 0.69 |
| 2:C:530:ARG:O | 3:D:1664:ASP:CB | 2.40 | 0.69 |
| 4:F:454:TYR:HA | 4:F:455:ILE:CA | 2.21 | 0.69 |
| 1:K:441:PHE:HA | 1:K:444:PRO:O | 1.93 | 0.69 |
| 4:R:158:ASN:HA | 4:R:321:LYS:O | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:V:1520:ARG:HA | 7:V:1541:ALA:HB2 | 1.74 | 0.69 |
| 4:X:451:GLU:CB | 4:X:451:GLU:N | 2.55 | 0.69 |
| 4:L:140:LYS:HA | 4:L:149:GLY:N | 2.08 | 0.69 |
| 4:X:140:LYS:HA | 4:X:149:GLY:N | 2.08 | 0.69 |
| 6:Z:408:SER:CA | 6:Z:410:LEU:H | 2.01 | 0.69 |
| 6:H:381:LYS:N | 6:H:381:LYS:CB | 2.55 | 0.69 |
| 5:S:341:ALA:H | 5:S:342:PRO:N | 1.87 | 0.69 |
| 1:A:441:PHE:HA | 1:A:444:PRO:O | 1.93 | 0.68 |
| 1:E:845:TYR:CB | 2:O:299:ILE:HA | 2.21 | 0.68 |
| 5:G:342:PRO:C | 5:G:343:ALA:C | 2.49 | 0.68 |
| 4:L:260:THR:CB | 4:L:260:THR:C | 2.60 | 0.68 |
| 4:F:140:LYS:HA | 4:F:149:GLY:N | 2.08 | 0.68 |
| 4:F:455:ILE:C | 4:F:457:ALA:N | 2.45 | 0.68 |
| 5:M:342:PRO:C | 5:M:343:ALA:C | 2.49 | 0.68 |
| 4:R:260:THR:CB | 4:R:260:THR:C | 2.60 | 0.68 |
| 1:W:441:PHE:HA | 1:W:444:PRO:O | 1.93 | 0.68 |
| 1:E:441:PHE:HA | 1:E:444:PRO:O | 1.93 | 0.68 |
| 4:L:451:GLU:N | 4:L:451:GLU:CB | 2.55 | 0.68 |
| 4:F:158:ASN:HA | 4:F:321:LYS:O | 1.92 | 0.68 |
| 4:F:451:GLU:CB | 4:F:451:GLU:N | 2.55 | 0.68 |
| 1:B:441:PHE:HA | 1:B:444:PRO:O | 1.93 | 0.68 |
| 4:R:140:LYS:HA | 4:R:149:GLY:N | 2.08 | 0.68 |
| 4:F:260:THR:CB | 4:F:260:THR:C | 2.61 | 0.68 |
| 5:G:341:ALA:H | 5:G:342:PRO:N | 1.87 | 0.68 |
| 2:C:676:ALA:CA | 1:K:846:ILE:O | 2.41 | 0.67 |
| 1:Q:441:PHE:HA | 1:Q:444:PRO:O | 1.93 | 0.67 |
| 2:C:535:TYR:N | 3:D:1664:ASP:H | 1.93 | 0.67 |
| 4:L:422:ASN:CB | 4:L:423:ALA:HB2 | 2.24 | 0.67 |
| 7:J:643:ALA:HB1 | 7:J:658:MET:N | 2.08 | 0.67 |
| 4:L:260:THR:CB | 4:L:260:THR:N | 2.57 | 0.67 |
| 4:F:422:ASN:CB | 4:F:423:ALA:HB2 | 2.24 | 0.67 |
| 2:O:781:ARG:HA | 1:W:92:GLU:C | 2.15 | 0.67 |
| 1:Q:942:PRO:HA | 1:Q:943:GLN:CB | 2.17 | 0.67 |
| 4:L:448:ARG:O | 4:L:449:SER:C | 2.32 | 0.67 |
| 5:S:342:PRO:C | 5:S:343:ALA:C | 2.49 | 0.67 |
| 4:X:260:THR:CB | 4:X:260:THR:N | 2.57 | 0.67 |
| 4:R:328:VAL:CA | 4:R:328:VAL:O | 2.40 | 0.67 |
| 4:X:328:VAL:CA | 4:X:328:VAL:O | 2.40 | 0.67 |
| 3:D:644:ALA:CA | 3:D:706:ALA:HB2 | 2.25 | 0.66 |
| 4:R:422:ASN:CB | 4:R:423:ALA:HB2 | 2.24 | 0.66 |
| 4:R:260:THR:CB | 4:R:260:THR:N | 2.57 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:V:643:ALA:HB1 | 7:V:658:MET:N | 2.08 | 0.66 |
| 2:C:535:TYR:HA | 3:D:1663:GLN:HA | 1.74 | 0.66 |
| 4:F:448:ARG:O | 4:F:449:SER:C | 2.32 | 0.66 |
| 4:F:486:GLU:C | 4:F:487:ASP:C | 2.54 | 0.66 |
| 4:R:486:GLU:C | 4:R:487:ASP:C | 2.54 | 0.66 |
| 7:V:858:TYR:CB | 7:V:867:LEU:H | 2.08 | 0.66 |
| 4:X:422:ASN:CB | 4:X:423:ALA:HB2 | 2.24 | 0.66 |
| 2:C:305:LEU:HA | 1:Q:848:ASP:C | 2.16 | 0.66 |
| 1:E:852:VAL:N | 2:O:305:LEU:O | 2.27 | 0.66 |
| 4:L:486:GLU:C | 4:L:487:ASP:C | 2.54 | 0.66 |
| 5:Y:341:ALA:H | 5:Y:342:PRO:N | 1.87 | 0.66 |
| 4:F:260:THR:CB | 4:F:260:THR:N | 2.57 | 0.66 |
| 3:P:644:ALA:HA | 3:P:706:ALA:CB | 2.26 | 0.66 |
| 4:X:399:SER:C | 4:X:401:TYR:N | 2.37 | 0.66 |
| 4:X:486:GLU:C | 4:X:487:ASP:C | 2.54 | 0.66 |
| 5:Y:379:HIS:N | 5:Y:379:HIS:HA | 2.05 | 0.66 |
| 2:C:675:ARG:CA | 1:K:849:ASN:CB | 2.73 | 0.66 |
| 7:J:858:TYR:CB | 7:J:867:LEU:H | 2.08 | 0.65 |
| 3:P:644:ALA:CA | 3:P:706:ALA:HB2 | 2.25 | 0.65 |
| 7:J:846:ALA:CB | 7:J:852:ILE:H | 2.01 | 0.65 |
| 4:X:299:ASN:C | 4:X:299:ASN:CB | 2.64 | 0.65 |
| 3:D:644:ALA:HA | 3:D:706:ALA:CB | 2.26 | 0.65 |
| 2:O:655:ALA:CB | 3:P:1447:THR:O | 2.45 | 0.65 |
| 7:J:643:ALA:HB1 | 7:J:658:MET:C | 2.16 | 0.65 |
| 7:V:643:ALA:HB1 | 7:V:658:MET:C | 2.15 | 0.65 |
| 2:C:483:GLU:CB | 3:D:1658:ALA:HB2 | 2.27 | 0.65 |
| 7:V:251:ARG:HA | 7:V:254:VAL:O | 1.97 | 0.65 |
| 4:X:448:ARG:O | 4:X:449:SER:C | 2.32 | 0.64 |
| 4:F:299:ASN:C | 4:F:299:ASN:CB | 2.64 | 0.64 |
| 4:X:454:TYR:CB | 4:X:454:TYR:H | 2.10 | 0.64 |
| 7:J:251:ARG:HA | 7:J:254:VAL:O | 1.97 | 0.64 |
| 4:X:472:GLU:N | 4:X:472:GLU:C | 2.51 | 0.64 |
| 4:L:472:GLU:N | 4:L:472:GLU:C | 2.51 | 0.64 |
| 4:F:328:VAL:CA | 4:F:328:VAL:O | 2.40 | 0.64 |
| 4:R:400:GLY:C | 4:R:401:TYR:C | 2.56 | 0.64 |
| 1:E:942:PRO:HA | 1:E:943:GLN:CB | 2.17 | 0.64 |
| 4:F:400:GLY:C | 4:F:401:TYR:C | 2.56 | 0.64 |
| 3:P:1489:HIS:CB | 3:P:1492:GLY:H | 2.11 | 0.64 |
| 7:V:846:ALA:CB | 7:V:852:ILE:H | 2.01 | 0.64 |
| 2:C:523:LEU:CA | 3:D:1613:VAL:CB | 2.76 | 0.64 |
| 2:C:531:LEU:HA | 3:D:1664:ASP:CB | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:1489:HIS:CB | 3:D:1492:GLY:H | 2.11 | 0.64 |
| 4:L:400:GLY:C | 4:L:401:TYR:C | 2.56 | 0.64 |
| 4:R:472:GLU:N | 4:R:472:GLU:C | 2.51 | 0.64 |
| 7:V:1177:VAL:CB | 7:V:1198:LEU:H | 2.10 | 0.64 |
| 2:C:524:ARG:O | 3:D:1610:PRO:CB | 2.45 | 0.64 |
| 7:V:792:MET:HA | 7:V:803:GLY:N | 2.13 | 0.64 |
| 1:E:851:ALA:HB3 | 2:O:305:LEU:O | 1.96 | 0.64 |
| 3:D:1664:ASP:N | 3:D:1667:ALA:HB2 | 2.13 | 0.63 |
| 1:E:847:ARG:O | 2:O:305:LEU:N | 2.24 | 0.63 |
| 1:E:1165:TYR:C | 1:K:727:PHE:HA | 2.12 | 0.63 |
| 4:F:454:TYR:CB | 4:F:454:TYR:H | 2.10 | 0.63 |
| 4:L:299:ASN:C | 4:L:299:ASN:CB | 2.64 | 0.63 |
| 2:C:534:LEU:CA | 3:D:1668:GLY:H | 2.11 | 0.63 |
| 4:F:449:SER:O | 4:F:451:GLU:C | 2.37 | 0.63 |
| 5:G:378:SER:C | 5:G:378:SER:CB | 2.67 | 0.63 |
| 4:L:367:THR:C | 4:L:367:THR:N | 2.52 | 0.63 |
| 3:P:1664:ASP:N | 3:P:1667:ALA:HB2 | 2.13 | 0.63 |
| 7:J:1177:VAL:CB | 7:J:1198:LEU:H | 2.10 | 0.63 |
| 2:O:784:GLN:CB | 1:W:131:GLY:C | 2.67 | 0.63 |
| 4:X:400:GLY:C | 4:X:401:TYR:C | 2.56 | 0.63 |
| 4:F:472:GLU:N | 4:F:472:GLU:C | 2.51 | 0.63 |
| 4:R:449:SER:O | 4:R:451:GLU:C | 2.37 | 0.63 |
| 1:W:942:PRO:HA | 1:W:943:GLN:CB | 2.17 | 0.63 |
| 5:Y:378:SER:C | 5:Y:378:SER:CB | 2.67 | 0.63 |
| 2:C:677:GLN:C | 1:K:847:ARG:CB | 2.51 | 0.63 |
| 4:R:299:ASN:C | 4:R:299:ASN:CB | 2.64 | 0.63 |
| 2:C:534:LEU:HA | 3:D:1668:GLY:H | 1.64 | 0.63 |
| 3:D:174:THR:HA | 3:D:181:GLY:HA3 | 1.80 | 0.63 |
| 3:P:174:THR:HA | 3:P:181:GLY:HA3 | 1.80 | 0.63 |
| 2:O:783:SER:CA | 1:W:92:GLU:N | 2.54 | 0.63 |
| 7:J:1177:VAL:N | 7:J:1197:GLN:HA | 2.15 | 0.62 |
| 2:O:19:GLU:CB | 2:O:20:THR:HA | 2.30 | 0.62 |
| 7:V:1177:VAL:N | 7:V:1197:GLN:HA | 2.14 | 0.62 |
| 2:C:305:LEU:CA | 1:Q:848:ASP:C | 2.67 | 0.62 |
| 2:C:306:PRO:O | 1:Q:850:ALA:HB3 | 1.99 | 0.62 |
| 4:F:367:THR:C | 4:F:367:THR:N | 2.52 | 0.62 |
| 4:R:483:ASP:CB | 4:R:483:ASP:N | 2.60 | 0.62 |
| 2:U:19:GLU:CB | 2:U:20:THR:HA | 2.30 | 0.62 |
| 2:O:784:GLN:CB | 1:W:132:GLY:HA2 | 2.29 | 0.62 |
| 1:W:50:SER:C | 1:W:58:SER:HA | 2.20 | 0.62 |
| 4:X:449:SER:O | 4:X:451:GLU:C | 2.37 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:50:SER:C | 1:E:58:SER:HA | 2.20 | 0.62 |
| 7:J:792:MET:HA | 7:J:803:GLY:N | 2.13 | 0.62 |
| 1:A:50:SER:C | 1:A:58:SER:HA | 2.20 | 0.62 |
| 5:G:379:HIS:N | 5:G:379:HIS:HA | 2.05 | 0.62 |
| 4:L:449:SER:O | 4:L:451:GLU:C | 2.37 | 0.62 |
| 4:R:367:THR:C | 4:R:367:THR:N | 2.52 | 0.62 |
| 4:F:399:SER:C | 4:F:401:TYR:N | 2.37 | 0.61 |
| 1:K:50:SER:C | 1:K:58:SER:HA | 2.20 | 0.61 |
| 1:B:50:SER:C | 1:B:58:SER:HA | 2.20 | 0.61 |
| 2:I:19:GLU:CB | 2:I:20:THR:HA | 2.30 | 0.61 |
| 1:E:1165:TYR:CA | 1:K:727:PHE:N | 2.47 | 0.61 |
| 5:M:378:SER:C | 5:M:378:SER:CB | 2.67 | 0.61 |
| 1:Q:50:SER:C | 1:Q:58:SER:HA | 2.20 | 0.61 |
| 4:L:487:ASP:C | 4:L:487:ASP:CB | 2.69 | 0.61 |
| 4:X:367:THR:C | 4:X:367:THR:N | 2.52 | 0.61 |
| 2:O:654:SER:N | 3:P:1454:ALA:O | 2.32 | 0.61 |
| 4:R:487:ASP:C | 4:R:487:ASP:CB | 2.69 | 0.61 |
| 7:J:794:ALA:HB3 | 7:J:804:GLN:HA | 1.82 | 0.61 |
| 5:M:326:LEU:CB | 5:M:327:ARG:HA | 2.31 | 0.61 |
| 2:U:215:LEU:C | 2:U:217:ASP:H | 2.04 | 0.61 |
| 7:V:794:ALA:HB3 | 7:V:804:GLN:HA | 1.82 | 0.61 |
| 2:I:215:LEU:C | 2:I:217:ASP:H | 2.04 | 0.61 |
| 5:S:276:SER:C | 5:S:276:SER:CB | 2.68 | 0.61 |
| 4:X:487:ASP:C | 4:X:487:ASP:CB | 2.69 | 0.61 |
| 5:S:342:PRO:C | 5:S:344:ASP:N | 2.55 | 0.61 |
| 5:Y:326:LEU:CB | 5:Y:327:ARG:HA | 2.31 | 0.61 |
| 4:F:487:ASP:C | 4:F:487:ASP:CB | 2.69 | 0.60 |
| 5:G:326:LEU:CB | 5:G:327:ARG:HA | 2.31 | 0.60 |
| 2:C:19:GLU:CB | 2:C:20:THR:HA | 2.30 | 0.60 |
| 3:P:1485:ALA:O | 3:P:1486:CYS:C | 2.34 | 0.60 |
| 5:Y:342:PRO:C | 5:Y:344:ASP:N | 2.55 | 0.60 |
| 5:G:342:PRO:C | 5:G:344:ASP:N | 2.54 | 0.60 |
| 4:L:453:TYR:O | 4:L:454:TYR:C | 2.40 | 0.60 |
| 7:V:363:GLN:O | 7:V:366:ALA:HB3 | 2.01 | 0.60 |
| 1:B:312:MET:CB | 1:B:313:SER:HA | 2.32 | 0.60 |
| 3:D:644:ALA:HA | 3:D:706:ALA:HB2 | 1.83 | 0.60 |
| 4:F:453:TYR:O | 4:F:454:TYR:C | 2.40 | 0.60 |
| 7:J:94:GLN:C | 7:J:96:TYR:H | 2.04 | 0.60 |
| 7:J:363:GLN:O | 7:J:366:ALA:HB3 | 2.01 | 0.60 |
| 1:K:312:MET:CB | 1:K:313:SER:HA | 2.32 | 0.60 |
| 2:O:654:SER:O | 3:P:1455:PRO:N | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:312:MET:CB | 1:Q:313:SER:HA | 2.32 | 0.60 |
| 4:R:448:ARG:O | 4:R:449:SER:C | 2.32 | 0.60 |
| 4:X:453:TYR:O | 4:X:454:TYR:C | 2.40 | 0.60 |
| 5:M:342:PRO:C | 5:M:344:ASP:N | 2.55 | 0.60 |
| 5:S:326:LEU:CB | 5:S:327:ARG:HA | 2.31 | 0.60 |
| 1:A:312:MET:CB | 1:A:313:SER:HA | 2.32 | 0.60 |
| 2:C:303:ALA:HB3 | 1:Q:849:ASN:H | 1.50 | 0.60 |
| 7:J:846:ALA:HB1 | 7:J:852:ILE:CB | 2.31 | 0.60 |
| 2:C:215:LEU:C | 2:C:217:ASP:H | 2.04 | 0.60 |
| 4:F:450:GLU:N | 4:F:451:GLU:N | 2.50 | 0.60 |
| 7:J:471:MET:O | 7:J:535:SER:HA | 2.01 | 0.60 |
| 5:M:327:ARG:CB | 5:M:327:ARG:C | 2.71 | 0.60 |
| 4:R:453:TYR:O | 4:R:454:TYR:C | 2.40 | 0.60 |
| 1:E:312:MET:CB | 1:E:313:SER:HA | 2.32 | 0.59 |
| 2:O:215:LEU:C | 2:O:217:ASP:H | 2.04 | 0.59 |
| 4:R:450:GLU:N | 4:R:451:GLU:N | 2.50 | 0.59 |
| 5:S:327:ARG:CB | 5:S:327:ARG:C | 2.71 | 0.59 |
| 7:V:471:MET:O | 7:V:535:SER:HA | 2.01 | 0.59 |
| 1:W:312:MET:CB | 1:W:313:SER:HA | 2.32 | 0.59 |
| 3:D:1485:ALA:O | 3:D:1486:CYS:C | 2.34 | 0.59 |
| 3:D:1542:PRO:O | 3:D:1545:PRO:N | 2.35 | 0.59 |
| 5:S:378:SER:C | 5:S:378:SER:CB | 2.67 | 0.59 |
| 7:V:846:ALA:HB1 | 7:V:852:ILE:CB | 2.31 | 0.59 |
| 5:G:327:ARG:CB | 5:G:327:ARG:C | 2.71 | 0.59 |
| 3:P:644:ALA:HA | 3:P:706:ALA:HB2 | 1.83 | 0.59 |
| 4:X:491:VAL:C | 4:X:493:HIS:N | 2.56 | 0.59 |
| 2:O:655:ALA:HB1 | 3:P:1447:THR:O | 2.02 | 0.59 |
| 7:V:94:GLN:C | 7:V:96:TYR:H | 2.04 | 0.59 |
| 5:Y:327:ARG:CB | 5:Y:327:ARG:C | 2.71 | 0.59 |
| 2:C:306:PRO:C | 1:Q:850:ALA:H | 2.05 | 0.59 |
| 3:P:1542:PRO:O | 3:P:1545:PRO:N | 2.35 | 0.59 |
| 4:R:399:SER:O | 4:R:400:GLY:HA3 | 2.00 | 0.59 |
| 4:R:491:VAL:C | 4:R:493:HIS:N | 2.56 | 0.59 |
| 4:X:450:GLU:N | 4:X:451:GLU:N | 2.50 | 0.59 |
| 1:A:441:PHE:C | 1:A:443:LYS:H | 2.06 | 0.59 |
| 1:B:441:PHE:C | 1:B:443:LYS:H | 2.06 | 0.59 |
| 4:F:483:ASP:CB | 4:F:483:ASP:N | 2.60 | 0.58 |
| 5:M:325:ALA:C | 5:M:326:LEU:CA | 2.70 | 0.58 |
| 1:Q:441:PHE:C | 1:Q:443:LYS:H | 2.06 | 0.58 |
| 5:Y:339:TYR:O | 5:Y:340:ALA:CB | 2.51 | 0.58 |
| 2:O:783:SER:H | 1:W:92:GLU:N | 2.00 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Y:276:SER:C | 5:Y:276:SER:CB | 2.68 | 0.58 |
| 4:F:491:VAL:C | 4:F:493:HIS:N | 2.56 | 0.58 |
| 2:C:524:ARG:O | 3:D:1610:PRO:CA | 2.40 | 0.58 |
| 1:E:441:PHE:C | 1:E:443:LYS:H | 2.06 | 0.58 |
| 5:G:325:ALA:C | 5:G:326:LEU:CA | 2.70 | 0.58 |
| 5:G:339:TYR:CB | 5:G:341:ALA:H | 2.16 | 0.58 |
| 7:J:1373:SER:CB | 7:J:1426:HIS:HA | 2.34 | 0.58 |
| 5:M:339:TYR:O | 5:M:340:ALA:CB | 2.51 | 0.58 |
| 5:S:339:TYR:CB | 5:S:341:ALA:H | 2.16 | 0.58 |
| 1:W:441:PHE:C | 1:W:443:LYS:H | 2.06 | 0.58 |
| 5:Y:339:TYR:CB | 5:Y:341:ALA:H | 2.16 | 0.58 |
| 4:L:491:VAL:C | 4:L:493:HIS:N | 2.56 | 0.58 |
| 4:L:450:GLU:N | 4:L:451:GLU:N | 2.50 | 0.58 |
| 1:A:205:LEU:C | 1:A:207:SER:HA | 2.24 | 0.58 |
| 1:E:852:VAL:CB | 2:O:304:PRO:C | 2.72 | 0.58 |
| 5:G:339:TYR:O | 5:G:340:ALA:CB | 2.51 | 0.58 |
| 7:J:485:VAL:HA | 7:J:495:ARG:HA | 1.86 | 0.58 |
| 1:K:441:PHE:C | 1:K:443:LYS:H | 2.06 | 0.58 |
| 5:M:276:SER:C | 5:M:276:SER:CB | 2.68 | 0.58 |
| 1:E:205:LEU:C | 1:E:207:SER:HA | 2.25 | 0.58 |
| 5:M:339:TYR:CB | 5:M:341:ALA:H | 2.16 | 0.58 |
| 5:S:325:ALA:C | 5:S:326:LEU:CA | 2.70 | 0.58 |
| 4:F:399:SER:O | 4:F:400:GLY:HA3 | 2.00 | 0.57 |
| 7:V:485:VAL:HA | 7:V:495:ARG:HA | 1.86 | 0.57 |
| 5:G:342:PRO:O | 5:G:343:ALA:C | 2.43 | 0.57 |
| 1:K:205:LEU:C | 1:K:207:SER:HA | 2.25 | 0.57 |
| 1:Q:205:LEU:C | 1:Q:207:SER:HA | 2.25 | 0.57 |
| 7:V:1373:SER:CB | 7:V:1426:HIS:HA | 2.34 | 0.57 |
| 1:W:205:LEU:C | 1:W:207:SER:HA | 2.25 | 0.57 |
| 1:B:205:LEU:C | 1:B:207:SER:HA | 2.24 | 0.57 |
| 4:F:453:TYR:O | 4:F:455:ILE:CA | 2.53 | 0.57 |
| 5:M:342:PRO:O | 5:M:343:ALA:C | 2.43 | 0.57 |
| 4:X:453:TYR:O | 4:X:455:ILE:CA | 2.53 | 0.57 |
| 4:X:483:ASP:CB | 4:X:483:ASP:N | 2.60 | 0.57 |
| 2:C:534:LEU:CB | 3:D:1667:ALA:CA | 2.80 | 0.57 |
| 4:R:454:TYR:CB | 4:R:454:TYR:H | 2.10 | 0.57 |
| 5:S:339:TYR:O | 5:S:340:ALA:CB | 2.51 | 0.57 |
| 5:S:342:PRO:O | 5:S:343:ALA:C | 2.43 | 0.57 |
| 2:C:535:TYR:N | 3:D:1664:ASP:N | 2.52 | 0.57 |
| 2:C:681:ALA:H | 1:K:850:ALA:HA | 1.69 | 0.57 |
| 3:D:1489:HIS:O | 3:D:1491:ILE:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:S:379:HIS:N | 5:S:379:HIS:HA | 2.06 | 0.57 |
| 4:R:328:VAL:C | 4:R:328:VAL:CB | 2.67 | 0.57 |
| 7:J:1177:VAL:H | 7:J:1197:GLN:HA | 1.69 | 0.57 |
| 3:P:1664:ASP:O | 3:P:1667:ALA:HB3 | 2.04 | 0.57 |
| 5:Y:342:PRO:O | 5:Y:343:ALA:C | 2.43 | 0.57 |
| 1:E:847:ARG:O | 2:O:303:ALA:CB | 2.47 | 0.57 |
| 7:V:498:THR:HA | 7:V:515:GLN:CB | 2.35 | 0.57 |
| 7:V:1463:MET:C | 7:V:1465:GLU:H | 2.08 | 0.57 |
| 2:C:681:ALA:HB3 | 1:K:850:ALA:HA | 1.87 | 0.56 |
| 2:C:725:GLU:C | 2:C:727:VAL:H | 2.08 | 0.56 |
| 4:F:447:VAL:CB | 4:F:447:VAL:N | 2.62 | 0.56 |
| 2:I:725:GLU:C | 2:I:727:VAL:H | 2.08 | 0.56 |
| 3:P:1489:HIS:O | 3:P:1491:ILE:N | 2.38 | 0.56 |
| 4:R:453:TYR:O | 4:R:455:ILE:CA | 2.53 | 0.56 |
| 2:C:306:PRO:N | 1:Q:849:ASN:CB | 2.61 | 0.56 |
| 2:C:487:CYS:H | 3:D:1661:ARG:CB | 2.11 | 0.56 |
| 2:C:679:ILE:O | 1:K:851:ALA:C | 2.44 | 0.56 |
| 1:E:1165:TYR:HA | 1:K:727:PHE:CB | 2.29 | 0.56 |
| 4:L:453:TYR:O | 4:L:455:ILE:CA | 2.53 | 0.56 |
| 2:O:725:GLU:C | 2:O:727:VAL:H | 2.08 | 0.56 |
| 2:U:483:GLU:HA | 2:U:484:ARG:N | 2.20 | 0.56 |
| 2:U:725:GLU:C | 2:U:727:VAL:H | 2.08 | 0.56 |
| 2:C:676:ALA:O | 1:K:846:ILE:O | 2.21 | 0.56 |
| 1:E:1165:TYR:HA | 1:K:727:PHE:HA | 0.58 | 0.56 |
| 7:J:249:THR:HA | 7:J:253:LEU:N | 2.20 | 0.56 |
| 7:V:249:THR:HA | 7:V:253:LEU:N | 2.20 | 0.56 |
| 2:C:681:ALA:HB3 | 1:K:850:ALA:CB | 2.35 | 0.56 |
| 2:C:483:GLU:HA | 2:C:484:ARG:N | 2.21 | 0.56 |
| 2:I:483:GLU:HA | 2:I:484:ARG:N | 2.21 | 0.56 |
| 4:L:454:TYR:CB | 4:L:454:TYR:H | 2.10 | 0.56 |
| 2:O:483:GLU:HA | 2:O:484:ARG:N | 2.20 | 0.56 |
| 1:A:205:LEU:O | 1:A:207:SER:HA | 2.06 | 0.56 |
| 1:B:205:LEU:O | 1:B:207:SER:HA | 2.06 | 0.56 |
| 4:F:449:SER:O | 4:F:452:ARG:N | 2.38 | 0.56 |
| 5:G:276:SER:C | 5:G:276:SER:CB | 2.68 | 0.56 |
| 4:R:449:SER:O | 4:R:452:ARG:N | 2.38 | 0.56 |
| 4:X:449:SER:O | 4:X:452:ARG:N | 2.39 | 0.56 |
| 4:L:483:ASP:CB | 4:L:483:ASP:N | 2.60 | 0.56 |
| 2:C:306:PRO:CA | 1:Q:849:ASN:CA | 2.70 | 0.56 |
| 1:Q:376:ARG:C | 1:Q:380:ALA:HA | 2.27 | 0.56 |
| 1:A:376:ARG:C | 1:A:380:ALA:HA | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:376:ARG:C | 1:E:380:ALA:HA | 2.27 | 0.55 |
| 7:J:1463:MET:C | 7:J:1465:GLU:H | 2.08 | 0.55 |
| 7:V:1177:VAL:H | 7:V:1197:GLN:HA | 1.69 | 0.55 |
| 5:Y:325:ALA:C | 5:Y:326:LEU:CA | 2.70 | 0.55 |
| 1:B:376:ARG:C | 1:B:380:ALA:HA | 2.27 | 0.55 |
| 5:Y:313:ILE:O | 5:Y:316:ALA:HB3 | 2.07 | 0.55 |
| 2:U:303:ALA:HB1 | 2:U:306:PRO:HA | 1.87 | 0.55 |
| 4:X:328:VAL:C | 4:X:328:VAL:CB | 2.67 | 0.55 |
| 1:Q:205:LEU:O | 1:Q:207:SER:HA | 2.06 | 0.55 |
| 5:S:313:ILE:O | 5:S:316:ALA:HB3 | 2.07 | 0.55 |
| 1:K:205:LEU:O | 1:K:207:SER:HA | 2.06 | 0.55 |
| 5:S:378:SER:CA | 5:S:378:SER:O | 2.51 | 0.55 |
| 1:W:205:LEU:O | 1:W:207:SER:HA | 2.06 | 0.55 |
| 1:K:376:ARG:C | 1:K:380:ALA:HA | 2.27 | 0.55 |
| 4:L:399:SER:C | 4:L:401:TYR:N | 2.37 | 0.55 |
| 4:L:455:ILE:C | 4:L:456:ASP:C | 2.56 | 0.55 |
| 2:O:783:SER:CB | 1:W:91:PRO:CB | 2.85 | 0.55 |
| 4:X:404:GLN:O | 4:X:405:ALA:CB | 2.55 | 0.55 |
| 2:I:303:ALA:HB1 | 2:I:306:PRO:HA | 1.87 | 0.55 |
| 4:L:399:SER:O | 4:L:400:GLY:HA3 | 2.00 | 0.55 |
| 5:M:313:ILE:O | 5:M:316:ALA:HB3 | 2.07 | 0.55 |
| 7:V:846:ALA:HB2 | 7:V:849:ASN:CA | 2.36 | 0.55 |
| 6:H:406:LEU:HA | 6:H:409:PRO:N | 2.22 | 0.55 |
| 2:C:522:CYS:CB | 3:D:1663:GLN:O | 2.55 | 0.55 |
| 2:C:679:ILE:O | 1:K:850:ALA:O | 2.24 | 0.55 |
| 3:D:1489:HIS:O | 3:D:1490:GLU:C | 2.44 | 0.55 |
| 7:J:498:THR:HA | 7:J:515:GLN:CB | 2.35 | 0.54 |
| 7:V:249:THR:HA | 7:V:253:LEU:HA | 1.89 | 0.54 |
| 4:F:404:GLN:O | 4:F:405:ALA:CB | 2.55 | 0.54 |
| 7:J:846:ALA:HB2 | 7:J:849:ASN:CA | 2.36 | 0.54 |
| 4:R:404:GLN:O | 4:R:405:ALA:CB | 2.55 | 0.54 |
| 4:L:449:SER:O | 4:L:452:ARG:N | 2.38 | 0.54 |
| 6:T:406:LEU:HA | 6:T:409:PRO:N | 2.22 | 0.54 |
| 2:U:483:GLU:N | 2:U:484:ARG:N | 2.55 | 0.54 |
| 1:E:205:LEU:O | 1:E:207:SER:HA | 2.06 | 0.54 |
| 2:I:483:GLU:N | 2:I:484:ARG:N | 2.55 | 0.54 |
| 2:O:784:GLN:CB | 1:W:132:GLY:N | 2.70 | 0.54 |
| 2:C:483:GLU:N | 2:C:484:ARG:N | 2.56 | 0.54 |
| 6:N:406:LEU:HA | 6:N:409:PRO:N | 2.22 | 0.54 |
| 2:O:483:GLU:N | 2:O:484:ARG:N | 2.55 | 0.54 |
| 6:Z:406:LEU:HA | 6:Z:409:PRO:N | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:L:235:ASP:CB | 4:L:235:ASP:C | 2.68 | 0.54 |
| 6:N:462:GLY:CA | 6:N:462:GLY:O | 2.51 | 0.54 |
| 7:V:848:GLY:O | 7:V:890:LEU:HA | 2.08 | 0.54 |
| 2:C:534:LEU:CA | 3:D:1668:GLY:N | 2.70 | 0.54 |
| 4:F:298:GLN:C | 4:F:299:ASN:C | 2.67 | 0.54 |
| 7:J:644:HIS:C | 7:J:660:ALA:H | 2.11 | 0.54 |
| 4:L:404:GLN:O | 4:L:405:ALA:CB | 2.55 | 0.54 |
| 7:J:848:GLY:O | 7:J:890:LEU:HA | 2.08 | 0.54 |
| 7:V:829:PRO:HA | 7:V:832:ASN:HA | 1.90 | 0.54 |
| 1:W:376:ARG:C | 1:W:380:ALA:HA | 2.27 | 0.54 |
| 4:L:447:VAL:CB | 4:L:447:VAL:N | 2.62 | 0.54 |
| 7:V:644:HIS:C | 7:V:660:ALA:H | 2.11 | 0.54 |
| 1:B:22:ALA:HB1 | 1:B:780:ALA:CA | 2.38 | 0.54 |
| 1:E:181:ALA:O | 1:E:196:GLY:HA2 | 2.08 | 0.54 |
| 5:G:313:ILE:O | 5:G:316:ALA:HB3 | 2.07 | 0.54 |
| 6:H:462:GLY:CA | 6:H:462:GLY:O | 2.51 | 0.53 |
| 4:L:298:GLN:C | 4:L:299:ASN:C | 2.67 | 0.53 |
| 2:O:589:ASN:O | 1:W:850:ALA:CA | 2.52 | 0.53 |
| 3:P:1489:HIS:O | 3:P:1490:GLU:C | 2.44 | 0.53 |
| 4:R:485:LEU:HA | 4:R:488:ILE:CB | 2.39 | 0.53 |
| 4:X:298:GLN:C | 4:X:299:ASN:C | 2.67 | 0.53 |
| 1:A:181:ALA:O | 1:A:196:GLY:HA2 | 2.08 | 0.53 |
| 6:H:408:SER:CA | 6:H:410:LEU:N | 2.68 | 0.53 |
| 7:J:829:PRO:HA | 7:J:832:ASN:HA | 1.90 | 0.53 |
| 1:K:181:ALA:O | 1:K:196:GLY:HA2 | 2.08 | 0.53 |
| 4:X:404:GLN:O | 4:X:405:ALA:HB2 | 2.09 | 0.53 |
| 4:L:404:GLN:O | 4:L:405:ALA:HB2 | 2.08 | 0.53 |
| 1:Q:181:ALA:O | 1:Q:196:GLY:HA2 | 2.09 | 0.53 |
| 4:X:235:ASP:CB | 4:X:235:ASP:C | 2.68 | 0.53 |
| 4:L:485:LEU:HA | 4:L:488:ILE:CB | 2.38 | 0.53 |
| 1:Q:22:ALA:HB1 | 1:Q:780:ALA:CA | 2.38 | 0.53 |
| 1:E:22:ALA:HB1 | 1:E:780:ALA:CA | 2.38 | 0.53 |
| 5:Y:325:ALA:CA | 5:Y:326:LEU:N | 2.69 | 0.53 |
| 1:B:181:ALA:O | 1:B:196:GLY:HA2 | 2.09 | 0.53 |
| 2:C:306:PRO:CB | 1:Q:848:ASP:CB | 2.87 | 0.53 |
| 4:F:485:LEU:HA | 4:F:488:ILE:CB | 2.38 | 0.53 |
| 6:T:409:PRO:CA | 6:T:410:LEU:N | 2.72 | 0.53 |
| 2:C:303:ALA:C | 1:Q:849:ASN:N | 2.56 | 0.53 |
| 5:G:339:TYR:CA | 5:G:340:ALA:N | 2.68 | 0.53 |
| 1:W:22:ALA:HB1 | 1:W:780:ALA:CB | 2.39 | 0.53 |
| 4:X:399:SER:O | 4:X:400:GLY:HA3 | 2.00 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:M:378:SER:CA | 5:M:378:SER:O | 2.51 | 0.53 |
| 4:R:404:GLN:O | 4:R:405:ALA:HB2 | 2.09 | 0.53 |
| 4:X:459:LEU:CA | 4:X:460:LEU:N | 2.54 | 0.53 |
| 4:X:485:LEU:HA | 4:X:488:ILE:CB | 2.38 | 0.53 |
| 7:J:249:THR:HA | 7:J:253:LEU:HA | 1.89 | 0.52 |
| 3:P:1448:MET:C | 3:P:1450:GLU:HA | 2.29 | 0.52 |
| 1:Q:22:ALA:HB1 | 1:Q:780:ALA:CB | 2.39 | 0.52 |
| 4:R:298:GLN:C | 4:R:299:ASN:C | 2.67 | 0.52 |
| 3:P:1664:ASP:C | 3:P:1667:ALA:H | 2.12 | 0.52 |
| 4:R:447:VAL:CB | 4:R:447:VAL:N | 2.62 | 0.52 |
| 4:R:159:ILE:CB | 4:R:254:ARG:HA | 2.40 | 0.52 |
| 4:F:404:GLN:O | 4:F:405:ALA:HB2 | 2.08 | 0.52 |
| 6:H:408:SER:C | 6:H:409:PRO:C | 2.64 | 0.52 |
| 7:V:1519:GLN:O | 7:V:1541:ALA:HB2 | 2.09 | 0.52 |
| 1:K:370:PHE:HA | 1:K:386:THR:O | 2.10 | 0.52 |
| 5:M:379:HIS:N | 5:M:379:HIS:HA | 2.05 | 0.52 |
| 2:O:653:ILE:CB | 3:P:1456:GLU:HA | 2.40 | 0.52 |
| 6:T:408:SER:CA | 6:T:410:LEU:N | 2.68 | 0.52 |
| 7:V:389:LEU:HA | 7:V:397:LEU:O | 2.10 | 0.52 |
| 1:W:370:PHE:HA | 1:W:386:THR:O | 2.10 | 0.52 |
| 1:A:22:ALA:HB1 | 1:A:780:ALA:CA | 2.38 | 0.52 |
| 1:E:370:PHE:HA | 1:E:386:THR:O | 2.10 | 0.52 |
| 4:F:222:THR:O | 4:F:246:GLU:HA | 2.10 | 0.52 |
| 4:X:450:GLU:O | 4:X:451:GLU:CA | 2.33 | 0.52 |
| 1:B:22:ALA:HB1 | 1:B:780:ALA:CB | 2.39 | 0.52 |
| 2:O:783:SER:N | 1:W:92:GLU:N | 2.55 | 0.52 |
| 4:R:235:ASP:CB | 4:R:235:ASP:C | 2.68 | 0.52 |
| 7:V:1175:GLY:CA | 7:V:1197:GLN:H | 2.19 | 0.52 |
| 1:K:22:ALA:HB1 | 1:K:780:ALA:CB | 2.39 | 0.52 |
| 5:S:339:TYR:CA | 5:S:340:ALA:N | 2.68 | 0.52 |
| 1:W:181:ALA:O | 1:W:196:GLY:HA2 | 2.08 | 0.52 |
| 2:C:531:LEU:O | 3:D:1663:GLN:CA | 2.53 | 0.52 |
| 7:J:1519:GLN:O | 7:J:1541:ALA:HB2 | 2.09 | 0.52 |
| 3:P:1504:VAL:O | 3:P:1505:SER:C | 2.39 | 0.52 |
| 7:V:644:HIS:O | 7:V:659:ASN:HA | 2.10 | 0.52 |
| 1:A:370:PHE:HA | 1:A:386:THR:O | 2.10 | 0.51 |
| 1:E:22:ALA:HB1 | 1:E:780:ALA:CB | 2.39 | 0.51 |
| 7:J:644:HIS:O | 7:J:659:ASN:HA | 2.10 | 0.51 |
| 2:C:306:PRO:C | 1:Q:849:ASN:CB | 2.76 | 0.51 |
| 1:Q:370:PHE:HA | 1:Q:386:THR:O | 2.10 | 0.51 |
| 4:R:458:ASP:O | 4:R:460:LEU:CA | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:Y:378:SER:CA | 5:Y:378:SER:O | 2.51 | 0.51 |
| 1:B:370:PHE:HA | 1:B:386:THR:O | 2.10 | 0.51 |
| 4:R:399:SER:CA | 4:R:401:TYR:N | 2.73 | 0.51 |
| 5:S:325:ALA:CA | 5:S:326:LEU:N | 2.69 | 0.51 |
| 6:T:462:GLY:CA | 6:T:462:GLY:O | 2.50 | 0.51 |
| 4:X:222:THR:O | 4:X:246:GLU:HA | 2.10 | 0.51 |
| 6:H:409:PRO:CA | 6:H:410:LEU:N | 2.72 | 0.51 |
| 7:J:389:LEU:HA | 7:J:397:LEU:O | 2.10 | 0.51 |
| 6:Z:462:GLY:CA | 6:Z:462:GLY:O | 2.50 | 0.51 |
| 1:A:22:ALA:HB1 | 1:A:780:ALA:CB | 2.39 | 0.51 |
| 4:L:222:THR:O | 4:L:246:GLU:HA | 2.10 | 0.51 |
| 4:X:222:THR:C | 4:X:247:ARG:H | 2.14 | 0.51 |
| 7:J:1353:VAL:O | 7:J:1356:ALA:HB3 | 2.10 | 0.51 |
| 1:K:22:ALA:HB1 | 1:K:780:ALA:CA | 2.38 | 0.51 |
| 4:L:399:SER:CA | 4:L:401:TYR:N | 2.74 | 0.51 |
| 6:N:425:HIS:O | 6:N:426:ALA:HB2 | 2.11 | 0.51 |
| 7:V:1353:VAL:O | 7:V:1356:ALA:HB3 | 2.10 | 0.51 |
| 4:X:399:SER:CA | 4:X:401:TYR:N | 2.74 | 0.51 |
| 3:D:1448:MET:C | 3:D:1450:GLU:HA | 2.29 | 0.51 |
| 6:H:425:HIS:O | 6:H:426:ALA:HB2 | 2.11 | 0.51 |
| 1:E:376:ARG:O | 1:E:380:ALA:HA | 2.11 | 0.51 |
| 6:H:490:GLN:CB | 6:H:490:GLN:N | 2.58 | 0.51 |
| 7:J:249:THR:HA | 7:J:253:LEU:CA | 2.41 | 0.51 |
| 5:Y:345:TYR:C | 5:Y:348:ILE:H | 2.14 | 0.51 |
| 5:M:339:TYR:CA | 5:M:340:ALA:N | 2.68 | 0.51 |
| 4:R:222:THR:O | 4:R:246:GLU:HA | 2.10 | 0.51 |
| 6:T:425:HIS:O | 6:T:426:ALA:HB2 | 2.11 | 0.51 |
| 5:G:345:TYR:C | 5:G:348:ILE:H | 2.14 | 0.50 |
| 7:J:1175:GLY:HA2 | 7:J:1196:GLN:HA | 1.93 | 0.50 |
| 6:N:409:PRO:CA | 6:N:410:LEU:N | 2.72 | 0.50 |
| 3:P:1448:MET:O | 3:P:1451:ARG:N | 2.44 | 0.50 |
| 7:V:250:ASN:N | 7:V:253:LEU:HA | 2.26 | 0.50 |
| 1:W:22:ALA:HB1 | 1:W:780:ALA:CA | 2.38 | 0.50 |
| 6:Z:425:HIS:O | 6:Z:426:ALA:HB2 | 2.11 | 0.50 |
| 3:D:1448:MET:O | 3:D:1451:ARG:N | 2.44 | 0.50 |
| 1:K:376:ARG:O | 1:K:380:ALA:HA | 2.11 | 0.50 |
| 4:F:399:SER:CA | 4:F:401:TYR:N | 2.74 | 0.50 |
| 1:K:215:LEU:HA | 1:K:230:GLY:HA2 | 1.94 | 0.50 |
| 5:M:339:TYR:CB | 5:M:341:ALA:N | 2.75 | 0.50 |
| 2:O:784:GLN:CB | 1:W:132:GLY:CA | 2.88 | 0.50 |
| 7:V:249:THR:HA | 7:V:253:LEU:CA | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Z:409:PRO:CA | 6:Z:410:LEU:N | 2.72 | 0.50 |
| 2:C:675:ARG:HA | 1:K:849:ASN:CB | 2.40 | 0.50 |
| 1:E:215:LEU:HA | 1:E:230:GLY:HA2 | 1.94 | 0.50 |
| 4:L:328:VAL:C | 4:L:328:VAL:CB | 2.67 | 0.50 |
| 5:M:345:TYR:C | 5:M:348:ILE:H | 2.14 | 0.50 |
| 6:N:408:SER:C | 6:N:409:PRO:C | 2.65 | 0.50 |
| 4:X:447:VAL:CB | 4:X:447:VAL:N | 2.62 | 0.50 |
| 1:B:376:ARG:O | 1:B:380:ALA:HA | 2.11 | 0.50 |
| 4:F:458:ASP:O | 4:F:460:LEU:CA | 2.58 | 0.50 |
| 7:V:1175:GLY:HA2 | 7:V:1196:GLN:HA | 1.93 | 0.50 |
| 1:W:376:ARG:O | 1:W:380:ALA:HA | 2.11 | 0.50 |
| 2:C:447:ASP:C | 2:C:448:TYR:HA | 2.32 | 0.50 |
| 5:G:326:LEU:N | 5:G:326:LEU:CB | 2.72 | 0.50 |
| 7:J:250:ASN:N | 7:J:253:LEU:HA | 2.26 | 0.50 |
| 7:J:1175:GLY:CA | 7:J:1197:GLN:H | 2.19 | 0.50 |
| 5:M:326:LEU:N | 5:M:326:LEU:CB | 2.72 | 0.50 |
| 1:Q:376:ARG:O | 1:Q:380:ALA:HA | 2.11 | 0.50 |
| 5:S:326:LEU:N | 5:S:326:LEU:CB | 2.72 | 0.50 |
| 2:U:15:GLN:CA | 2:U:16:LEU:N | 2.71 | 0.50 |
| 4:X:329:GLY:N | 4:X:329:GLY:C | 2.62 | 0.50 |
| 6:Z:408:SER:CA | 6:Z:410:LEU:N | 2.68 | 0.50 |
| 4:F:222:THR:C | 4:F:247:ARG:H | 2.14 | 0.50 |
| 5:M:325:ALA:CA | 5:M:326:LEU:N | 2.68 | 0.50 |
| 2:O:783:SER:N | 1:W:92:GLU:H | 2.10 | 0.50 |
| 1:Q:215:LEU:HA | 1:Q:230:GLY:HA2 | 1.94 | 0.50 |
| 5:S:345:TYR:C | 5:S:348:ILE:H | 2.14 | 0.50 |
| 6:N:490:GLN:CB | 6:N:490:GLN:N | 2.58 | 0.50 |
| 2:O:447:ASP:C | 2:O:448:TYR:HA | 2.33 | 0.50 |
| 3:P:324:GLY:O | 3:P:327:ALA:HB3 | 2.12 | 0.50 |
| 6:Z:490:GLN:CB | 6:Z:490:GLN:N | 2.59 | 0.50 |
| 4:L:459:LEU:CA | 4:L:460:LEU:N | 2.54 | 0.49 |
| 5:S:339:TYR:CB | 5:S:341:ALA:N | 2.75 | 0.49 |
| 6:Z:408:SER:C | 6:Z:409:PRO:C | 2.64 | 0.49 |
| 4:X:457:ALA:C | 4:X:459:LEU:N | 2.66 | 0.49 |
| 5:Y:339:TYR:CB | 5:Y:341:ALA:N | 2.75 | 0.49 |
| 2:C:469:THR:O | 2:C:470:ALA:HB3 | 2.13 | 0.49 |
| 2:O:469:THR:O | 2:O:470:ALA:HB3 | 2.12 | 0.49 |
| 6:T:380:GLU:C | 6:T:381:LYS:CA | 2.72 | 0.49 |
| 1:A:376:ARG:O | 1:A:380:ALA:HA | 2.11 | 0.49 |
| 2:C:675:ARG:O | 1:K:851:ALA:HB3 | 2.12 | 0.49 |
| 3:P:1489:HIS:C | 3:P:1491:ILE:N | 2.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:339:TYR:CB | 5:G:341:ALA:N | 2.75 | 0.49 |
| 4:L:222:THR:C | 4:L:247:ARG:H | 2.14 | 0.49 |
| 4:R:222:THR:C | 4:R:247:ARG:H | 2.14 | 0.49 |
| 4:X:488:ILE:N | 4:X:488:ILE:CB | 2.66 | 0.49 |
| 2:C:306:PRO:CB | 1:Q:848:ASP:C | 2.74 | 0.49 |
| 4:F:458:ASP:O | 4:F:459:LEU:C | 2.45 | 0.49 |
| 1:K:312:MET:CB | 1:K:313:SER:CA | 2.91 | 0.49 |
| 4:L:457:ALA:C | 4:L:459:LEU:N | 2.66 | 0.49 |
| 4:R:457:ALA:C | 4:R:459:LEU:N | 2.66 | 0.49 |
| 4:F:457:ALA:C | 4:F:459:LEU:N | 2.66 | 0.49 |
| 3:D:1489:HIS:C | 3:D:1491:ILE:N | 2.61 | 0.49 |
| 5:G:325:ALA:CA | 5:G:326:LEU:N | 2.69 | 0.49 |
| 2:O:15:GLN:N | 2:O:16:LEU:N | 2.61 | 0.49 |
| 2:O:234:LEU:C | 2:O:252:MET:HA | 2.33 | 0.49 |
| 1:W:215:LEU:HA | 1:W:230:GLY:HA2 | 1.94 | 0.49 |
| 4:X:458:ASP:O | 4:X:460:LEU:CA | 2.58 | 0.49 |
| 1:A:312:MET:CB | 1:A:313:SER:CA | 2.91 | 0.49 |
| 1:B:215:LEU:HA | 1:B:230:GLY:HA2 | 1.94 | 0.49 |
| 3:D:324:GLY:O | 3:D:327:ALA:HB3 | 2.12 | 0.49 |
| 2:I:447:ASP:C | 2:I:448:TYR:HA | 2.32 | 0.49 |
| 6:T:408:SER:C | 6:T:409:PRO:C | 2.64 | 0.49 |
| 2:U:469:THR:O | 2:U:470:ALA:HB3 | 2.12 | 0.49 |
| 4:L:458:ASP:C | 4:L:460:LEU:N | 2.66 | 0.49 |
| 2:U:447:ASP:C | 2:U:448:TYR:HA | 2.33 | 0.49 |
| 2:C:234:LEU:C | 2:C:252:MET:HA | 2.33 | 0.48 |
| 3:D:1509:GLN:O | 3:D:1510:GLN:C | 2.45 | 0.48 |
| 2:O:653:ILE:CB | 3:P:1456:GLU:CA | 2.91 | 0.48 |
| 3:P:69:LYS:O | 3:P:70:ALA:HB3 | 2.13 | 0.48 |
| 2:C:487:CYS:CB | 3:D:1661:ARG:CA | 2.85 | 0.48 |
| 5:M:378:SER:CB | 5:M:378:SER:O | 2.61 | 0.48 |
| 2:C:15:GLN:N | 2:C:16:LEU:N | 2.61 | 0.48 |
| 4:F:458:ASP:C | 4:F:460:LEU:N | 2.66 | 0.48 |
| 2:I:234:LEU:C | 2:I:252:MET:HA | 2.33 | 0.48 |
| 4:R:458:ASP:O | 4:R:459:LEU:C | 2.45 | 0.48 |
| 5:Y:326:LEU:N | 5:Y:326:LEU:CB | 2.72 | 0.48 |
| 5:Y:378:SER:CB | 5:Y:378:SER:O | 2.61 | 0.48 |
| 1:E:312:MET:CB | 1:E:313:SER:CA | 2.91 | 0.48 |
| 2:I:469:THR:O | 2:I:470:ALA:HB3 | 2.12 | 0.48 |
| 7:J:147:PHE:C | 7:J:149:ASP:H | 2.17 | 0.48 |
| 1:A:215:LEU:HA | 1:A:230:GLY:HA2 | 1.94 | 0.48 |
| 6:H:374:SER:CB | 6:H:374:SER:H | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:L:450:GLU:O | 4:L:451:GLU:CA | 2.33 | 0.48 |
| 3:P:644:ALA:HB2 | 3:P:702:PRO:O | 2.14 | 0.48 |
| 1:Q:312:MET:CB | 1:Q:313:SER:CA | 2.91 | 0.48 |
| 4:X:493:HIS:CB | 4:X:493:HIS:C | 2.60 | 0.48 |
| 4:F:492:GLU:CA | 4:F:492:GLU:O | 2.53 | 0.48 |
| 5:G:378:SER:CA | 5:G:378:SER:O | 2.51 | 0.48 |
| 2:I:15:GLN:N | 2:I:16:LEU:N | 2.61 | 0.48 |
| 7:J:1175:GLY:HA3 | 7:J:1197:GLN:N | 2.23 | 0.48 |
| 2:U:234:LEU:C | 2:U:252:MET:HA | 2.33 | 0.48 |
| 1:W:312:MET:CB | 1:W:313:SER:CA | 2.91 | 0.48 |
| 2:C:19:GLU:CB | 2:C:20:THR:CA | 2.92 | 0.48 |
| 5:G:378:SER:CB | 5:G:378:SER:O | 2.61 | 0.48 |
| 2:O:591:GLY:HA2 | 1:W:853:ASP:CB | 2.44 | 0.48 |
| 4:X:455:ILE:C | 4:X:457:ALA:H | 2.15 | 0.48 |
| 4:F:490:LEU:O | 4:F:493:HIS:N | 2.43 | 0.48 |
| 5:G:325:ALA:C | 5:G:325:ALA:CB | 2.77 | 0.48 |
| 4:L:493:HIS:CB | 4:L:493:HIS:C | 2.60 | 0.48 |
| 2:O:231:THR:C | 2:O:233:VAL:H | 2.17 | 0.48 |
| 5:S:378:SER:CB | 5:S:378:SER:O | 2.61 | 0.48 |
| 7:V:1157:SER:CB | 7:V:1222:SER:CB | 2.92 | 0.48 |
| 7:V:1175:GLY:HA3 | 7:V:1197:GLN:N | 2.23 | 0.48 |
| 1:E:852:VAL:CB | 2:O:304:PRO:CA | 2.89 | 0.48 |
| 4:F:235:ASP:CB | 4:F:235:ASP:C | 2.68 | 0.48 |
| 1:K:1352:LEU:C | 1:K:1354:LEU:H | 2.17 | 0.48 |
| 4:L:488:ILE:N | 4:L:488:ILE:CB | 2.66 | 0.48 |
| 7:V:1465:GLU:O | 7:V:1474:MET:N | 2.47 | 0.48 |
| 2:C:231:THR:C | 2:C:233:VAL:H | 2.18 | 0.48 |
| 3:D:69:LYS:O | 3:D:70:ALA:HB3 | 2.13 | 0.48 |
| 7:J:1157:SER:CB | 7:J:1222:SER:CB | 2.92 | 0.48 |
| 4:R:367:THR:CA | 4:R:367:THR:O | 2.53 | 0.48 |
| 2:U:15:GLN:N | 2:U:16:LEU:N | 2.61 | 0.48 |
| 3:D:644:ALA:HB2 | 3:D:702:PRO:O | 2.14 | 0.47 |
| 4:F:158:ASN:CA | 4:F:321:LYS:O | 2.62 | 0.47 |
| 2:U:807:THR:C | 2:U:809:ALA:H | 2.16 | 0.47 |
| 1:B:312:MET:CB | 1:B:313:SER:CA | 2.91 | 0.47 |
| 4:F:140:LYS:CA | 4:F:149:GLY:HA2 | 2.45 | 0.47 |
| 2:I:807:THR:C | 2:I:809:ALA:H | 2.16 | 0.47 |
| 2:O:19:GLU:CB | 2:O:20:THR:CA | 2.92 | 0.47 |
| 7:V:147:PHE:C | 7:V:149:ASP:H | 2.17 | 0.47 |
| 5:Y:339:TYR:CA | 5:Y:340:ALA:N | 2.68 | 0.47 |
| 2:C:681:ALA:HB3 | 1:K:850:ALA:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:328:VAL:C | 4:F:328:VAL:CB | 2.67 | 0.47 |
| 4:L:197:LYS:CB | 4:L:201:GLU:CB | 2.92 | 0.47 |
| 4:R:140:LYS:CA | 4:R:149:GLY:HA2 | 2.45 | 0.47 |
| 6:T:477:ILE:O | 6:T:480:ALA:HB3 | 2.14 | 0.47 |
| 3:D:644:ALA:HB2 | 3:D:702:PRO:C | 2.35 | 0.47 |
| 6:N:408:SER:CA | 6:N:410:LEU:N | 2.68 | 0.47 |
| 2:O:807:THR:C | 2:O:809:ALA:H | 2.17 | 0.47 |
| 3:P:644:ALA:HB2 | 3:P:702:PRO:C | 2.35 | 0.47 |
| 4:X:490:LEU:O | 4:X:493:HIS:N | 2.43 | 0.47 |
| 2:C:807:THR:C | 2:C:809:ALA:H | 2.16 | 0.47 |
| 2:I:19:GLU:CB | 2:I:20:THR:CA | 2.92 | 0.47 |
| 4:R:197:LYS:CB | 4:R:201:GLU:CB | 2.92 | 0.47 |
| 5:S:322:ALA:O | 5:S:325:ALA:HB3 | 2.14 | 0.47 |
| 5:Y:322:ALA:O | 5:Y:325:ALA:HB3 | 2.14 | 0.47 |
| 7:J:1386:LYS:CB | 7:J:1388:LEU:HA | 2.45 | 0.47 |
| 7:J:1465:GLU:O | 7:J:1474:MET:N | 2.47 | 0.47 |
| 5:M:340:ALA:O | 5:M:341:ALA:CB | 2.62 | 0.47 |
| 4:R:211:GLU:HA | 4:R:214:HIS:CB | 2.45 | 0.47 |
| 2:C:487:CYS:CA | 3:D:1661:ARG:CB | 2.87 | 0.47 |
| 3:D:49:ASP:C | 3:D:51:ILE:H | 2.18 | 0.47 |
| 3:D:1486:CYS:O | 3:D:1487:ASP:C | 2.50 | 0.47 |
| 3:D:1517:SER:O | 3:D:1518:ASN:C | 2.51 | 0.47 |
| 1:E:852:VAL:CB | 2:O:305:LEU:H | 2.25 | 0.47 |
| 4:F:197:LYS:CB | 4:F:201:GLU:CB | 2.92 | 0.47 |
| 4:F:488:ILE:N | 4:F:488:ILE:CB | 2.66 | 0.47 |
| 4:L:140:LYS:HA | 4:L:149:GLY:CA | 2.45 | 0.47 |
| 4:L:140:LYS:CA | 4:L:149:GLY:HA2 | 2.45 | 0.47 |
| 4:L:458:ASP:O | 4:L:460:LEU:CA | 2.58 | 0.47 |
| 3:P:1489:HIS:O | 3:P:1492:GLY:N | 2.48 | 0.47 |
| 4:R:492:GLU:CB | 4:R:492:GLU:O | 2.63 | 0.47 |
| 7:V:1386:LYS:CB | 7:V:1388:LEU:HA | 2.45 | 0.47 |
| 1:W:1352:LEU:C | 1:W:1354:LEU:H | 2.17 | 0.47 |
| 5:Y:340:ALA:O | 5:Y:341:ALA:CB | 2.63 | 0.47 |
| 2:C:538:LYS:HA | 3:D:1671:GLN:C | 1.95 | 0.47 |
| 5:G:322:ALA:O | 5:G:325:ALA:HB3 | 2.14 | 0.47 |
| 6:H:477:ILE:O | 6:H:480:ALA:HB3 | 2.15 | 0.47 |
| 3:P:49:ASP:C | 3:P:51:ILE:H | 2.18 | 0.47 |
| 1:Q:1352:LEU:C | 1:Q:1354:LEU:H | 2.17 | 0.47 |
| 5:S:340:ALA:O | 5:S:341:ALA:CB | 2.63 | 0.47 |
| 1:W:340:LYS:C | 1:W:342:ILE:HA | 2.35 | 0.47 |
| 4:X:367:THR:C | 4:X:367:THR:CB | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1352:LEU:C | 1:E:1354:LEU:H | 2.17 | 0.47 |
| 6:H:380:GLU:C | 6:H:381:LYS:CA | 2.72 | 0.47 |
| 7:J:1436:ALA:C | 7:J:1438:ARG:H | 2.18 | 0.47 |
| 2:U:19:GLU:CB | 2:U:20:THR:CA | 2.92 | 0.47 |
| 4:X:492:GLU:CB | 4:X:492:GLU:O | 2.63 | 0.47 |
| 6:Z:477:ILE:O | 6:Z:480:ALA:HB3 | 2.14 | 0.47 |
| 1:A:38:ARG:HA | 1:A:484:THR:CB | 2.45 | 0.47 |
| 2:C:681:ALA:HB3 | 1:K:850:ALA:CA | 2.45 | 0.47 |
| 4:F:492:GLU:CB | 4:F:492:GLU:O | 2.63 | 0.47 |
| 5:G:340:ALA:O | 5:G:341:ALA:CB | 2.63 | 0.47 |
| 4:L:490:LEU:O | 4:L:493:HIS:N | 2.43 | 0.47 |
| 1:Q:38:ARG:HA | 1:Q:484:THR:CB | 2.45 | 0.47 |
| 4:X:140:LYS:CA | 4:X:149:GLY:HA2 | 2.44 | 0.47 |
| 1:A:340:LYS:C | 1:A:342:ILE:HA | 2.35 | 0.46 |
| 7:J:1373:SER:CB | 7:J:1426:HIS:CB | 2.93 | 0.46 |
| 3:P:1509:GLN:O | 3:P:1510:GLN:C | 2.45 | 0.46 |
| 1:B:38:ARG:HA | 1:B:484:THR:CB | 2.45 | 0.46 |
| 3:D:1542:PRO:C | 3:D:1544:PRO:N | 2.68 | 0.46 |
| 1:E:340:LYS:C | 1:E:342:ILE:HA | 2.35 | 0.46 |
| 6:N:406:LEU:C | 6:N:408:SER:N | 2.62 | 0.46 |
| 4:R:140:LYS:HA | 4:R:149:GLY:CA | 2.44 | 0.46 |
| 4:R:158:ASN:CA | 4:R:321:LYS:O | 2.62 | 0.46 |
| 4:R:458:ASP:C | 4:R:460:LEU:N | 2.66 | 0.46 |
| 1:W:38:ARG:HA | 1:W:484:THR:CB | 2.45 | 0.46 |
| 4:X:197:LYS:CB | 4:X:201:GLU:CB | 2.92 | 0.46 |
| 4:X:211:GLU:HA | 4:X:214:HIS:CB | 2.45 | 0.46 |
| 4:X:489:LYS:O | 4:X:492:GLU:N | 2.48 | 0.46 |
| 3:D:1489:HIS:O | 3:D:1492:GLY:N | 2.48 | 0.46 |
| 4:L:211:GLU:HA | 4:L:214:HIS:CB | 2.46 | 0.46 |
| 4:R:490:LEU:O | 4:R:493:HIS:N | 2.43 | 0.46 |
| 5:S:325:ALA:C | 5:S:325:ALA:CB | 2.77 | 0.46 |
| 7:V:1436:ALA:C | 7:V:1438:ARG:H | 2.18 | 0.46 |
| 4:X:140:LYS:HA | 4:X:149:GLY:CA | 2.44 | 0.46 |
| 2:C:535:TYR:CB | 3:D:1662:CYS:O | 2.63 | 0.46 |
| 4:F:140:LYS:HA | 4:F:149:GLY:CA | 2.44 | 0.46 |
| 5:M:322:ALA:O | 5:M:325:ALA:HB3 | 2.14 | 0.46 |
| 5:M:374:GLN:HA | 5:M:377:ASN:CB | 2.46 | 0.46 |
| 3:P:1447:THR:O | 3:P:1448:MET:C | 2.53 | 0.46 |
| 2:U:231:THR:C | 2:U:233:VAL:H | 2.17 | 0.46 |
| 7:V:1437:VAL:O | 7:V:1487:ALA:HB1 | 2.15 | 0.46 |
| 4:X:158:ASN:CA | 4:X:321:LYS:O | 2.62 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Z:374:SER:CB | 6:Z:374:SER:H | 2.25 | 0.46 |
| 4:F:452:ARG:C | 4:F:453:TYR:C | 2.74 | 0.46 |
| 4:F:489:LYS:O | 4:F:492:GLU:N | 2.48 | 0.46 |
| 1:K:340:LYS:C | 1:K:342:ILE:HA | 2.35 | 0.46 |
| 4:L:492:GLU:CB | 4:L:492:GLU:O | 2.63 | 0.46 |
| 1:Q:340:LYS:C | 1:Q:342:ILE:HA | 2.35 | 0.46 |
| 2:C:15:GLN:CA | 2:C:16:LEU:N | 2.71 | 0.46 |
| 7:J:469:ASP:O | 7:J:537:SER:HA | 2.16 | 0.46 |
| 5:S:374:GLN:HA | 5:S:377:ASN:CB | 2.46 | 0.46 |
| 7:V:469:ASP:O | 7:V:537:SER:HA | 2.16 | 0.46 |
| 7:V:1373:SER:CB | 7:V:1426:HIS:CB | 2.93 | 0.46 |
| 3:D:1493:ARG:O | 3:D:1494:MET:C | 2.47 | 0.46 |
| 1:E:38:ARG:HA | 1:E:484:THR:CB | 2.45 | 0.46 |
| 5:Y:374:GLN:HA | 5:Y:377:ASN:CB | 2.46 | 0.46 |
| 4:F:140:LYS:CA | 4:F:149:GLY:CA | 2.94 | 0.46 |
| 4:R:493:HIS:CB | 4:R:493:HIS:C | 2.61 | 0.46 |
| 5:Y:325:ALA:C | 5:Y:325:ALA:CB | 2.77 | 0.46 |
| 4:F:211:GLU:HA | 4:F:214:HIS:CB | 2.45 | 0.46 |
| 5:G:374:GLN:HA | 5:G:377:ASN:CB | 2.46 | 0.46 |
| 2:I:231:THR:C | 2:I:233:VAL:H | 2.17 | 0.46 |
| 2:O:15:GLN:CA | 2:O:16:LEU:N | 2.71 | 0.46 |
| 4:X:458:ASP:C | 4:X:460:LEU:N | 2.66 | 0.46 |
| 4:L:452:ARG:C | 4:L:453:TYR:C | 2.74 | 0.45 |
| 6:N:477:ILE:O | 6:N:480:ALA:HB3 | 2.15 | 0.45 |
| 3:P:1482:CYS:O | 3:P:1485:ALA:HB3 | 2.16 | 0.45 |
| 3:P:1542:PRO:C | 3:P:1544:PRO:N | 2.68 | 0.45 |
| 4:R:140:LYS:CA | 4:R:149:GLY:CA | 2.94 | 0.45 |
| 4:R:447:VAL:CB | 4:R:447:VAL:C | 2.77 | 0.45 |
| 4:X:367:THR:CA | 4:X:367:THR:O | 2.53 | 0.45 |
| 1:K:38:ARG:HA | 1:K:484:THR:CB | 2.45 | 0.45 |
| 3:P:1486:CYS:O | 3:P:1487:ASP:C | 2.50 | 0.45 |
| 4:R:489:LYS:O | 4:R:492:GLU:N | 2.48 | 0.45 |
| 4:X:452:ARG:C | 4:X:453:TYR:C | 2.74 | 0.45 |
| 4:L:450:GLU:C | 4:L:451:GLU:C | 2.73 | 0.45 |
| 2:C:307:GLY:N | 1:Q:849:ASN:CB | 2.79 | 0.45 |
| 4:L:140:LYS:CA | 4:L:149:GLY:CA | 2.94 | 0.45 |
| 4:L:367:THR:CA | 4:L:367:THR:O | 2.53 | 0.45 |
| 5:M:342:PRO:O | 5:M:344:ASP:N | 2.50 | 0.45 |
| 2:O:234:LEU:CB | 2:O:250:VAL:O | 2.65 | 0.45 |
| 3:P:1487:ASP:O | 3:P:1490:GLU:N | 2.49 | 0.45 |
| 3:P:1491:ILE:O | 3:P:1492:GLY:C | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:452:ARG:C | 4:R:453:TYR:C | 2.74 | 0.45 |
| 4:R:459:LEU:CA | 4:R:460:LEU:N | 2.54 | 0.45 |
| 1:W:395:GLY:N | 1:W:400:SER:CB | 2.80 | 0.45 |
| 4:X:453:TYR:N | 4:X:453:TYR:C | 2.70 | 0.45 |
| 1:B:340:LYS:C | 1:B:342:ILE:HA | 2.35 | 0.45 |
| 3:D:1472:SER:O | 3:D:1473:TYR:C | 2.55 | 0.45 |
| 3:D:1537:GLN:C | 3:D:1539:LEU:N | 2.69 | 0.45 |
| 4:F:453:TYR:N | 4:F:453:TYR:C | 2.70 | 0.45 |
| 7:J:192:GLY:C | 7:J:194:LEU:H | 2.20 | 0.45 |
| 2:O:655:ALA:O | 3:P:1447:THR:CB | 2.64 | 0.45 |
| 3:P:1494:MET:CB | 3:P:1551:TYR:CB | 2.95 | 0.45 |
| 4:R:405:ALA:HB3 | 4:R:406:ASP:H | 1.17 | 0.45 |
| 2:U:303:ALA:HB1 | 2:U:306:PRO:CA | 2.46 | 0.45 |
| 4:X:140:LYS:CA | 4:X:149:GLY:CA | 2.94 | 0.45 |
| 1:A:395:GLY:N | 1:A:400:SER:CB | 2.80 | 0.45 |
| 2:C:234:LEU:CB | 2:C:250:VAL:O | 2.65 | 0.45 |
| 4:F:486:GLU:C | 4:F:488:ILE:N | 2.70 | 0.45 |
| 2:I:503:LEU:O | 2:I:504:LYS:CB | 2.64 | 0.45 |
| 7:J:1437:VAL:O | 7:J:1487:ALA:HB1 | 2.15 | 0.45 |
| 4:L:486:GLU:C | 4:L:488:ILE:N | 2.70 | 0.45 |
| 6:N:374:SER:CB | 6:N:374:SER:H | 2.25 | 0.45 |
| 2:U:503:LEU:O | 2:U:504:LYS:CB | 2.64 | 0.45 |
| 3:D:1447:THR:O | 3:D:1448:MET:C | 2.53 | 0.45 |
| 3:D:1494:MET:CB | 3:D:1551:TYR:CB | 2.95 | 0.45 |
| 2:I:303:ALA:HB1 | 2:I:306:PRO:CA | 2.46 | 0.45 |
| 4:L:489:LYS:O | 4:L:492:GLU:N | 2.48 | 0.45 |
| 1:B:395:GLY:N | 1:B:400:SER:CB | 2.80 | 0.45 |
| 1:B:404:LYS:HA | 1:B:405:PRO:HA | 1.70 | 0.45 |
| 2:C:524:ARG:CA | 3:D:1610:PRO:HA | 2.47 | 0.45 |
| 4:F:493:HIS:CB | 4:F:493:HIS:C | 2.61 | 0.45 |
| 4:L:453:TYR:N | 4:L:453:TYR:C | 2.70 | 0.45 |
| 2:O:653:ILE:CB | 3:P:1456:GLU:CB | 2.95 | 0.45 |
| 7:V:846:ALA:CB | 7:V:852:ILE:CB | 2.95 | 0.45 |
| 4:X:486:GLU:C | 4:X:488:ILE:N | 2.70 | 0.45 |
| 2:C:503:LEU:O | 2:C:504:LYS:CB | 2.64 | 0.45 |
| 1:E:1164:GLN:CA | 1:K:726:GLN:CB | 2.94 | 0.45 |
| 4:L:158:ASN:CA | 4:L:321:LYS:O | 2.62 | 0.45 |
| 5:M:332:PRO:O | 5:M:335:LEU:HA | 2.17 | 0.45 |
| 5:S:342:PRO:O | 5:S:344:ASP:N | 2.50 | 0.45 |
| 2:C:531:LEU:C | 3:D:1664:ASP:N | 2.62 | 0.45 |
| 2:C:675:ARG:CB | 1:K:848:ASP:CB | 2.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:342:PRO:O | 5:G:344:ASP:N | 2.49 | 0.45 |
| 7:J:1329:ASN:CB | 7:J:1389:ASP:N | 2.80 | 0.45 |
| 4:L:140:LYS:CB | 4:L:149:GLY:HA2 | 2.47 | 0.45 |
| 7:V:794:ALA:C | 7:V:807:GLY:H | 2.20 | 0.45 |
| 7:V:1329:ASN:CB | 7:V:1389:ASP:N | 2.80 | 0.45 |
| 4:X:140:LYS:CB | 4:X:149:GLY:HA2 | 2.47 | 0.45 |
| 7:J:250:ASN:H | 7:J:253:LEU:HA | 1.82 | 0.44 |
| 6:T:490:GLN:CB | 6:T:490:GLN:N | 2.58 | 0.44 |
| 2:U:234:LEU:CB | 2:U:250:VAL:O | 2.65 | 0.44 |
| 7:V:192:GLY:C | 7:V:194:LEU:H | 2.20 | 0.44 |
| 3:D:1518:ASN:O | 3:D:1519:SER:C | 2.55 | 0.44 |
| 4:F:329:GLY:N | 4:F:329:GLY:C | 2.62 | 0.44 |
| 2:I:234:LEU:CB | 2:I:250:VAL:O | 2.65 | 0.44 |
| 7:J:811:ILE:CB | 7:J:866:ALA:HB1 | 2.47 | 0.44 |
| 4:L:447:VAL:O | 4:L:450:GLU:CA | 2.65 | 0.44 |
| 3:P:1513:LEU:O | 3:P:1514:LEU:C | 2.50 | 0.44 |
| 3:P:1517:SER:O | 3:P:1518:ASN:C | 2.51 | 0.44 |
| 3:P:1518:ASN:O | 3:P:1519:SER:C | 2.55 | 0.44 |
| 4:X:222:THR:CB | 4:X:222:THR:O | 2.62 | 0.44 |
| 4:X:450:GLU:C | 4:X:451:GLU:C | 2.73 | 0.44 |
| 5:Y:332:PRO:O | 5:Y:335:LEU:HA | 2.17 | 0.44 |
| 2:C:588:GLU:HA | 2:C:592:SER:O | 2.18 | 0.44 |
| 2:C:678:GLY:CA | 1:K:847:ARG:CB | 2.83 | 0.44 |
| 3:D:1491:ILE:O | 3:D:1492:GLY:C | 2.53 | 0.44 |
| 7:J:846:ALA:CB | 7:J:852:ILE:CB | 2.95 | 0.44 |
| 1:K:395:GLY:N | 1:K:400:SER:CB | 2.80 | 0.44 |
| 2:O:230:MET:HA | 2:O:233:VAL:CB | 2.48 | 0.44 |
| 4:R:492:GLU:C | 4:R:493:HIS:CA | 2.84 | 0.44 |
| 6:T:374:SER:CB | 6:T:374:SER:H | 2.26 | 0.44 |
| 4:X:447:VAL:O | 4:X:450:GLU:CA | 2.65 | 0.44 |
| 2:C:230:MET:HA | 2:C:233:VAL:CB | 2.48 | 0.44 |
| 1:E:395:GLY:N | 1:E:400:SER:CB | 2.80 | 0.44 |
| 2:O:588:GLU:HA | 2:O:592:SER:O | 2.18 | 0.44 |
| 4:R:488:ILE:N | 4:R:488:ILE:CB | 2.66 | 0.44 |
| 5:S:332:PRO:O | 5:S:335:LEU:HA | 2.17 | 0.44 |
| 1:A:404:LYS:HA | 1:A:405:PRO:HA | 1.70 | 0.44 |
| 2:C:303:ALA:HB1 | 2:C:306:PRO:CA | 2.46 | 0.44 |
| 4:F:405:ALA:HB3 | 4:F:406:ASP:H | 1.17 | 0.44 |
| 4:F:447:VAL:O | 4:F:450:GLU:CA | 2.65 | 0.44 |
| 7:J:1373:SER:CB | 7:J:1426:HIS:CA | 2.96 | 0.44 |
| 5:M:325:ALA:C | 5:M:325:ALA:CB | 2.77 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:453:TYR:N | 4:R:453:TYR:C | 2.70 | 0.44 |
| 7:V:811:ILE:CB | 7:V:866:ALA:HB1 | 2.47 | 0.44 |
| 2:C:487:CYS:N | 3:D:1661:ARG:CB | 2.77 | 0.44 |
| 3:D:1482:CYS:O | 3:D:1485:ALA:HB3 | 2.17 | 0.44 |
| 3:D:1536:LEU:O | 3:D:1539:LEU:CB | 2.66 | 0.44 |
| 4:F:367:THR:CA | 4:F:367:THR:O | 2.53 | 0.44 |
| 4:F:450:GLU:C | 4:F:451:GLU:C | 2.73 | 0.44 |
| 7:J:794:ALA:C | 7:J:807:GLY:H | 2.20 | 0.44 |
| 2:O:503:LEU:O | 2:O:504:LYS:CB | 2.64 | 0.44 |
| 3:P:1512:TRP:O | 3:P:1515:TYR:N | 2.51 | 0.44 |
| 1:Q:395:GLY:N | 1:Q:400:SER:CB | 2.80 | 0.44 |
| 4:R:486:GLU:C | 4:R:488:ILE:N | 2.70 | 0.44 |
| 5:Y:342:PRO:O | 5:Y:344:ASP:N | 2.49 | 0.44 |
| 4:F:459:LEU:CA | 4:F:460:LEU:N | 2.54 | 0.44 |
| 1:Q:1355:ASP:CB | 1:Q:1358:CYS:CB | 2.96 | 0.44 |
| 4:R:447:VAL:O | 4:R:450:GLU:CA | 2.65 | 0.44 |
| 1:W:1355:ASP:CB | 1:W:1358:CYS:CB | 2.96 | 0.44 |
| 4:F:140:LYS:CB | 4:F:149:GLY:HA2 | 2.47 | 0.44 |
| 5:G:332:PRO:O | 5:G:335:LEU:HA | 2.17 | 0.44 |
| 4:L:222:THR:CB | 4:L:222:THR:O | 2.62 | 0.44 |
| 4:R:140:LYS:CB | 4:R:149:GLY:HA2 | 2.47 | 0.44 |
| 3:D:1512:TRP:O | 3:D:1515:TYR:N | 2.51 | 0.44 |
| 1:K:1355:ASP:CB | 1:K:1358:CYS:CB | 2.96 | 0.44 |
| 4:R:367:THR:C | 4:R:367:THR:CB | 2.78 | 0.44 |
| 5:G:374:GLN:O | 5:G:377:ASN:CB | 2.66 | 0.43 |
| 1:K:942:PRO:HA | 1:K:943:GLN:HA | 1.48 | 0.43 |
| 5:M:374:GLN:O | 5:M:377:ASN:CB | 2.66 | 0.43 |
| 3:P:1536:LEU:O | 3:P:1539:LEU:CB | 2.66 | 0.43 |
| 5:S:374:GLN:O | 5:S:377:ASN:CB | 2.66 | 0.43 |
| 2:U:588:GLU:HA | 2:U:592:SER:O | 2.18 | 0.43 |
| 7:V:250:ASN:H | 7:V:253:LEU:HA | 1.82 | 0.43 |
| 5:Y:374:GLN:O | 5:Y:377:ASN:CB | 2.66 | 0.43 |
| 2:I:588:GLU:HA | 2:I:592:SER:O | 2.18 | 0.43 |
| 7:V:846:ALA:HB2 | 7:V:849:ASN:C | 2.38 | 0.43 |
| 7:V:858:TYR:CB | 7:V:865:PRO:N | 2.81 | 0.43 |
| 5:Y:366:GLU:CB | 5:Y:367:LEU:N | 2.81 | 0.43 |
| 1:E:1355:ASP:CB | 1:E:1358:CYS:CB | 2.96 | 0.43 |
| 4:X:492:GLU:CA | 4:X:492:GLU:O | 2.53 | 0.43 |
| 7:J:520:GLN:O | 7:J:530:VAL:HA | 2.18 | 0.43 |
| 7:J:846:ALA:HB2 | 7:J:849:ASN:C | 2.38 | 0.43 |
| 2:O:589:ASN:C | 1:W:850:ALA:N | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:V:520:GLN:O | 7:V:530:VAL:HA | 2.19 | 0.43 |
| 7:V:1373:SER:CB | 7:V:1426:HIS:CA | 2.96 | 0.43 |
| 7:J:1519:GLN:CB | 7:J:1539:THR:N | 2.81 | 0.43 |
| 3:P:1542:PRO:O | 3:P:1544:PRO:N | 2.52 | 0.43 |
| 2:U:230:MET:HA | 2:U:233:VAL:CB | 2.48 | 0.43 |
| 4:X:450:GLU:O | 4:X:451:GLU:O | 2.36 | 0.43 |
| 4:F:492:GLU:C | 4:F:493:HIS:CA | 2.84 | 0.43 |
| 4:L:492:GLU:C | 4:L:493:HIS:CA | 2.84 | 0.43 |
| 4:R:222:THR:CB | 4:R:222:THR:O | 2.62 | 0.43 |
| 4:R:483:ASP:C | 4:R:486:GLU:H | 2.22 | 0.43 |
| 3:D:1542:PRO:O | 3:D:1544:PRO:N | 2.51 | 0.43 |
| 1:E:1170:SER:N | 1:K:576:TYR:CB | 2.68 | 0.43 |
| 1:K:404:LYS:HA | 1:K:405:PRO:HA | 1.70 | 0.43 |
| 4:L:200:THR:C | 4:L:202:ILE:N | 2.70 | 0.43 |
| 2:O:480:PHE:C | 2:O:484:ARG:CB | 2.87 | 0.43 |
| 3:P:1544:PRO:C | 3:P:1546:LEU:N | 2.72 | 0.43 |
| 7:V:1519:GLN:CB | 7:V:1539:THR:N | 2.81 | 0.43 |
| 6:Z:380:GLU:C | 6:Z:381:LYS:CA | 2.72 | 0.43 |
| 4:F:140:LYS:O | 4:F:149:GLY:HA3 | 2.19 | 0.43 |
| 4:F:222:THR:CB | 4:F:222:THR:O | 2.62 | 0.43 |
| 5:G:318:GLU:C | 5:G:320:LYS:N | 2.71 | 0.43 |
| 2:I:230:MET:HA | 2:I:233:VAL:CB | 2.48 | 0.43 |
| 7:J:794:ALA:HB3 | 7:J:803:GLY:O | 2.19 | 0.43 |
| 4:L:140:LYS:O | 4:L:149:GLY:HA3 | 2.19 | 0.43 |
| 4:L:450:GLU:O | 4:L:451:GLU:O | 2.36 | 0.43 |
| 3:P:1493:ARG:O | 3:P:1494:MET:C | 2.47 | 0.43 |
| 3:P:1506:VAL:O | 3:P:1508:LYS:N | 2.47 | 0.43 |
| 7:V:1175:GLY:CA | 7:V:1196:GLN:HA | 2.49 | 0.43 |
| 4:X:140:LYS:O | 4:X:149:GLY:HA3 | 2.19 | 0.43 |
| 2:C:480:PHE:C | 2:C:484:ARG:CB | 2.87 | 0.43 |
| 3:D:644:ALA:HB1 | 3:D:706:ALA:HB2 | 2.01 | 0.43 |
| 1:E:1170:SER:CB | 1:K:576:TYR:CB | 2.96 | 0.43 |
| 4:L:198:LYS:C | 4:L:200:THR:N | 2.58 | 0.43 |
| 6:N:380:GLU:C | 6:N:381:LYS:CA | 2.72 | 0.43 |
| 3:P:1537:GLN:C | 3:P:1539:LEU:N | 2.69 | 0.43 |
| 2:U:724:GLN:C | 2:U:726:SER:H | 2.22 | 0.43 |
| 7:V:829:PRO:C | 7:V:832:ASN:H | 2.22 | 0.43 |
| 4:X:447:VAL:O | 4:X:450:GLU:N | 2.52 | 0.43 |
| 3:D:1664:ASP:N | 3:D:1667:ALA:CB | 2.82 | 0.43 |
| 2:I:724:GLN:C | 2:I:726:SER:H | 2.23 | 0.43 |
| 4:R:447:VAL:O | 4:R:450:GLU:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:483:ASP:C | 4:X:486:GLU:H | 2.22 | 0.43 |
| 3:D:1504:VAL:O | 3:D:1505:SER:C | 2.39 | 0.42 |
| 7:V:794:ALA:HB3 | 7:V:803:GLY:O | 2.19 | 0.42 |
| 6:Z:463:ALA:N | 6:Z:463:ALA:C | 2.65 | 0.42 |
| 3:D:644:ALA:CB | 3:D:706:ALA:HB2 | 2.49 | 0.42 |
| 3:D:1485:ALA:O | 3:D:1487:ASP:N | 2.52 | 0.42 |
| 4:F:455:ILE:C | 4:F:457:ALA:H | 2.15 | 0.42 |
| 4:F:483:ASP:C | 4:F:486:GLU:H | 2.22 | 0.42 |
| 3:P:1502:ARG:O | 3:P:1503:ILE:C | 2.58 | 0.42 |
| 7:V:1385:ARG:O | 7:V:1390:ALA:HB3 | 2.18 | 0.42 |
| 7:V:1460:SER:C | 7:V:1463:MET:H | 2.22 | 0.42 |
| 4:X:198:LYS:C | 4:X:200:THR:N | 2.58 | 0.42 |
| 3:D:1544:PRO:C | 3:D:1546:LEU:N | 2.72 | 0.42 |
| 4:F:422:ASN:CB | 4:F:423:ALA:CB | 2.94 | 0.42 |
| 4:L:447:VAL:O | 4:L:450:GLU:N | 2.52 | 0.42 |
| 4:L:483:ASP:C | 4:L:486:GLU:H | 2.22 | 0.42 |
| 4:L:489:LYS:O | 4:L:492:GLU:CB | 2.67 | 0.42 |
| 3:P:1537:GLN:O | 3:P:1538:SER:C | 2.56 | 0.42 |
| 4:R:492:GLU:CA | 4:R:492:GLU:O | 2.53 | 0.42 |
| 6:T:406:LEU:C | 6:T:408:SER:N | 2.61 | 0.42 |
| 4:X:489:LYS:O | 4:X:492:GLU:CB | 2.68 | 0.42 |
| 6:Z:494:LEU:O | 6:Z:498:LYS:CB | 2.68 | 0.42 |
| 7:J:844:HIS:O | 7:J:848:GLY:HA2 | 2.19 | 0.42 |
| 7:J:1385:ARG:O | 7:J:1390:ALA:HB3 | 2.19 | 0.42 |
| 3:P:644:ALA:HB1 | 3:P:706:ALA:HB2 | 2.01 | 0.42 |
| 4:R:140:LYS:O | 4:R:149:GLY:HA3 | 2.19 | 0.42 |
| 4:R:200:THR:C | 4:R:202:ILE:N | 2.70 | 0.42 |
| 4:R:450:GLU:O | 4:R:451:GLU:O | 2.36 | 0.42 |
| 4:X:422:ASN:CB | 4:X:423:ALA:CB | 2.94 | 0.42 |
| 3:D:1544:PRO:O | 3:D:1546:LEU:N | 2.52 | 0.42 |
| 2:I:480:PHE:C | 2:I:484:ARG:CB | 2.87 | 0.42 |
| 3:P:644:ALA:CB | 3:P:706:ALA:HB2 | 2.49 | 0.42 |
| 3:P:1544:PRO:O | 3:P:1546:LEU:N | 2.52 | 0.42 |
| 4:R:489:LYS:O | 4:R:492:GLU:CB | 2.68 | 0.42 |
| 2:U:480:PHE:C | 2:U:484:ARG:CB | 2.87 | 0.42 |
| 7:V:844:HIS:O | 7:V:848:GLY:HA2 | 2.19 | 0.42 |
| 1:B:326:ALA:CB | 1:B:387:LEU:CB | 2.95 | 0.42 |
| 4:F:465:GLN:O | 4:F:466:HIS:C | 2.57 | 0.42 |
| 7:J:858:TYR:CB | 7:J:865:PRO:N | 2.81 | 0.42 |
| 3:P:1472:SER:O | 3:P:1473:TYR:C | 2.55 | 0.42 |
| 4:R:458:ASP:C | 4:R:459:LEU:C | 2.79 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:481:ARG:HA | 3:D:1593:GLU:CB | 2.50 | 0.42 |
| 3:D:1487:ASP:O | 3:D:1490:GLU:N | 2.49 | 0.42 |
| 1:E:404:LYS:HA | 1:E:405:PRO:HA | 1.70 | 0.42 |
| 4:F:200:THR:C | 4:F:202:ILE:N | 2.70 | 0.42 |
| 6:H:494:LEU:O | 6:H:498:LYS:CB | 2.68 | 0.42 |
| 2:I:480:PHE:O | 2:I:484:ARG:CB | 2.68 | 0.42 |
| 6:N:494:LEU:O | 6:N:498:LYS:CB | 2.68 | 0.42 |
| 3:P:1485:ALA:O | 3:P:1487:ASP:N | 2.52 | 0.42 |
| 6:T:494:LEU:O | 6:T:498:LYS:CB | 2.68 | 0.42 |
| 2:U:480:PHE:O | 2:U:484:ARG:CB | 2.68 | 0.42 |
| 3:D:1513:LEU:O | 3:D:1514:LEU:C | 2.50 | 0.42 |
| 7:J:829:PRO:C | 7:J:832:ASN:H | 2.22 | 0.42 |
| 6:N:490:GLN:CB | 6:N:490:GLN:O | 2.66 | 0.42 |
| 2:O:784:GLN:CB | 1:W:131:GLY:O | 2.68 | 0.42 |
| 3:P:1664:ASP:N | 3:P:1667:ALA:CB | 2.82 | 0.42 |
| 7:V:581:SER:C | 7:V:583:ALA:H | 2.23 | 0.42 |
| 4:X:332:GLU:O | 4:X:335:ARG:CB | 2.68 | 0.42 |
| 4:X:492:GLU:C | 4:X:493:HIS:CA | 2.84 | 0.42 |
| 2:C:724:GLN:C | 2:C:726:SER:H | 2.23 | 0.42 |
| 3:D:1491:ILE:C | 3:D:1493:ARG:N | 2.72 | 0.42 |
| 4:F:458:ASP:C | 4:F:459:LEU:C | 2.79 | 0.42 |
| 7:J:1175:GLY:CA | 7:J:1196:GLN:HA | 2.49 | 0.42 |
| 4:L:332:GLU:O | 4:L:335:ARG:CB | 2.68 | 0.42 |
| 4:X:200:THR:C | 4:X:202:ILE:N | 2.70 | 0.42 |
| 6:Z:406:LEU:C | 6:Z:408:SER:N | 2.62 | 0.42 |
| 4:F:447:VAL:O | 4:F:450:GLU:N | 2.52 | 0.42 |
| 4:R:329:GLY:N | 4:R:329:GLY:C | 2.62 | 0.42 |
| 4:R:450:GLU:C | 4:R:451:GLU:C | 2.73 | 0.42 |
| 6:T:493:ALA:O | 6:T:497:ARG:CB | 2.68 | 0.42 |
| 2:U:279:HIS:HA | 2:U:283:LEU:HA | 2.02 | 0.42 |
| 7:V:859:ILE:H | 7:V:865:PRO:CA | 2.33 | 0.42 |
| 7:V:1175:GLY:CA | 7:V:1197:GLN:N | 2.82 | 0.42 |
| 2:C:234:LEU:C | 2:C:252:MET:N | 2.74 | 0.41 |
| 2:C:480:PHE:O | 2:C:484:ARG:CB | 2.68 | 0.41 |
| 4:F:450:GLU:O | 4:F:451:GLU:O | 2.36 | 0.41 |
| 5:G:379:HIS:N | 5:G:379:HIS:CB | 2.72 | 0.41 |
| 7:J:1460:SER:C | 7:J:1463:MET:H | 2.22 | 0.41 |
| 6:N:493:ALA:O | 6:N:497:ARG:CB | 2.68 | 0.41 |
| 2:O:724:GLN:C | 2:O:726:SER:H | 2.22 | 0.41 |
| 7:V:1465:GLU:O | 7:V:1475:ARG:N | 2.51 | 0.41 |
| 2:C:679:ILE:C | 1:K:850:ALA:O | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:279:HIS:HA | 2:I:283:LEU:HA | 2.02 | 0.41 |
| 7:J:1246:PHE:CB | 7:J:1275:HIS:N | 2.83 | 0.41 |
| 4:L:447:VAL:CB | 4:L:447:VAL:C | 2.77 | 0.41 |
| 2:O:480:PHE:O | 2:O:484:ARG:CB | 2.68 | 0.41 |
| 4:R:255:ARG:O | 4:R:292:GLN:CB | 2.69 | 0.41 |
| 4:F:460:LEU:CB | 6:H:470:PRO:C | 2.89 | 0.41 |
| 5:G:366:GLU:CB | 5:G:367:LEU:N | 2.81 | 0.41 |
| 4:L:459:LEU:C | 4:L:459:LEU:N | 2.63 | 0.41 |
| 5:M:366:GLU:CB | 5:M:367:LEU:N | 2.81 | 0.41 |
| 3:P:1489:HIS:CB | 3:P:1492:GLY:N | 2.81 | 0.41 |
| 2:U:234:LEU:C | 2:U:252:MET:N | 2.74 | 0.41 |
| 4:F:367:THR:C | 4:F:367:THR:CB | 2.78 | 0.41 |
| 4:F:489:LYS:O | 4:F:492:GLU:CB | 2.68 | 0.41 |
| 2:I:234:LEU:C | 2:I:252:MET:N | 2.73 | 0.41 |
| 7:J:581:SER:C | 7:J:583:ALA:H | 2.23 | 0.41 |
| 4:L:458:ASP:O | 4:L:459:LEU:C | 2.45 | 0.41 |
| 4:L:460:LEU:O | 4:L:461:ARG:O | 2.39 | 0.41 |
| 3:P:1492:GLY:O | 3:P:1495:LEU:N | 2.53 | 0.41 |
| 4:R:422:ASN:CB | 4:R:423:ALA:CB | 2.94 | 0.41 |
| 5:S:366:GLU:CB | 5:S:367:LEU:N | 2.81 | 0.41 |
| 4:F:332:GLU:O | 4:F:335:ARG:CB | 2.68 | 0.41 |
| 6:H:463:ALA:N | 6:H:463:ALA:C | 2.65 | 0.41 |
| 4:R:332:GLU:O | 4:R:335:ARG:CB | 2.68 | 0.41 |
| 7:V:1246:PHE:CB | 7:V:1275:HIS:N | 2.83 | 0.41 |
| 4:X:460:LEU:CB | 6:Z:470:PRO:C | 2.89 | 0.41 |
| 6:Z:493:ALA:O | 6:Z:497:ARG:CB | 2.68 | 0.41 |
| 1:A:326:ALA:CB | 1:A:387:LEU:CB | 2.95 | 0.41 |
| 3:D:1544:PRO:C | 3:D:1546:LEU:H | 2.24 | 0.41 |
| 4:F:460:LEU:O | 4:F:461:ARG:O | 2.39 | 0.41 |
| 6:H:406:LEU:C | 6:H:408:SER:N | 2.61 | 0.41 |
| 4:L:458:ASP:C | 4:L:459:LEU:C | 2.79 | 0.41 |
| 2:O:234:LEU:C | 2:O:252:MET:N | 2.74 | 0.41 |
| 4:R:460:LEU:CB | 6:T:470:PRO:C | 2.89 | 0.41 |
| 7:V:551:HIS:C | 7:V:553:VAL:H | 2.24 | 0.41 |
| 7:V:1462:PHE:O | 7:V:1465:GLU:CB | 2.69 | 0.41 |
| 4:X:458:ASP:C | 4:X:459:LEU:C | 2.78 | 0.41 |
| 4:X:460:LEU:O | 4:X:461:ARG:O | 2.39 | 0.41 |
| 3:D:1502:ARG:O | 3:D:1503:ILE:C | 2.58 | 0.41 |
| 2:I:303:ALA:CB | 2:I:306:PRO:HA | 2.50 | 0.41 |
| 7:J:859:ILE:H | 7:J:865:PRO:CA | 2.33 | 0.41 |
| 6:N:463:ALA:N | 6:N:463:ALA:C | 2.65 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:T:408:SER:C | 6:T:410:LEU:N | 2.74 | 0.41 |
| 2:U:303:ALA:CB | 2:U:306:PRO:HA | 2.50 | 0.41 |
| 4:X:453:TYR:O | 4:X:455:ILE:N | 2.54 | 0.41 |
| 6:Z:408:SER:C | 6:Z:410:LEU:N | 2.74 | 0.41 |
| 3:D:1515:TYR:O | 3:D:1516:LEU:C | 2.57 | 0.41 |
| 7:J:1462:PHE:O | 7:J:1465:GLU:CB | 2.69 | 0.41 |
| 4:L:148:TRP:C | 4:L:150:THR:N | 2.74 | 0.41 |
| 4:L:460:LEU:CB | 6:N:470:PRO:C | 2.89 | 0.41 |
| 3:P:254:GLU:C | 3:P:256:VAL:H | 2.24 | 0.41 |
| 3:P:1563:VAL:O | 3:P:1569:GLY:HA3 | 2.21 | 0.41 |
| 2:C:173:PRO:CB | 3:D:1687:GLY:CA | 2.90 | 0.41 |
| 2:C:214:GLU:O | 2:C:215:LEU:CB | 2.68 | 0.41 |
| 2:C:535:TYR:N | 3:D:1663:GLN:HA | 2.31 | 0.41 |
| 3:D:254:GLU:C | 3:D:256:VAL:H | 2.24 | 0.41 |
| 3:D:1506:VAL:O | 3:D:1508:LYS:N | 2.47 | 0.41 |
| 3:D:1537:GLN:O | 3:D:1538:SER:C | 2.56 | 0.41 |
| 4:F:198:LYS:C | 4:F:200:THR:N | 2.58 | 0.41 |
| 6:H:493:ALA:O | 6:H:497:ARG:CB | 2.68 | 0.41 |
| 2:I:214:GLU:O | 2:I:215:LEU:CB | 2.68 | 0.41 |
| 7:J:860:TYR:CB | 7:J:868:PRO:N | 2.84 | 0.41 |
| 4:L:453:TYR:O | 4:L:455:ILE:N | 2.54 | 0.41 |
| 4:L:465:GLN:O | 4:L:466:HIS:C | 2.57 | 0.41 |
| 5:M:344:ASP:O | 5:M:348:ILE:N | 2.54 | 0.41 |
| 6:N:360:ALA:O | 6:N:363:ARG:CB | 2.69 | 0.41 |
| 6:N:408:SER:C | 6:N:410:LEU:N | 2.74 | 0.41 |
| 2:O:214:GLU:O | 2:O:215:LEU:CB | 2.68 | 0.41 |
| 1:Q:404:LYS:HA | 1:Q:405:PRO:HA | 1.70 | 0.41 |
| 5:S:318:GLU:C | 5:S:320:LYS:N | 2.71 | 0.41 |
| 6:T:490:GLN:CB | 6:T:490:GLN:O | 2.66 | 0.41 |
| 2:U:214:GLU:O | 2:U:215:LEU:CB | 2.68 | 0.41 |
| 1:W:1170:SER:C | 1:W:1172:GLN:H | 2.24 | 0.41 |
| 7:J:551:HIS:C | 7:J:553:VAL:H | 2.24 | 0.41 |
| 1:K:542:HIS:O | 1:K:543:GLN:CB | 2.69 | 0.41 |
| 4:L:329:GLY:N | 4:L:329:GLY:C | 2.62 | 0.41 |
| 3:P:1544:PRO:C | 3:P:1546:LEU:H | 2.24 | 0.41 |
| 1:Q:350:ASN:HA | 1:Q:353:SER:O | 2.21 | 0.41 |
| 4:R:460:LEU:O | 4:R:461:ARG:O | 2.38 | 0.41 |
| 5:S:344:ASP:O | 5:S:348:ILE:N | 2.54 | 0.41 |
| 5:Y:344:ASP:O | 5:Y:348:ILE:N | 2.54 | 0.41 |
| 3:D:1492:GLY:O | 3:D:1495:LEU:N | 2.53 | 0.40 |
| 1:E:852:VAL:HA | 2:O:305:LEU:CB | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:344:ASP:O | 5:G:348:ILE:N | 2.54 | 0.40 |
| 5:Y:379:HIS:N | 5:Y:379:HIS:CB | 2.72 | 0.40 |
| 6:Z:360:ALA:O | 6:Z:363:ARG:CB | 2.69 | 0.40 |
| 3:D:1539:LEU:O | 3:D:1540:LEU:C | 2.40 | 0.40 |
| 4:F:450:GLU:O | 4:F:451:GLU:CA | 2.33 | 0.40 |
| 5:M:318:GLU:C | 5:M:320:LYS:N | 2.71 | 0.40 |
| 4:R:455:ILE:C | 4:R:457:ALA:H | 2.15 | 0.40 |
| 7:V:860:TYR:CB | 7:V:868:PRO:N | 2.84 | 0.40 |
| 1:W:350:ASN:HA | 1:W:353:SER:O | 2.21 | 0.40 |
| 4:X:465:GLN:O | 4:X:466:HIS:C | 2.57 | 0.40 |
| 1:B:350:ASN:HA | 1:B:353:SER:O | 2.21 | 0.40 |
| 1:E:542:HIS:O | 1:E:543:GLN:CB | 2.69 | 0.40 |
| 5:G:325:ALA:C | 5:G:325:ALA:HA | 2.15 | 0.40 |
| 1:Q:1170:SER:C | 1:Q:1172:GLN:H | 2.24 | 0.40 |
| 6:T:490:GLN:HA | 6:T:493:ALA:H | 1.87 | 0.40 |
| 5:Y:318:GLU:C | 5:Y:320:LYS:N | 2.71 | 0.40 |
| 2:C:307:GLY:H | 1:Q:849:ASN:CB | 2.35 | 0.40 |
| 1:E:849:ASN:H | 2:O:303:ALA:HA | 1.87 | 0.40 |
| 7:J:155:ARG:CB | 7:J:158:TYR:CB | 3.00 | 0.40 |
| 7:J:1467:HIS:CB | 7:J:1475:ARG:CA | 2.96 | 0.40 |
| 3:P:1491:ILE:C | 3:P:1493:ARG:N | 2.72 | 0.40 |
| 4:X:459:LEU:C | 4:X:459:LEU:N | 2.63 | 0.40 |
| 5:Y:342:PRO:C | 5:Y:344:ASP:H | 2.25 | 0.40 |
| 1:A:542:HIS:O | 1:A:543:GLN:CB | 2.69 | 0.40 |
| 2:I:231:THR:C | 2:I:233:VAL:N | 2.75 | 0.40 |
| 7:J:1175:GLY:CA | 7:J:1197:GLN:N | 2.82 | 0.40 |
| 4:L:140:LYS:O | 4:L:149:GLY:CA | 2.70 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 612/1391 (44%) | 562 (92%) | 38 (6%) | 12 (2%) | 7 | 38 |
| 1 | B | 612/1391 (44%) | 562 (92%) | 38 (6%) | 12 (2%) | 7 | 38 |
| 1 | E | 1027/1391 (74%) | 947 (92%) | 58 (6%) | 22 (2%) | 7 | 36 |
| 1 | K | 1027/1391 (74%) | 947 (92%) | 58 (6%) | 22 (2%) | 7 | 36 |
| 1 | Q | 1027/1391 (74%) | 947 (92%) | 58 (6%) | 22 (2%) | 7 | 36 |
| 1 | W | 1027/1391 (74%) | 947 (92%) | 58 (6%) | 22 (2%) | 7 | 36 |
| 2 | C | 618/819 (76%) | 516 (84%) | 59 (10%) | 43 (7%) | 1 | 14 |
| 2 | I | 618/819 (76%) | 516 (84%) | 58 (9%) | 44 (7%) | 1 | 14 |
| 2 | O | 618/819 (76%) | 516 (84%) | 59 (10%) | 43 (7%) | 1 | 14 |
| 2 | U | 618/819 (76%) | 516 (84%) | 59 (10%) | 43 (7%) | 1 | 14 |
| 3 | D | 972/2012 (48%) | 899 (92%) | 59 (6%) | 14 (1%) | 11 | 46 |
| 3 | P | 972/2012 (48%) | 899 (92%) | 59 (6%) | 14 (1%) | 11 | 46 |
| 4 | F | 329/507 (65%) | 286 (87%) | 21 (6%) | 22 (7%) | 1 | 15 |
| 4 | L | 329/507 (65%) | 286 (87%) | 21 (6%) | 22 (7%) | 1 | 15 |
| 4 | R | 329/507 (65%) | 286 (87%) | 21 (6%) | 22 (7%) | 1 | 15 |
| 4 | X | 329/507 (65%) | 286 (87%) | 21 (6%) | 22 (7%) | 1 | 15 |
| 5 | G | 169/599 (28%) | 153 (90%) | 10 (6%) | 6 (4%) | 3 | 25 |
| 5 | M | 169/599 (28%) | 153 (90%) | 11 (6%) | 5 (3%) | 4 | 28 |
| 5 | S | 169/599 (28%) | 153 (90%) | 11 (6%) | 5 (3%) | 4 | 28 |
| 5 | Y | 169/599 (28%) | 153 (90%) | 11 (6%) | 5 (3%) | 4 | 28 |
| 6 | H | 167/522 (32%) | 152 (91%) | 8 (5%) | 7 (4%) | 3 | 22 |
| 6 | N | 167/522 (32%) | 152 (91%) | 8 (5%) | 7 (4%) | 3 | 22 |
| 6 | T | 167/522 (32%) | 152 (91%) | 8 (5%) | 7 (4%) | 3 | 22 |
| 6 | Z | 167/522 (32%) | 152 (91%) | 8 (5%) | 7 (4%) | 3 | 22 |
| 7 | J | 1232/1749 (70%) | 1111 (90%) | 75 (6%) | 46 (4%) | 3 | 24 |
| 7 | V | 1232/1749 (70%) | 1111 (90%) | 75 (6%) | 46 (4%) | 3 | 24 |
| All | All | 14872/25656 (58%) | 13360 (90%) | 970 (6%) | 542 (4%) | 6 | 25 |

All (542) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 332 | ARG |
| 1 | A | 443 | LYS |
| 1 | A | 543 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 802 | GLN |
| 1 | B | 332 | ARG |
| 1 | B | 443 | LYS |
| 1 | B | 543 | GLN |
| 1 | B | 802 | GLN |
| 2 | C | 24 | SER |
| 2 | C | 252 | MET |
| 2 | C | 278 | LEU |
| 2 | C | 301 | LEU |
| 2 | C | 382 | ASN |
| 2 | C | 383 | THR |
| 2 | C | 587 | LEU |
| 2 | C | 592 | SER |
| 2 | C | 603 | SER |
| 2 | C | 623 | GLU |
| 2 | C | 652 | GLN |
| 2 | C | 655 | ALA |
| 2 | C | 656 | PRO |
| 2 | C | 661 | GLU |
| 2 | C | 662 | ARG |
| 2 | C | 723 | ASN |
| 2 | C | 764 | LYS |
| 3 | D | 453 | ASN |
| 3 | D | 1451 | ARG |
| 3 | D | 1637 | GLN |
| 3 | D | 1662 | CYS |
| 3 | D | 1664 | ASP |
| 1 | E | 332 | ARG |
| 1 | E | 443 | LYS |
| 1 | E | 543 | GLN |
| 1 | E | 802 | GLN |
| 1 | E | 1320 | PRO |
| 1 | E | 1343 | ASN |
| 1 | E | 1351 | ASN |
| 1 | E | 1369 | SER |
| 4 | F | 148 | TRP |
| 4 | F | 222 | THR |
| 4 | F | 318 | ASP |
| 4 | F | 403 | ILE |
| 4 | F | 405 | ALA |
| 4 | F | 451 | GLU |
| 4 | F | 453 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | F | 454 | TYR |
| 4 | F | 458 | ASP |
| 4 | F | 464 | LYS |
| 5 | G | 276 | SER |
| 5 | G | 327 | ARG |
| 5 | G | 335 | LEU |
| 6 | H | 426 | ALA |
| 6 | H | 466 | ASP |
| 2 | I | 24 | SER |
| 2 | I | 252 | MET |
| 2 | I | 278 | LEU |
| 2 | I | 301 | LEU |
| 2 | I | 382 | ASN |
| 2 | I | 383 | THR |
| 2 | I | 587 | LEU |
| 2 | I | 592 | SER |
| 2 | I | 603 | SER |
| 2 | I | 623 | GLU |
| 2 | I | 652 | GLN |
| 2 | I | 655 | ALA |
| 2 | I | 656 | PRO |
| 2 | I | 661 | GLU |
| 2 | I | 662 | ARG |
| 2 | I | 723 | ASN |
| 2 | I | 764 | LYS |
| 7 | J | 30 | SER |
| 7 | J | 113 | GLN |
| 7 | J | 160 | ASP |
| 7 | J | 254 | VAL |
| 7 | J | 288 | ASP |
| 7 | J | 397 | LEU |
| 7 | J | 481 | LYS |
| 7 | J | 559 | ILE |
| 7 | J | 581 | SER |
| 7 | J | 660 | ALA |
| 7 | J | 755 | SER |
| 7 | J | 835 | SER |
| 7 | J | 883 | PRO |
| 7 | J | 1299 | ASP |
| 7 | J | 1388 | LEU |
| 7 | J | 1479 | VAL |
| 1 | K | 332 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 443 | LYS |
| 1 | K | 543 | GLN |
| 1 | K | 802 | GLN |
| 1 | K | 1320 | PRO |
| 1 | K | 1343 | ASN |
| 1 | K | 1351 | ASN |
| 1 | K | 1369 | SER |
| 4 | L | 148 | TRP |
| 4 | L | 222 | THR |
| 4 | L | 318 | ASP |
| 4 | L | 403 | ILE |
| 4 | L | 405 | ALA |
| 4 | L | 451 | GLU |
| 4 | L | 453 | TYR |
| 4 | L | 454 | TYR |
| 4 | L | 458 | ASP |
| 4 | L | 464 | LYS |
| 5 | M | 276 | SER |
| 5 | M | 327 | ARG |
| 5 | M | 335 | LEU |
| 6 | N | 426 | ALA |
| 6 | N | 466 | ASP |
| 2 | O | 24 | SER |
| 2 | O | 252 | MET |
| 2 | O | 278 | LEU |
| 2 | O | 301 | LEU |
| 2 | O | 382 | ASN |
| 2 | O | 383 | THR |
| 2 | O | 587 | LEU |
| 2 | O | 592 | SER |
| 2 | O | 603 | SER |
| 2 | O | 623 | GLU |
| 2 | O | 652 | GLN |
| 2 | O | 655 | ALA |
| 2 | O | 656 | PRO |
| 2 | O | 661 | GLU |
| 2 | O | 662 | ARG |
| 2 | O | 723 | ASN |
| 2 | O | 764 | LYS |
| 3 | P | 453 | ASN |
| 3 | P | 1451 | ARG |
| 3 | P | 1637 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 1662 | CYS |
| 3 | P | 1664 | ASP |
| 1 | Q | 332 | ARG |
| 1 | Q | 443 | LYS |
| 1 | Q | 543 | GLN |
| 1 | Q | 802 | GLN |
| 1 | Q | 1320 | PRO |
| 1 | Q | 1343 | ASN |
| 1 | Q | 1351 | ASN |
| 1 | Q | 1369 | SER |
| 4 | R | 148 | TRP |
| 4 | R | 222 | THR |
| 4 | R | 318 | ASP |
| 4 | R | 403 | ILE |
| 4 | R | 405 | ALA |
| 4 | R | 451 | GLU |
| 4 | R | 453 | TYR |
| 4 | R | 454 | TYR |
| 4 | R | 458 | ASP |
| 4 | R | 464 | LYS |
| 5 | S | 276 | SER |
| 5 | S | 327 | ARG |
| 5 | S | 335 | LEU |
| 6 | T | 426 | ALA |
| 6 | T | 466 | ASP |
| 2 | U | 24 | SER |
| 2 | U | 252 | MET |
| 2 | U | 278 | LEU |
| 2 | U | 301 | LEU |
| 2 | U | 382 | ASN |
| 2 | U | 383 | THR |
| 2 | U | 587 | LEU |
| 2 | U | 592 | SER |
| 2 | U | 603 | SER |
| 2 | U | 623 | GLU |
| 2 | U | 652 | GLN |
| 2 | U | 655 | ALA |
| 2 | U | 656 | PRO |
| 2 | U | 661 | GLU |
| 2 | U | 662 | ARG |
| 2 | U | 723 | ASN |
| 2 | U | 764 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | V | 30 | SER |
| 7 | V | 113 | GLN |
| 7 | V | 160 | ASP |
| 7 | V | 254 | VAL |
| 7 | V | 288 | ASP |
| 7 | V | 397 | LEU |
| 7 | V | 481 | LYS |
| 7 | V | 559 | ILE |
| 7 | V | 581 | SER |
| 7 | V | 660 | ALA |
| 7 | V | 755 | SER |
| 7 | V | 835 | SER |
| 7 | V | 883 | PRO |
| 7 | V | 1299 | ASP |
| 7 | V | 1388 | LEU |
| 7 | V | 1479 | VAL |
| 1 | W | 332 | ARG |
| 1 | W | 443 | LYS |
| 1 | W | 543 | GLN |
| 1 | W | 802 | GLN |
| 1 | W | 1320 | PRO |
| 1 | W | 1343 | ASN |
| 1 | W | 1351 | ASN |
| 1 | W | 1369 | SER |
| 4 | X | 148 | TRP |
| 4 | X | 222 | THR |
| 4 | X | 318 | ASP |
| 4 | X | 403 | ILE |
| 4 | X | 405 | ALA |
| 4 | X | 451 | GLU |
| 4 | X | 453 | TYR |
| 4 | X | 454 | TYR |
| 4 | X | 458 | ASP |
| 4 | X | 464 | LYS |
| 5 | Y | 276 | SER |
| 5 | Y | 327 | ARG |
| 5 | Y | 335 | LEU |
| 6 | Z | 426 | ALA |
| 6 | Z | 466 | ASP |
| 1 | A | 260 | SER |
| 1 | A | 312 | MET |
| 1 | A | 415 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 260 | SER |
| 1 | B | 312 | MET |
| 1 | B | 415 | LYS |
| 2 | C | 23 | ILE |
| 2 | C | 179 | ASP |
| 2 | C | 215 | LEU |
| 2 | C | 219 | SER |
| 2 | C | 354 | GLU |
| 2 | C | 368 | GLU |
| 2 | C | 402 | ASN |
| 2 | C | 404 | SER |
| 2 | C | 559 | ASP |
| 2 | C | 602 | THR |
| 2 | C | 649 | VAL |
| 2 | C | 679 | ILE |
| 2 | C | 726 | SER |
| 2 | C | 754 | ASN |
| 3 | D | 39 | LEU |
| 3 | D | 881 | GLN |
| 1 | E | 260 | SER |
| 1 | E | 312 | MET |
| 1 | E | 415 | LYS |
| 1 | E | 961 | GLY |
| 1 | E | 1235 | LEU |
| 1 | E | 1346 | ARG |
| 4 | F | 204 | SER |
| 4 | F | 221 | GLN |
| 4 | F | 301 | PRO |
| 4 | F | 461 | ARG |
| 4 | F | 492 | GLU |
| 5 | G | 326 | LEU |
| 5 | G | 378 | SER |
| 6 | H | 411 | GLU |
| 6 | H | 494 | LEU |
| 2 | I | 23 | ILE |
| 2 | I | 179 | ASP |
| 2 | I | 215 | LEU |
| 2 | I | 219 | SER |
| 2 | I | 354 | GLU |
| 2 | I | 368 | GLU |
| 2 | I | 402 | ASN |
| 2 | I | 404 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 559 | ASP |
| 2 | I | 602 | THR |
| 2 | I | 649 | VAL |
| 2 | I | 679 | ILE |
| 2 | I | 726 | SER |
| 2 | I | 754 | ASN |
| 7 | J | 157 | GLU |
| 7 | J | 367 | SER |
| 7 | J | 506 | GLY |
| 7 | J | 552 | VAL |
| 7 | J | 834 | VAL |
| 7 | J | 845 | GLY |
| 7 | J | 1245 | LEU |
| 7 | J | 1312 | ILE |
| 7 | J | 1323 | SER |
| 7 | J | 1519 | GLN |
| 1 | K | 260 | SER |
| 1 | K | 312 | MET |
| 1 | K | 415 | LYS |
| 1 | K | 961 | GLY |
| 1 | K | 1235 | LEU |
| 1 | K | 1346 | ARG |
| 4 | L | 204 | SER |
| 4 | L | 221 | GLN |
| 4 | L | 301 | PRO |
| 4 | L | 461 | ARG |
| 4 | L | 492 | GLU |
| 5 | M | 326 | LEU |
| 5 | M | 378 | SER |
| 6 | N | 411 | GLU |
| 6 | N | 494 | LEU |
| 2 | O | 23 | ILE |
| 2 | O | 179 | ASP |
| 2 | O | 215 | LEU |
| 2 | O | 219 | SER |
| 2 | O | 354 | GLU |
| 2 | O | 368 | GLU |
| 2 | O | 402 | ASN |
| 2 | O | 404 | SER |
| 2 | O | 559 | ASP |
| 2 | O | 602 | THR |
| 2 | O | 649 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | O | 679 | ILE |
| 2 | O | 726 | SER |
| 2 | O | 754 | ASN |
| 3 | P | 39 | LEU |
| 3 | P | 881 | GLN |
| 1 | Q | 260 | SER |
| 1 | Q | 312 | MET |
| 1 | Q | 415 | LYS |
| 1 | Q | 961 | GLY |
| 1 | Q | 1235 | LEU |
| 1 | Q | 1346 | ARG |
| 4 | R | 204 | SER |
| 4 | R | 221 | GLN |
| 4 | R | 301 | PRO |
| 4 | R | 461 | ARG |
| 4 | R | 492 | GLU |
| 5 | S | 326 | LEU |
| 5 | S | 378 | SER |
| 6 | T | 411 | GLU |
| 6 | T | 494 | LEU |
| 2 | U | 23 | ILE |
| 2 | U | 179 | ASP |
| 2 | U | 215 | LEU |
| 2 | U | 219 | SER |
| 2 | U | 354 | GLU |
| 2 | U | 368 | GLU |
| 2 | U | 402 | ASN |
| 2 | U | 404 | SER |
| 2 | U | 559 | ASP |
| 2 | U | 602 | THR |
| 2 | U | 649 | VAL |
| 2 | U | 679 | ILE |
| 2 | U | 726 | SER |
| 2 | U | 754 | ASN |
| 7 | V | 157 | GLU |
| 7 | V | 367 | SER |
| 7 | V | 506 | GLY |
| 7 | V | 552 | VAL |
| 7 | V | 834 | VAL |
| 7 | V | 845 | GLY |
| 7 | V | 1245 | LEU |
| 7 | V | 1312 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | V | 1323 | SER |
| 7 | V | 1519 | GLN |
| 1 | W | 260 | SER |
| 1 | W | 312 | MET |
| 1 | W | 415 | LYS |
| 1 | W | 961 | GLY |
| 1 | W | 1235 | LEU |
| 1 | W | 1346 | ARG |
| 4 | X | 204 | SER |
| 4 | X | 221 | GLN |
| 4 | X | 301 | PRO |
| 4 | X | 461 | ARG |
| 4 | X | 492 | GLU |
| 5 | Y | 326 | LEU |
| 5 | Y | 378 | SER |
| 6 | Z | 411 | GLU |
| 6 | Z | 494 | LEU |
| 1 | A | 204 | PRO |
| 1 | B | 204 | PRO |
| 2 | C | 308 | LEU |
| 2 | C | 482 | MET |
| 2 | C | 734 | PHE |
| 3 | D | 437 | ARG |
| 1 | E | 204 | PRO |
| 1 | E | 1365 | GLN |
| 4 | F | 299 | ASN |
| 6 | H | 465 | ALA |
| 2 | I | 308 | LEU |
| 2 | I | 482 | MET |
| 2 | I | 734 | PHE |
| 7 | J | 425 | PRO |
| 7 | J | 697 | SER |
| 7 | J | 1220 | LYS |
| 7 | J | 1328 | GLN |
| 7 | J | 1373 | SER |
| 7 | J | 1377 | THR |
| 7 | J | 1466 | TRP |
| 1 | K | 204 | PRO |
| 1 | K | 1365 | GLN |
| 4 | L | 299 | ASN |
| 6 | N | 465 | ALA |
| 2 | O | 308 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | O | 482 | MET |
| 2 | O | 734 | PHE |
| 3 | P | 437 | ARG |
| 1 | Q | 204 | PRO |
| 1 | Q | 1365 | GLN |
| 4 | R | 299 | ASN |
| 6 | T | 465 | ALA |
| 2 | U | 308 | LEU |
| 2 | U | 482 | MET |
| 2 | U | 734 | PHE |
| 7 | V | 425 | PRO |
| 7 | V | 697 | SER |
| 7 | V | 1220 | LYS |
| 7 | V | 1328 | GLN |
| 7 | V | 1373 | SER |
| 7 | V | 1377 | THR |
| 7 | V | 1466 | TRP |
| 1 | W | 204 | PRO |
| 1 | W | 1365 | GLN |
| 4 | X | 299 | ASN |
| 6 | Z | 465 | ALA |
| 1 | A | 40 | TYR |
| 1 | B | 40 | TYR |
| 2 | C | 446 | GLU |
| 2 | C | 561 | GLN |
| 3 | D | 637 | SER |
| 3 | D | 1450 | GLU |
| 1 | E | 40 | TYR |
| 4 | F | 206 | GLN |
| 4 | F | 234 | PRO |
| 4 | F | 450 | GLU |
| 4 | F | 459 | LEU |
| 2 | I | 446 | GLU |
| 2 | I | 561 | GLN |
| 7 | J | 414 | PRO |
| 7 | J | 420 | PHE |
| 7 | J | 640 | PRO |
| 7 | J | 1325 | ARG |
| 7 | J | 1542 | SER |
| 1 | K | 40 | TYR |
| 4 | L | 206 | GLN |
| 4 | L | 234 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | L | 450 | GLU |
| 4 | L | 459 | LEU |
| 2 | O | 446 | GLU |
| 2 | O | 561 | GLN |
| 3 | P | 637 | SER |
| 3 | P | 1450 | GLU |
| 1 | Q | 40 | TYR |
| 4 | R | 206 | GLN |
| 4 | R | 234 | PRO |
| 4 | R | 450 | GLU |
| 4 | R | 459 | LEU |
| 2 | U | 446 | GLU |
| 2 | U | 561 | GLN |
| 7 | V | 414 | PRO |
| 7 | V | 420 | PHE |
| 7 | V | 640 | PRO |
| 7 | V | 1325 | ARG |
| 7 | V | 1542 | SER |
| 1 | W | 40 | TYR |
| 4 | X | 234 | PRO |
| 4 | X | 450 | GLU |
| 4 | X | 459 | LEU |
| 6 | Z | 497 | ARG |
| 1 | A | 278 | PRO |
| 1 | B | 278 | PRO |
| 2 | C | 460 | PHE |
| 2 | C | 800 | PRO |
| 3 | D | 58 | PRO |
| 3 | D | 536 | VAL |
| 3 | D | 659 | ILE |
| 3 | D | 1519 | SER |
| 1 | E | 278 | PRO |
| 1 | E | 910 | GLN |
| 4 | F | 145 | GLN |
| 6 | H | 464 | PRO |
| 6 | H | 497 | ARG |
| 2 | I | 460 | PHE |
| 2 | I | 800 | PRO |
| 7 | J | 151 | ARG |
| 7 | J | 1437 | VAL |
| 1 | K | 278 | PRO |
| 1 | K | 910 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | N | 464 | PRO |
| 6 | N | 497 | ARG |
| 2 | O | 460 | PHE |
| 2 | O | 800 | PRO |
| 3 | P | 58 | PRO |
| 3 | P | 536 | VAL |
| 3 | P | 659 | ILE |
| 3 | P | 1519 | SER |
| 1 | Q | 278 | PRO |
| 1 | Q | 910 | GLN |
| 6 | T | 464 | PRO |
| 6 | T | 497 | ARG |
| 2 | U | 460 | PHE |
| 2 | U | 800 | PRO |
| 7 | V | 151 | ARG |
| 7 | V | 1437 | VAL |
| 1 | W | 278 | PRO |
| 1 | W | 910 | GLN |
| 4 | X | 206 | GLN |
| 6 | Z | 464 | PRO |
| 1 | A | 158 | GLN |
| 1 | B | 158 | GLN |
| 2 | C | 22 | GLY |
| 2 | C | 31 | ARG |
| 2 | C | 429 | SER |
| 1 | E | 158 | GLN |
| 5 | G | 377 | ASN |
| 2 | I | 22 | GLY |
| 2 | I | 31 | ARG |
| 2 | I | 429 | SER |
| 7 | J | 482 | PRO |
| 7 | J | 1176 | SER |
| 1 | K | 158 | GLN |
| 4 | L | 145 | GLN |
| 2 | O | 22 | GLY |
| 2 | O | 31 | ARG |
| 2 | O | 429 | SER |
| 1 | Q | 158 | GLN |
| 4 | R | 145 | GLN |
| 2 | U | 22 | GLY |
| 2 | U | 31 | ARG |
| 2 | U | 429 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | V | 482 | PRO |
| 7 | V | 1176 | SER |
| 1 | W | 158 | GLN |
| 4 | X | 145 | GLN |
| 2 | C | 430 | SER |
| 2 | I | 430 | SER |
| 2 | O | 430 | SER |
| 2 | U | 430 | SER |
| 7 | J | 156 | VAL |
| 7 | J | 582 | ILE |
| 7 | V | 156 | VAL |
| 7 | V | 582 | ILE |
| 1 | E | 942 | PRO |
| 1 | K | 942 | PRO |
| 1 | Q | 942 | PRO |
| 1 | W | 942 | PRO |
| 1 | A | 76 | PRO |
| 1 | B | 76 | PRO |
| 2 | C | 276 | GLY |
| 1 | E | 76 | PRO |
| 2 | I | 276 | GLY |
| 7 | J | 368 | GLY |
| 7 | J | 1221 | VAL |
| 1 | K | 76 | PRO |
| 2 | O | 276 | GLY |
| 1 | Q | 76 | PRO |
| 2 | U | 276 | GLY |
| 7 | V | 368 | GLY |
| 7 | V | 1221 | VAL |
| 1 | W | 76 | PRO |
| 4 | F | 424 | PRO |
| 2 | I | 346 | GLY |
| 4 | L | 424 | PRO |
| 4 | R | 424 | PRO |
| 4 | X | 424 | PRO |

### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 4 | F | 6 |
| 4 | L | 6 |
| 4 | R | 6 |
| 4 | X | 6 |
| 2 | C | 3 |
| 2 | I | 3 |
| 2 | O | 3 |
| 2 | U | 3 |
| 5 | M | 3 |
| 5 | Y | 3 |
| 5 | G | 3 |
| 5 | S | 3 |
| 6 | H | 3 |
| 6 | N | 3 |
| 6 | T | 3 |
| 6 | Z | 3 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 483:GLU | C | 484:ARG | N | 4.02 |
| 1 | I | 483:GLU | C | 484:ARG | N | 4.02 |
| 1 | O | 483:GLU | C | 484:ARG | N | 4.02 |
| 1 | U | 483:GLU | C | 484:ARG | N | 4.02 |
| 1 | C | 447:ASP | C | 448:TYR | N | 3.63 |
| 1 | I | 447:ASP | C | 448:TYR | N | 3.63 |
| 1 | O | 447:ASP | C | 448:TYR | N | 3.63 |
| 1 | U | 447:ASP | C | 448:TYR | N | 3.63 |
| 1 | M | 379:HIS | C | 380:ILE | N | 1.99 |
| 1 | Y | 379:HIS | C | 380:ILE | N | 1.99 |
| 1 | G | 379:HIS | C | 380:ILE | N | 1.98 |
| 1 | S | 379:HIS | C | 380:ILE | N | 1.98 |
| 1 | F | 458:ASP | C | 459:LEU | N | 1.82 |
| 1 | L | 458:ASP | C | 459:LEU | N | 1.82 |
| 1 | R | 458:ASP | C | 459:LEU | N | 1.82 |
| 1 | X | 458:ASP | C | 459:LEU | N | 1.82 |
| 1 | G | 339:TYR | C | 340:ALA | N | 1.72 |
| 1 | M | 339:TYR | C | 340:ALA | N | 1.72 |
| 1 | S | 339:TYR | C | 340:ALA | N | 1.72 |
| 1 | Y | 339:TYR | C | 340:ALA | N | 1.72 |
| 1 | F | 492:GLU | C | 493:HIS | N | 1.69 |
| 1 | H | 411:GLU | C | 412:GLU | N | 1.69 |
| 1 | L | 492:GLU | C | 493:HIS | N | 1.69 |
| 1 | N | 411:GLU | C | 412:GLU | N | 1.69 |
| 1 | R | 492:GLU | C | 493:HIS | N | 1.69 |
| 1 | T | 411:GLU | C | 412:GLU | N | 1.69 |
| 1 | X | 492:GLU | C | 493:HIS | N | 1.69 |
| 1 | Z | 411:GLU | C | 412:GLU | N | 1.69 |
| 1 | F | 454:TYR | C | 455:ILE | N | 1.64 |
| 1 | L | 454:TYR | C | 455:ILE | N | 1.64 |
| 1 | R | 454:TYR | C | 455:ILE | N | 1.64 |
| 1 | X | 454:TYR | C | 455:ILE | N | 1.63 |
| 1 | F | 221:GLN | C | 222:THR | N | 1.61 |
| 1 | L | 221:GLN | C | 222:THR | N | 1.61 |
| 1 | R | 221:GLN | C | 222:THR | N | 1.61 |
| 1 | X | 221:GLN | C | 222:THR | N | 1.61 |
| 1 | G | 378:SER | C | 379:HIS | N | 1.60 |
| 1 | M | 378:SER | C | 379:HIS | N | 1.60 |
| 1 | S | 378:SER | C | 379:HIS | N | 1.60 |
| 1 | Y | 378:SER | C | 379:HIS | N | 1.60 |
| 1 | H | 412:GLU | C | 413:LEU | N | 1.16 |
| 1 | N | 412:GLU | C | 413:LEU | N | 1.16 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | T | 412:GLU | C | 413:LEU | N | 1.16 |
| 1 | Z | 412:GLU | C | 413:LEU | N | 1.16 |
| 1 | C | 7:GLY | C | 8:GLU | N | 1.14 |
| 1 | I | 7:GLY | C | 8:GLU | N | 1.14 |
| 1 | O | 7:GLY | C | 8:GLU | N | 1.14 |
| 1 | U | 7:GLY | C | 8:GLU | N | 1.14 |
| 1 | H | 408:SER | C | 409:PRO | N | 1.13 |
| 1 | N | 408:SER | C | 409:PRO | N | 1.13 |
| 1 | T | 408:SER | C | 409:PRO | N | 1.13 |
| 1 | Z | 408:SER | C | 409:PRO | N | 1.13 |
| 1 | F | 455:ILE | C | 456:ASP | N | 0.99 |
| 1 | L | 455:ILE | C | 456:ASP | N | 0.99 |
| 1 | R | 455:ILE | C | 456:ASP | N | 0.99 |
| 1 | X | 455:ILE | C | 456:ASP | N | 0.99 |
| 1 | F | 459:LEU | C | 460:LEU | N | 0.98 |
| 1 | L | 459:LEU | C | 460:LEU | N | 0.98 |
| 1 | R | 459:LEU | C | 460:LEU | N | 0.98 |
| 1 | X | 459:LEU | C | 460:LEU | N | 0.98 |

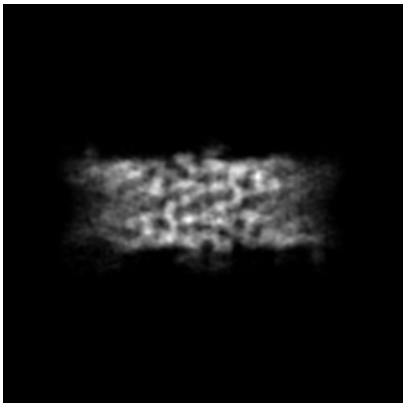
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8085. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

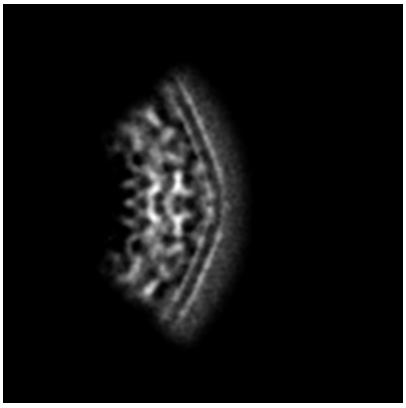
## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map



X

Y



Z

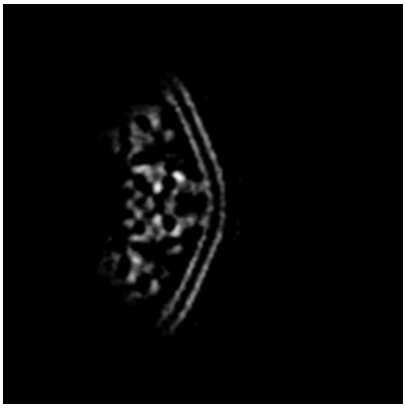
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

### 6.2.1 Primary map

X Index: 72

Y Index: 72

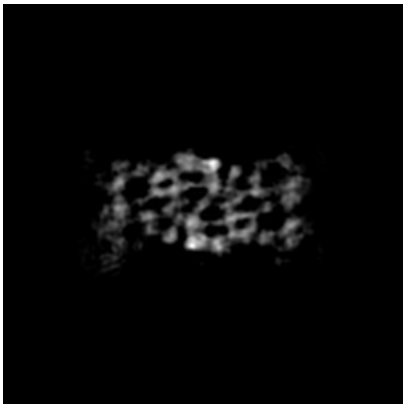


Z Index: 72

The images above show central slices of the map in three orthogonal directions.

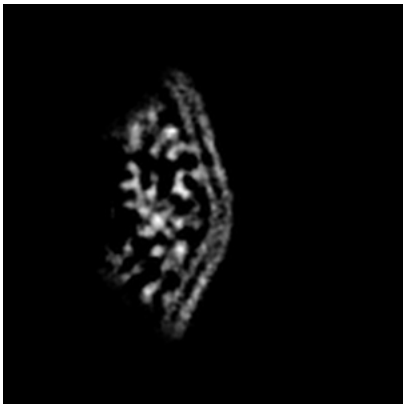
## 6.3 Largest variance slices (i)

### 6.3.1 Primary map



X Index: 53

Y Index: 76



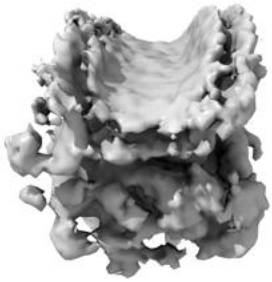
Z Index: 78

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 36.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

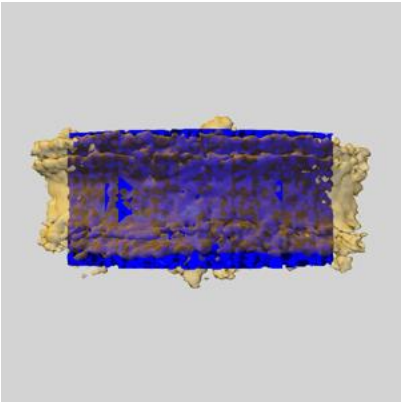
## 6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

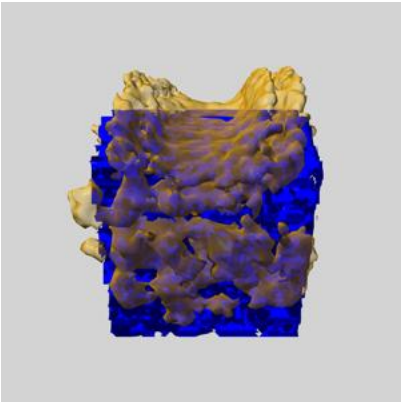
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

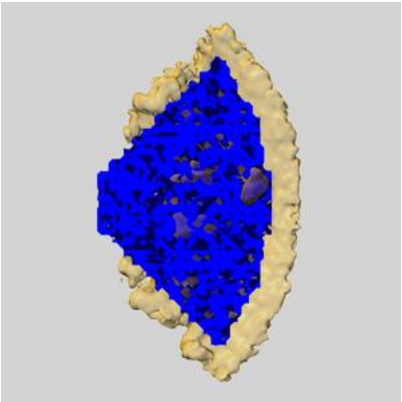
### 6.5.1 emd_8085_msk_1.map (i)



X



Y

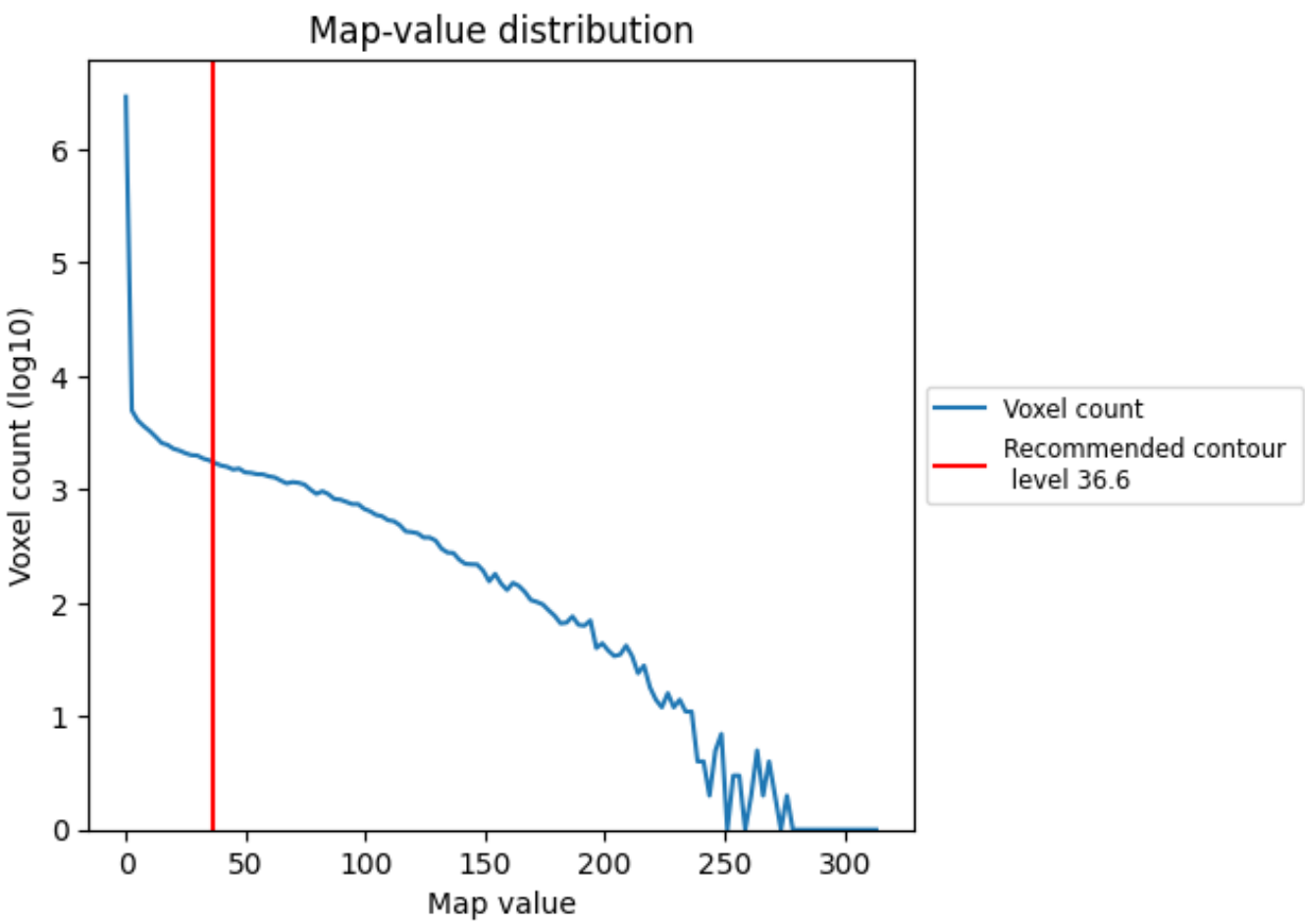


Z

# 7 Map analysis (i)

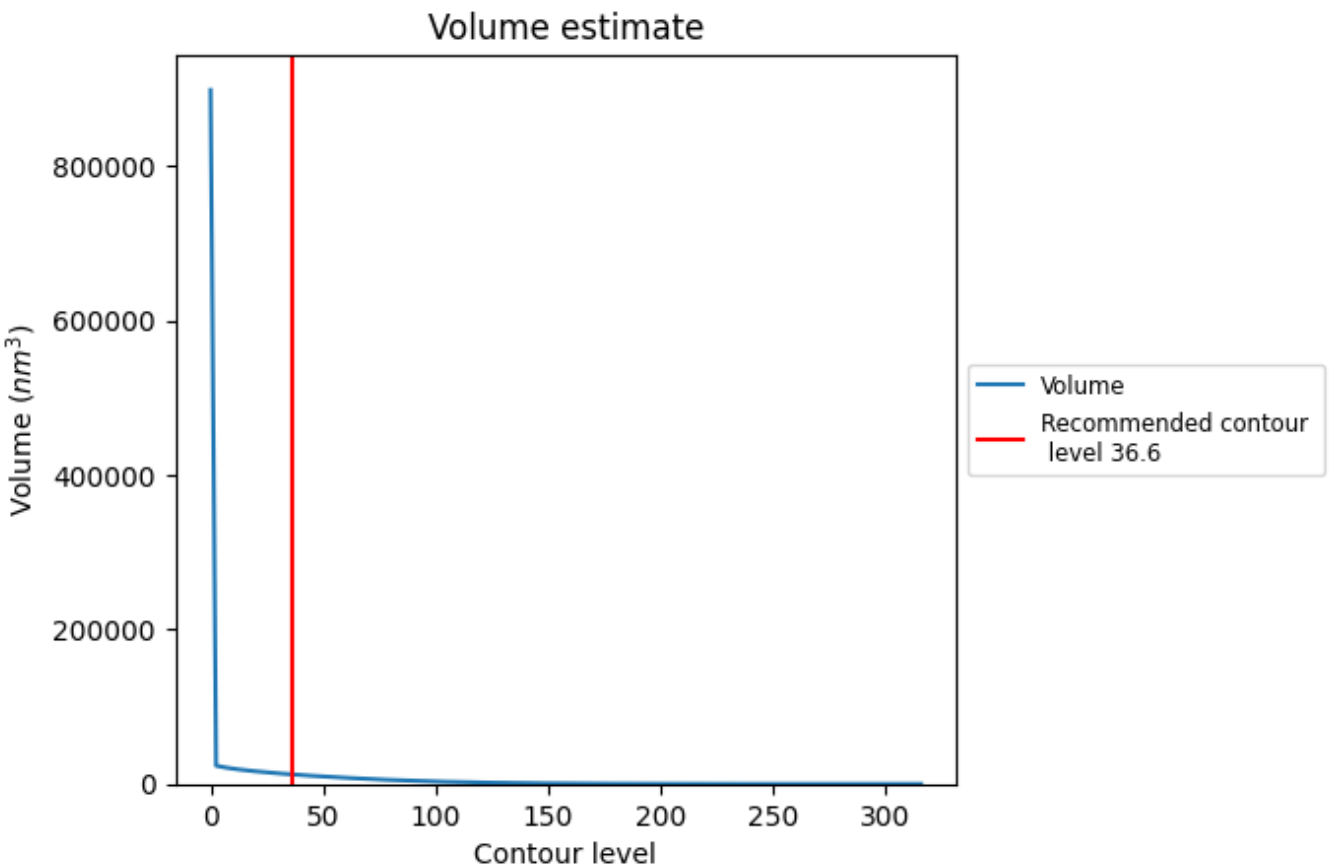
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

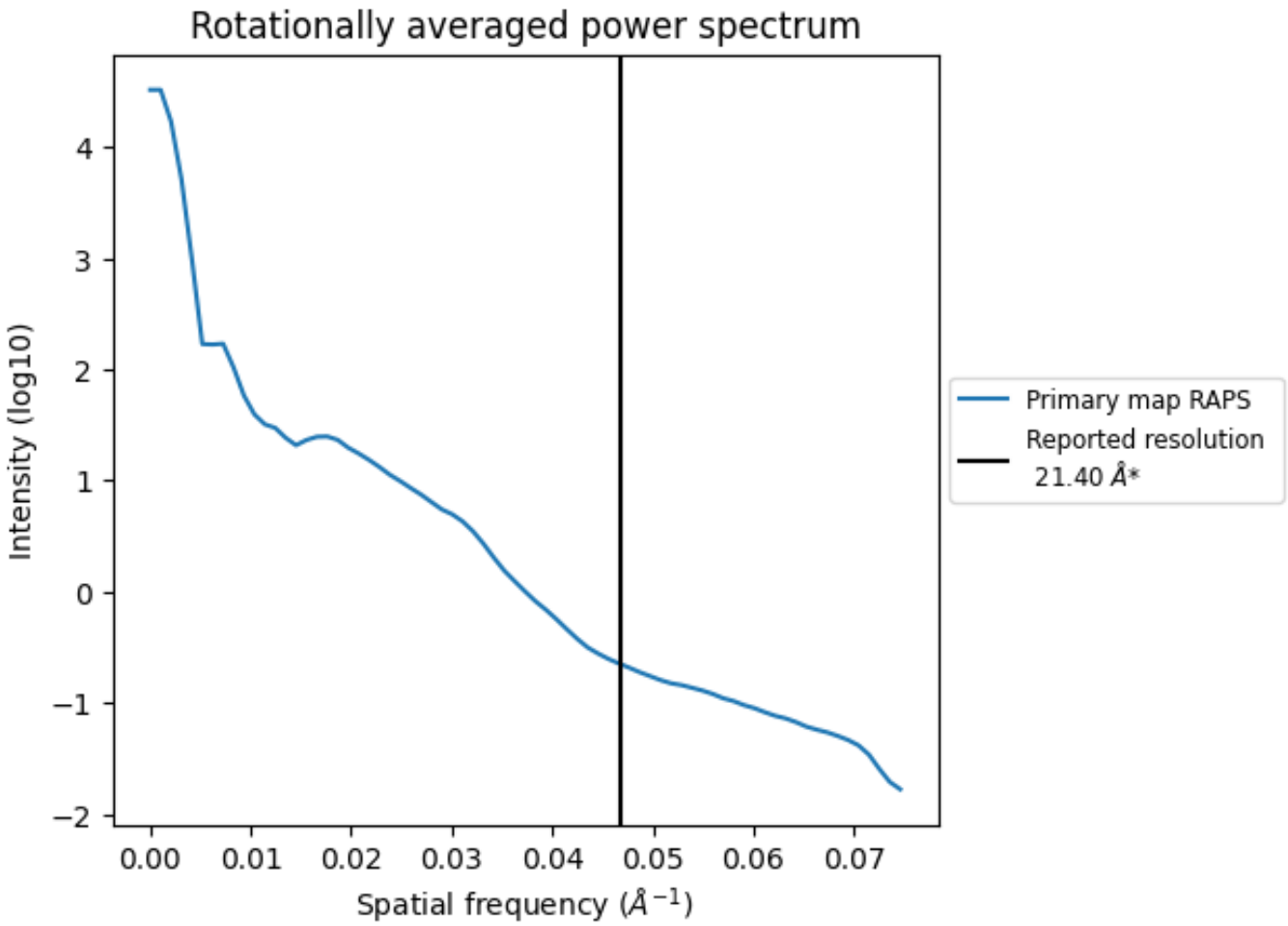
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 12255 $nm^3$; this corresponds to an approximate mass of 11070 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.047 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

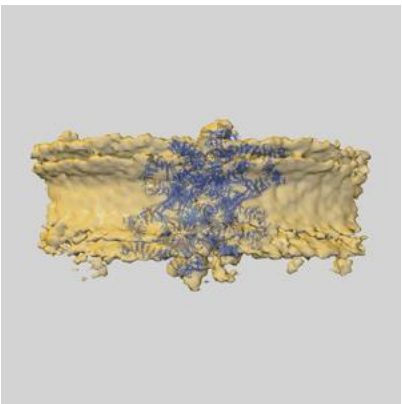
This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit (i)

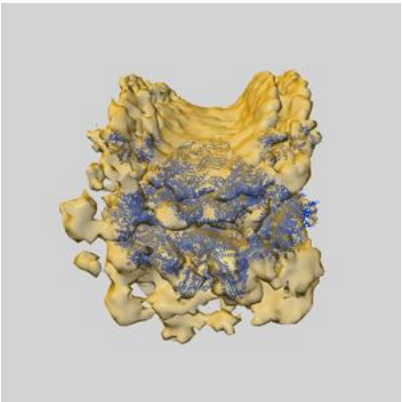
This section contains information regarding the fit between EMDB map EMD-8085 and PDB model 5IJO. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlays

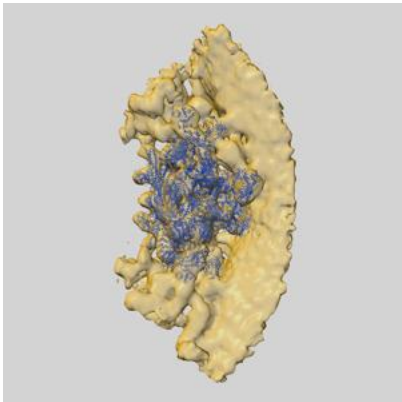
### 9.1.1 Map-model overlay (i)



X

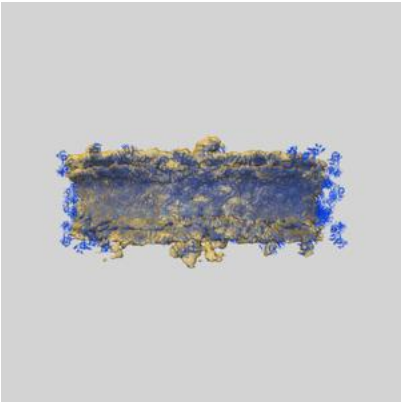


Y

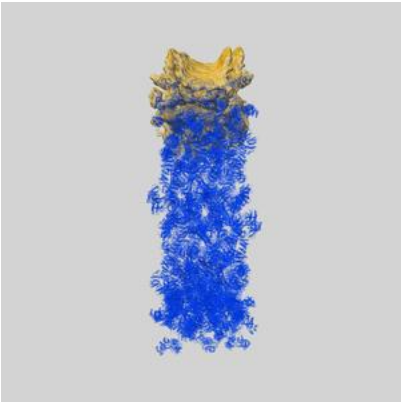


Z

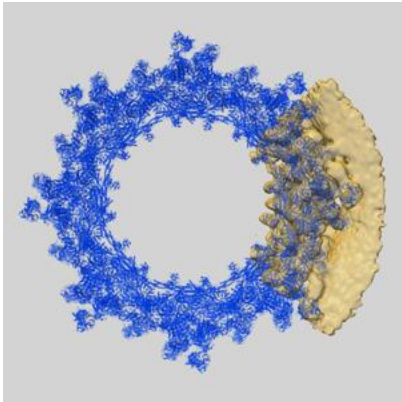
### 9.1.2 Map-model assembly overlay (i)



X



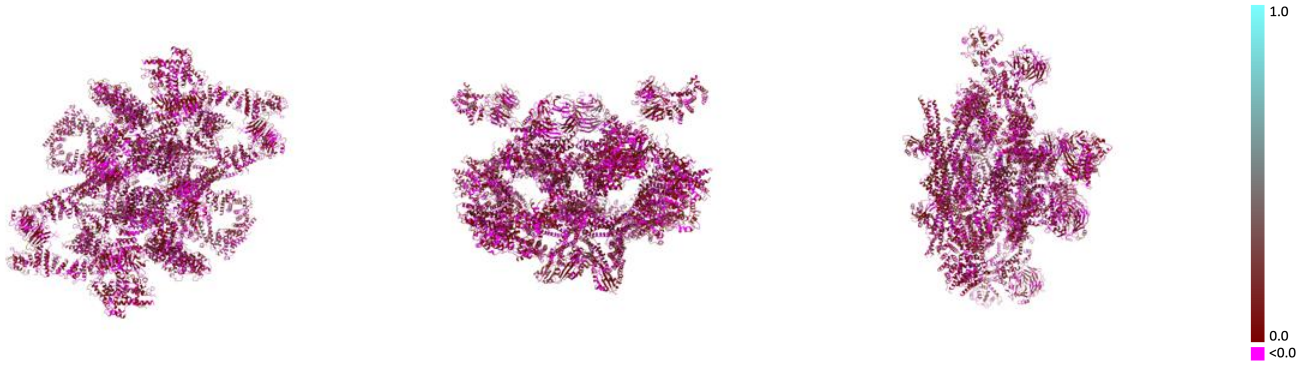
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 36.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

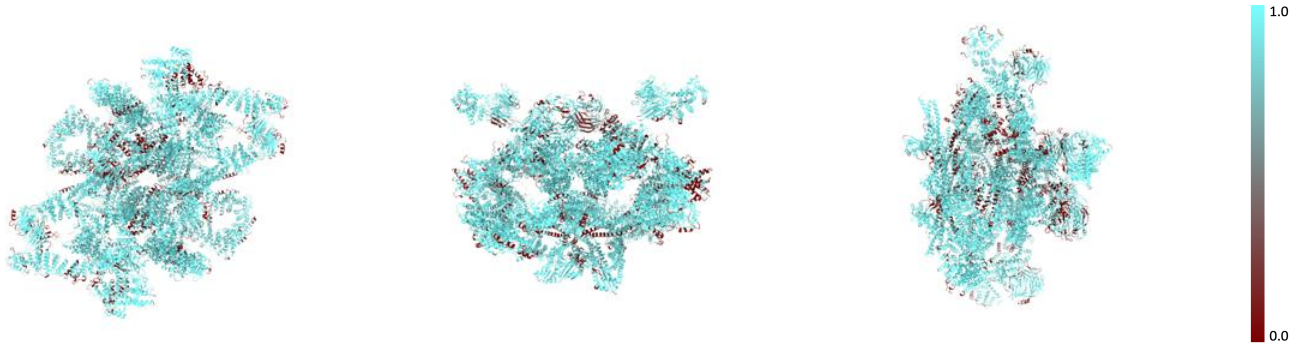
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

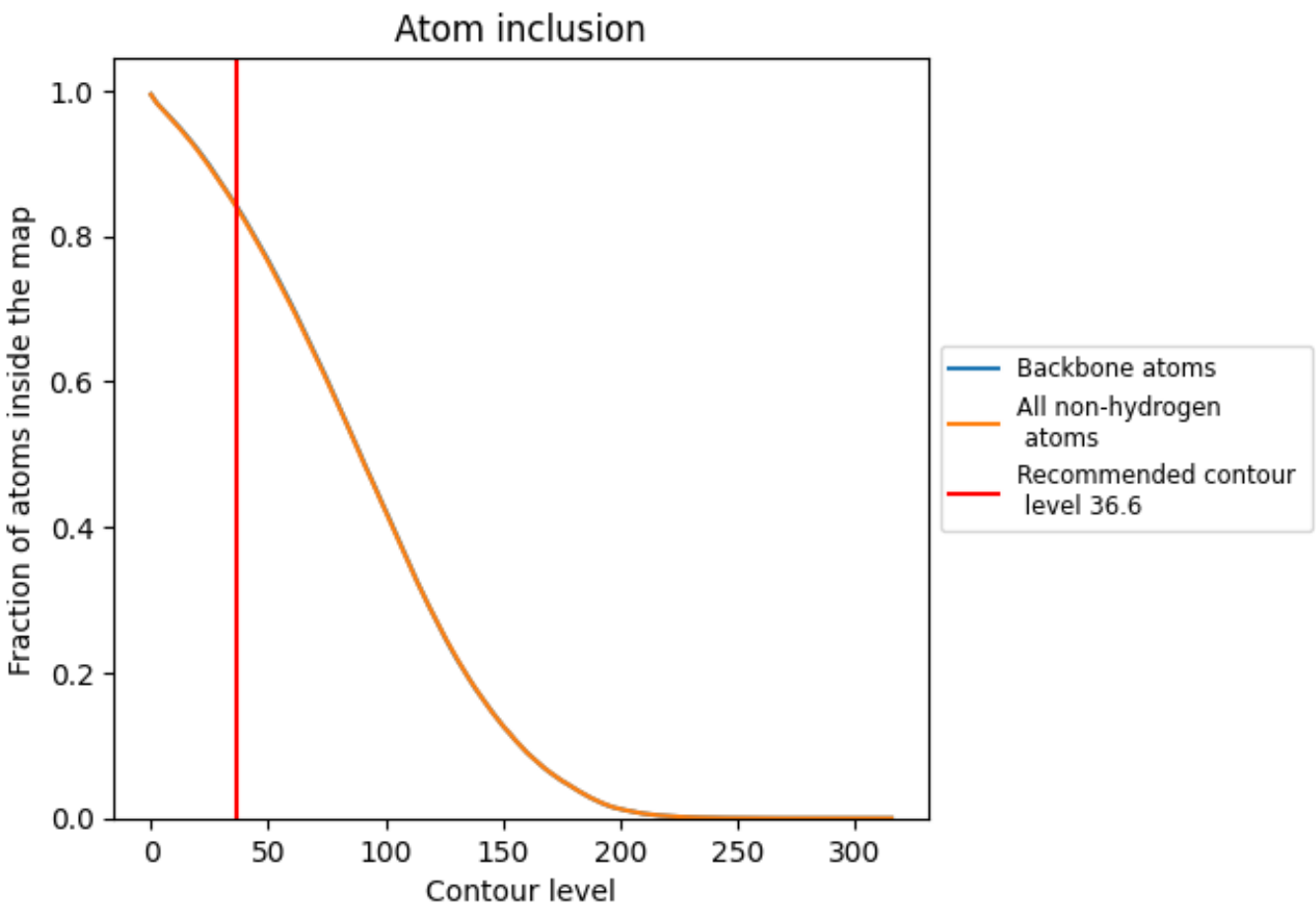
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (36.6).

## 9.4 Atom inclusion (i)




At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (36.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8392 | 0.0440 |
| A | 0.9291 | 0.0440 |
| B | 0.8787 | 0.0450 |
| C | 0.8493 | 0.0410 |
| D | 0.8983 | 0.0470 |
| E | 0.8658 | 0.0410 |
| F | 0.8100 | 0.0380 |
| G | 0.9039 | 0.0460 |
| H | 0.7993 | 0.0310 |
| I | 0.8271 | 0.0510 |
| J | 0.8785 | 0.0530 |
| K | 0.5460 | 0.0190 |
| L | 0.7986 | 0.0280 |
| M | 0.8453 | 0.0490 |
| N | 0.8729 | 0.0700 |
| O | 0.8782 | 0.0470 |
| P | 0.8971 | 0.0560 |
| Q | 0.8813 | 0.0440 |
| R | 0.7762 | 0.0310 |
| S | 0.9332 | 0.0600 |
| T | 0.7482 | 0.0470 |
| U | 0.8004 | 0.0440 |
| V | 0.9036 | 0.0520 |
| W | 0.7753 | 0.0350 |
| X | 0.8372 | 0.0380 |
| Y | 0.9004 | 0.0550 |
| Z | 0.8492 | 0.0460 |