# Full wwPDB EM Validation Report (i)

Nov 8, 2022 – 07:54 AM JST

| | | |
|---|---|---|
| PDB ID | : | 5YWP |
| EMDB ID | : | EMD-6855 |
| Title | : | JEV-2H4 Fab complex |
| Authors | : | Qiu, X.D.; Lei, Y.F.; Yang, P.; Gao, Q.; WANG, N.; Cao, L.; Yuan, S.; Wang, X.X.; Xu, Z.K.; Rao, Z.H. |
| Deposited on | : | 2017-11-29 |
| Resolution | : | 4.60 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:

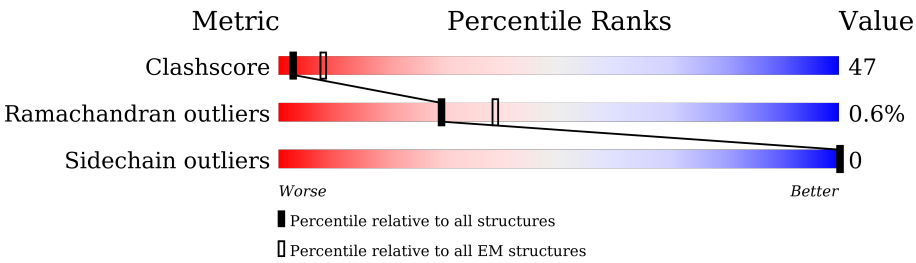
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 4.60 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 |
| Sidechain outliers | 154315 | 3826 |

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 | 500 | 82% 35% 64% |
| 1 | C | 500 | 83% 37% 62% . |
| 1 | E | 500 | 89% 29% 70% . |
| 2 | B | 74 | 88% 53% 46% . |
| 2 | D | 74 | 95% 47% 50% . |
| 2 | F | 74 | 97% 38% 61% . |
| 3 | M | 215 | 81% 29% 70% . |
| 3 | Q | 215 | 47% 24% 75% . |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | N | 218 | 34% 31% 69% |
| 4 | R | 218 | 57% 27% 72% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19561 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 JEV E protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 500 | 3753 | 2369 | 650 | 709 | 25 | 0 | 0 |
| 1 | C | 500 | 3753 | 2369 | 650 | 709 | 25 | 0 | 0 |
| 1 | E | 500 | 3753 | 2369 | 650 | 709 | 25 | 0 | 0 |

- Molecule 2 is a protein called JEV M protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 74 | 574 | 370 | 98 | 104 | 2 | 0 | 0 |
| 2 | D | 74 | 574 | 370 | 98 | 104 | 2 | 0 | 0 |
| 2 | F | 74 | 574 | 370 | 98 | 104 | 2 | 0 | 0 |

- Molecule 3 is a protein called 2H4 light chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | M | 215 | 1657 | 1029 | 287 | 334 | 7 | 0 | 0 |
| 3 | Q | 215 | 1657 | 1029 | 287 | 334 | 7 | 0 | 0 |

- Molecule 4 is a protein called 2H4 heavy chain.

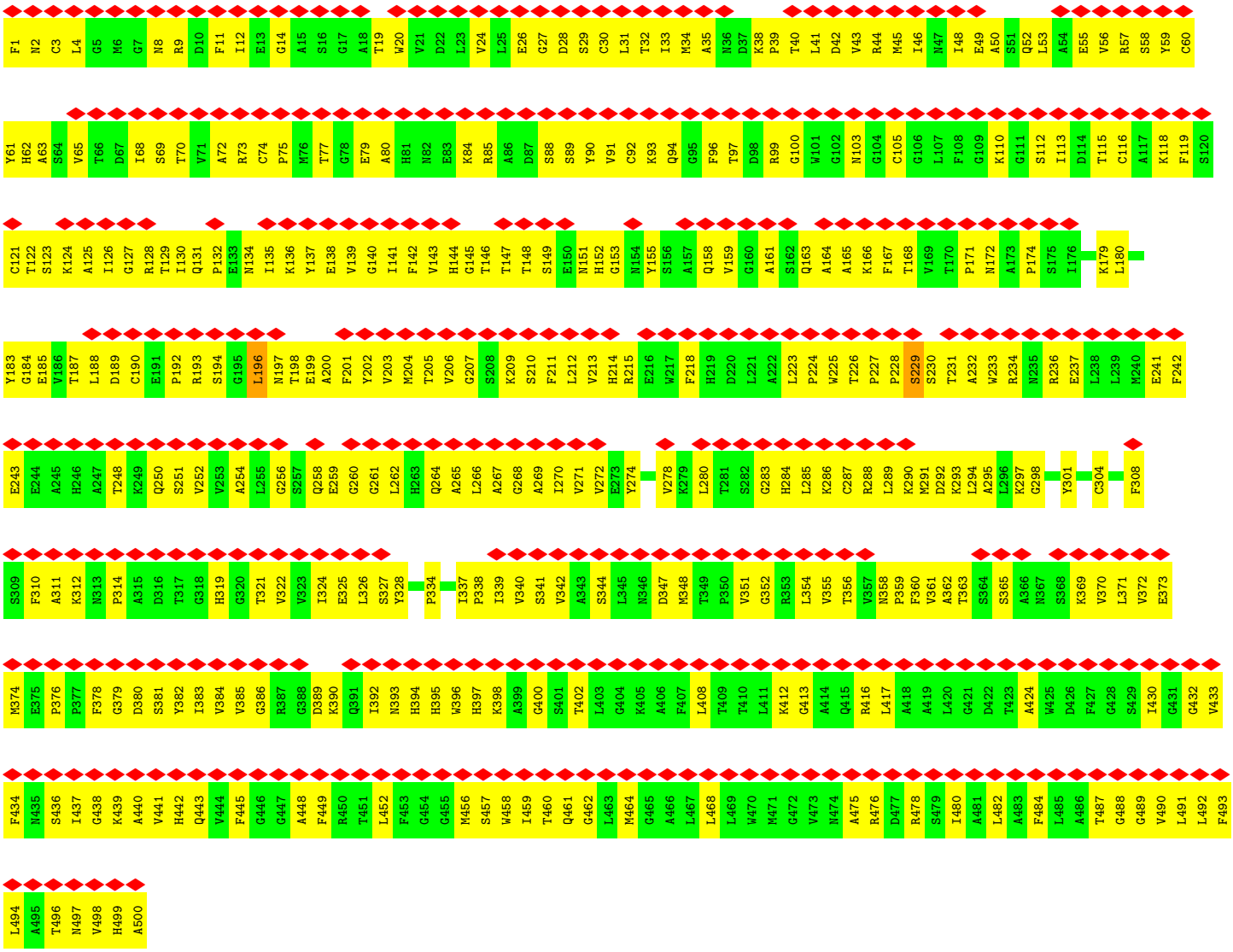
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | N | 218 | 1633 | 1041 | 264 | 320 | 8 | 0 | 0 |
| 4 | R | 218 | 1633 | 1041 | 264 | 320 | 8 | 0 | 0 |

# 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.

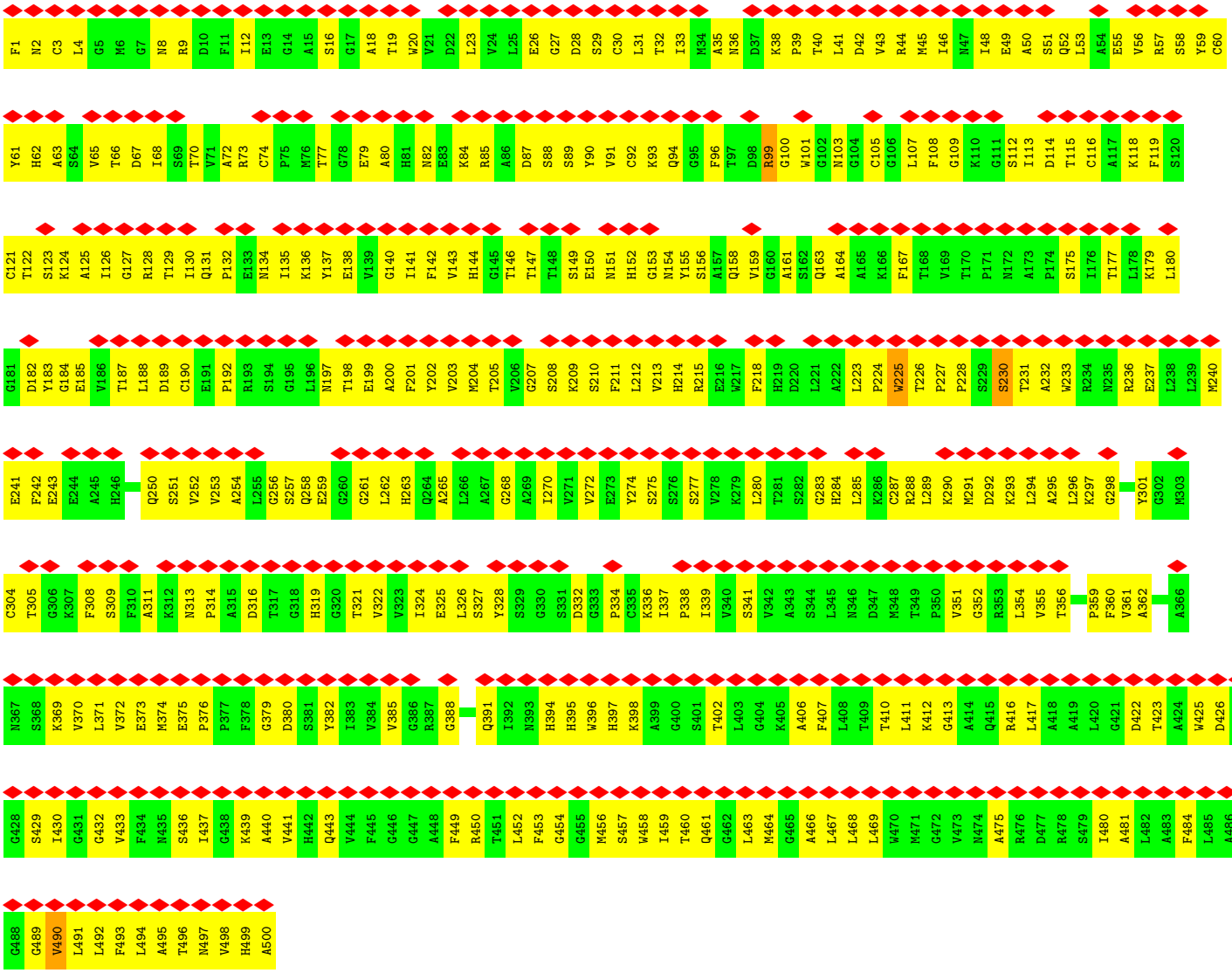
- Molecule 1: JEV E protein

Chain A: 82% 35% 64%



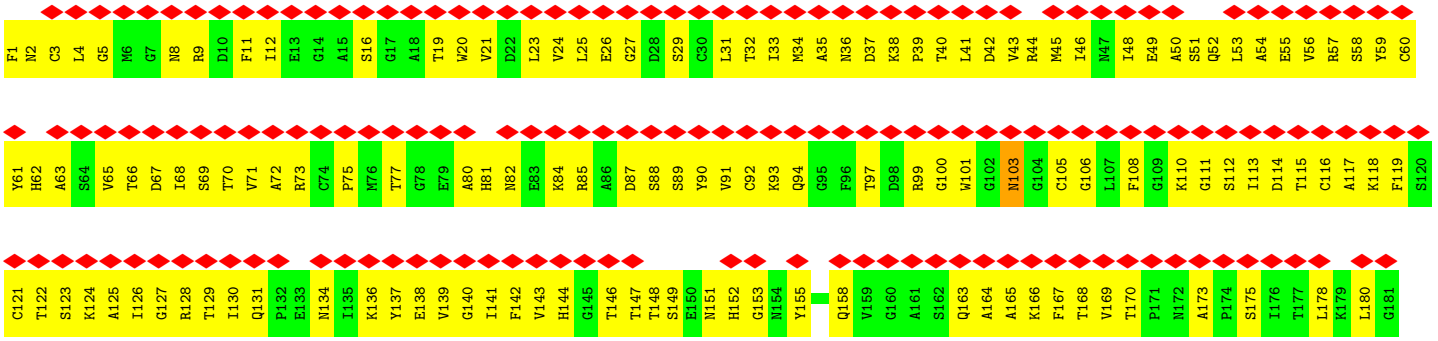

- Molecule 1: JEV E protein

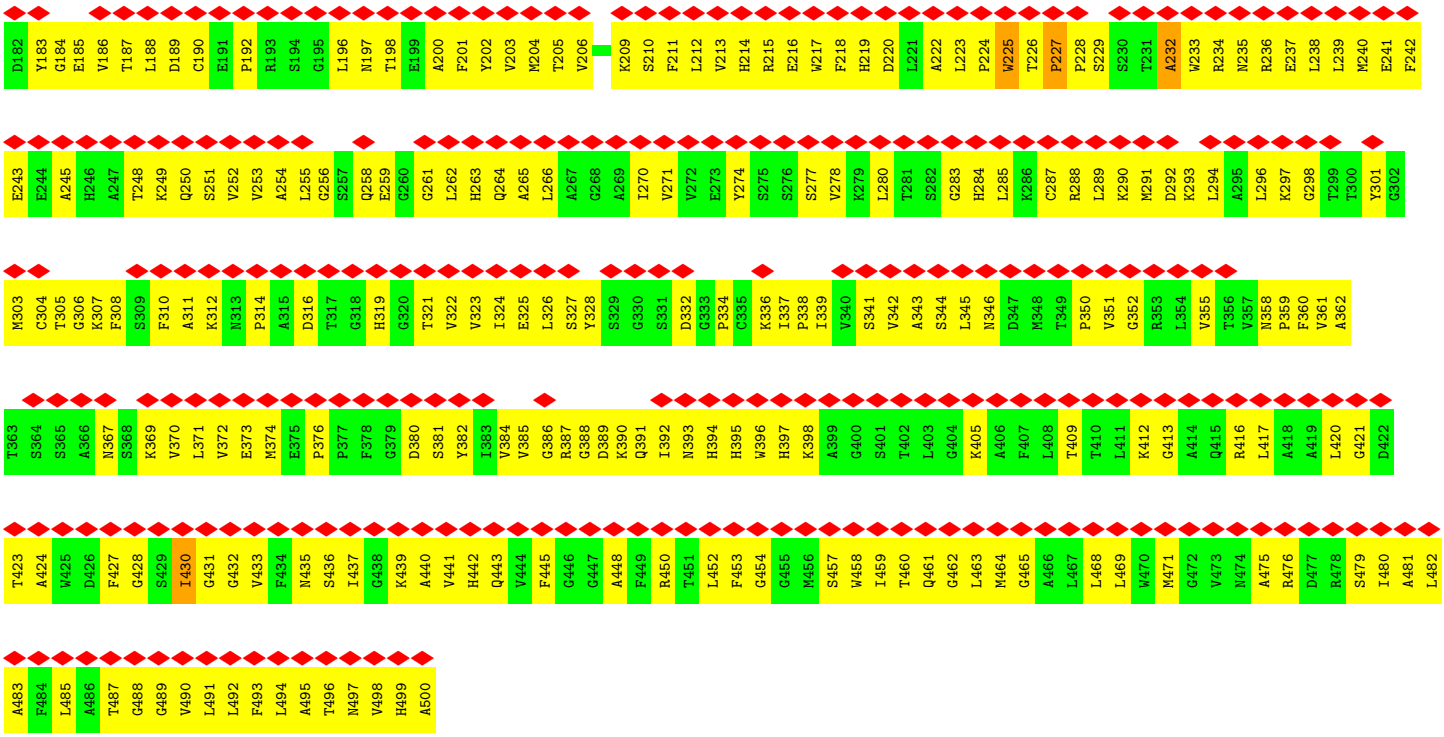
Chain C: 83%




- Molecule 1: JEV E protein

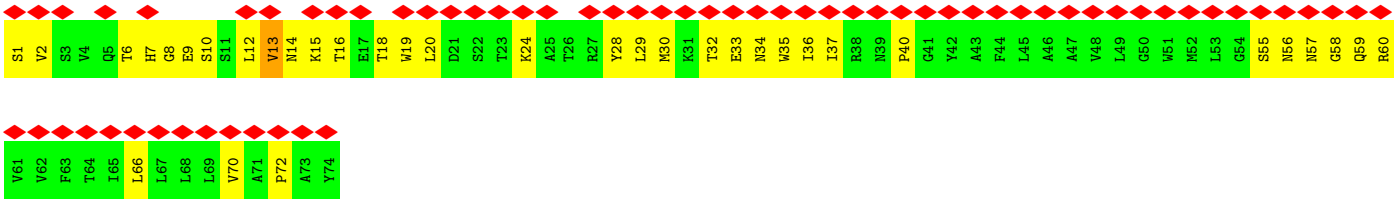
Chain E: 89%





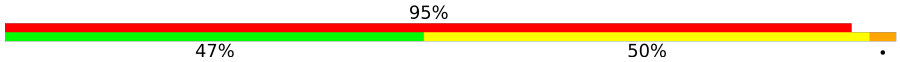

- Molecule 2: JEV M protein

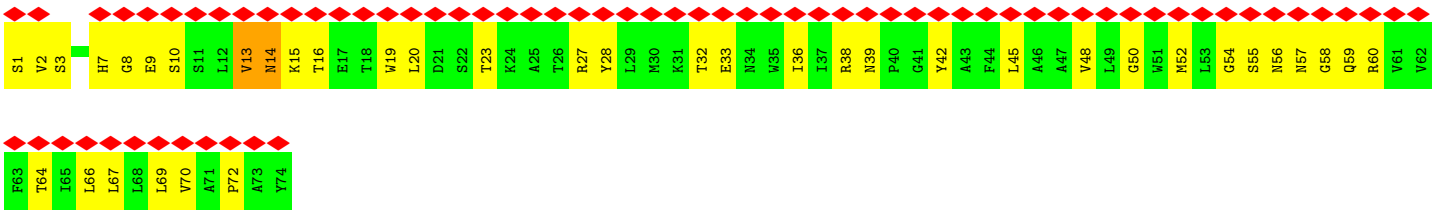
Chain B:




- Molecule 2: JEV M protein

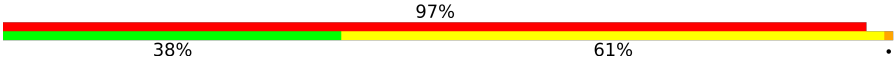
Chain D:

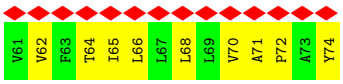


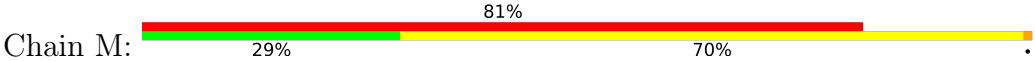

- Molecule 2: JEV M protein

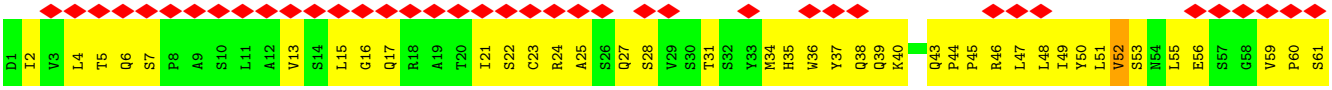
Chain F:

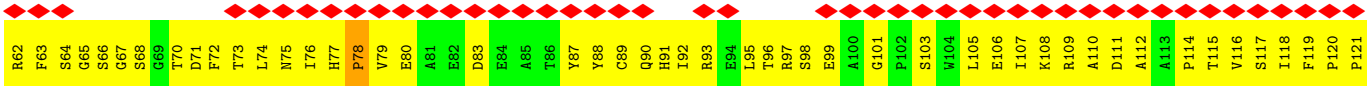


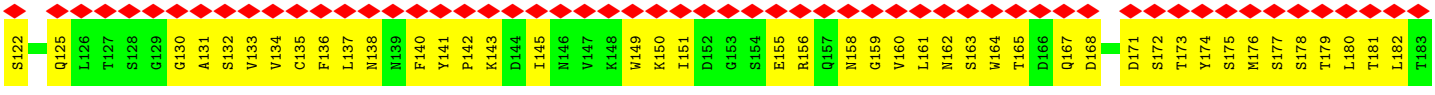


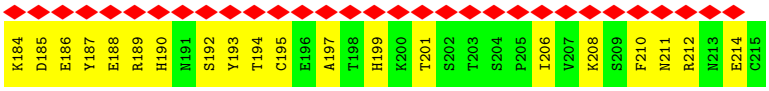

• Molecule 3: 2H4 light chain



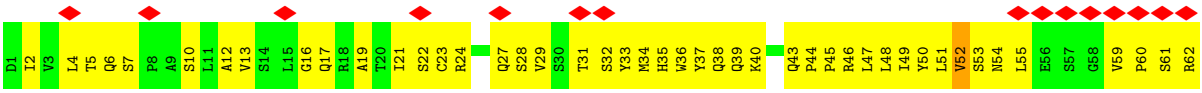



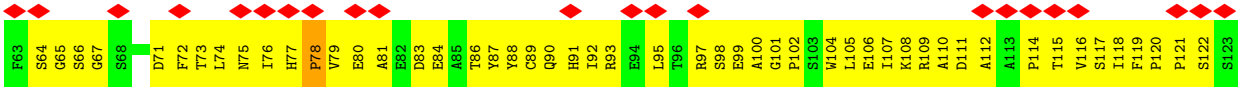



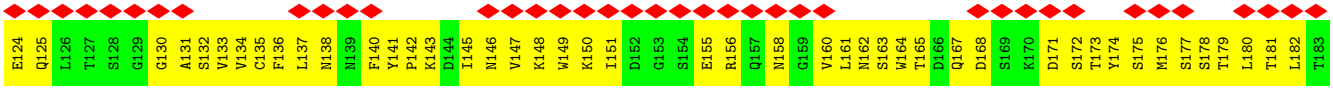



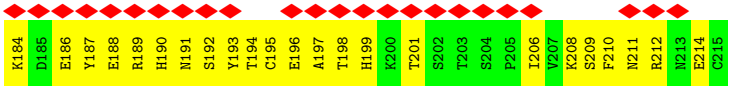




• Molecule 3: 2H4 light chain

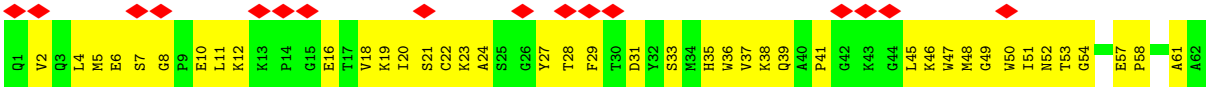


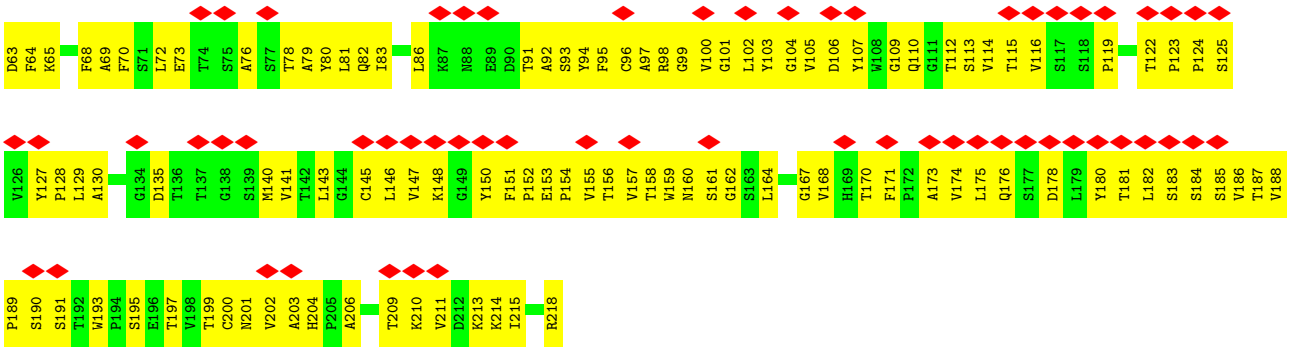



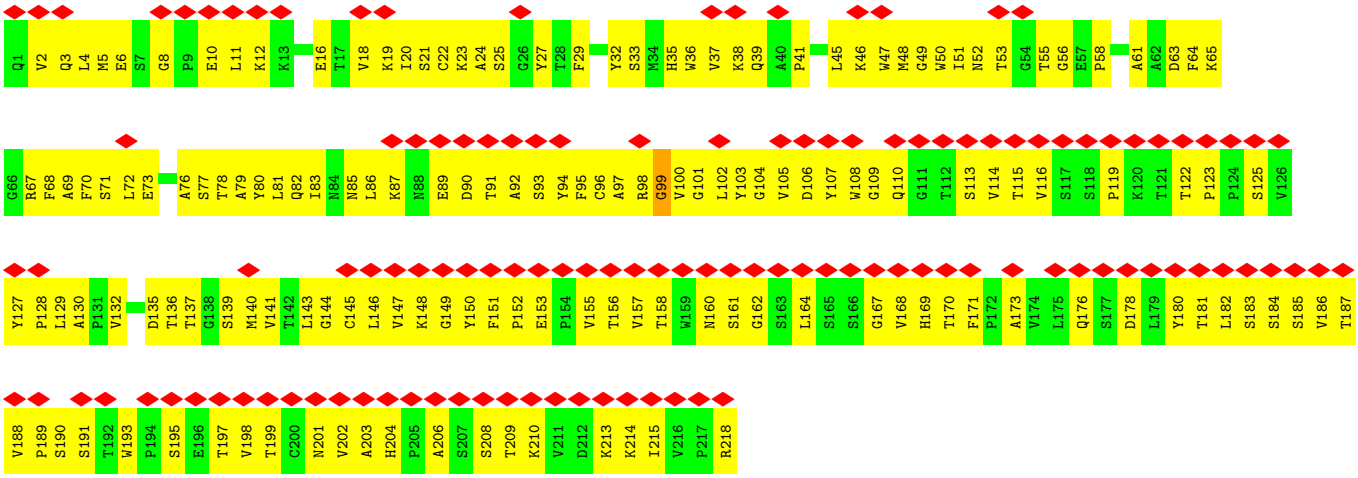

• Molecule 4: 2H4 heavy chain






- Molecule 4: 2H4 heavy chain

Chain R:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 26229 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.087 | Depositor |
| Minimum map value | -0.030 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.025 | Depositor |
| Map size (Å) | 993.6, 993.6, 993.6 | wwPDB |
| Map dimensions | 720, 720, 720 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.38, 1.38, 1.38 | 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 | 0.34 | 0/3835 | 0.55 | 0/5198 |
| 1 | C | 0.32 | 0/3835 | 0.54 | 0/5198 |
| 1 | E | 0.31 | 0/3835 | 0.56 | 0/5198 |
| 2 | B | 0.26 | 0/586 | 0.54 | 0/799 |
| 2 | D | 0.27 | 0/586 | 0.54 | 0/799 |
| 2 | F | 0.26 | 0/586 | 0.54 | 0/799 |
| 3 | M | 0.34 | 0/1696 | 0.56 | 0/2309 |
| 3 | Q | 0.34 | 0/1696 | 0.58 | 0/2309 |
| 4 | N | 0.37 | 0/1680 | 0.60 | 0/2299 |
| 4 | R | 0.36 | 0/1680 | 0.59 | 0/2299 |
| All | All | 0.33 | 0/20015 | 0.56 | 0/27207 |

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 | 3 |
| 1 | C | 0 | 3 |
| 1 | E | 0 | 5 |
| 2 | D | 0 | 1 |
| 3 | M | 0 | 1 |
| 4 | N | 0 | 1 |
| 4 | R | 0 | 1 |
| All | All | 0 | 15 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 196 | LEU | Peptide |
| 1 | A | 229 | SER | Peptide |
| 1 | A | 400 | GLY | Peptide |
| 1 | C | 225 | TRP | Peptide |
| 1 | C | 230 | SER | Peptide |
| 1 | C | 99 | ARG | Peptide |
| 2 | D | 14 | ASN | Peptide |
| 1 | E | 103 | ASN | Peptide |
| 1 | E | 225 | TRP | Peptide |
| 1 | E | 227 | PRO | Peptide |
| 1 | E | 229 | SER | Peptide |
| 1 | E | 232 | ALA | Peptide |
| 3 | M | 68 | SER | Peptide |
| 4 | N | 154 | PRO | Peptide |
| 4 | R | 99 | GLY | Peptide |

## 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 | 3753 | 0 | 3692 | 357 | 0 |
| 1 | C | 3753 | 0 | 3692 | 325 | 0 |
| 1 | E | 3753 | 0 | 3692 | 398 | 0 |
| 2 | B | 574 | 0 | 585 | 35 | 0 |
| 2 | D | 574 | 0 | 585 | 35 | 0 |
| 2 | F | 574 | 0 | 585 | 46 | 0 |
| 3 | M | 1657 | 0 | 1571 | 189 | 0 |
| 3 | Q | 1657 | 0 | 1571 | 211 | 0 |
| 4 | N | 1633 | 0 | 1585 | 180 | 0 |
| 4 | R | 1633 | 0 | 1585 | 203 | 0 |
| All | All | 19561 | 0 | 19143 | 1825 | 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 47.

All (1825) 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) |
|---|---|---|---|
| 1:A:33:ILE:HB | 1:A:41:LEU:HB2 | 1.46 | 0.95 |
| 1:C:33:ILE:HB | 1:C:41:LEU:HB2 | 1.49 | 0.94 |
| 1:E:42:ASP:HB2 | 1:E:142:PHE:HB3 | 1.49 | 0.94 |
| 1:E:355:VAL:H | 1:E:374:MET:HA | 1.28 | 0.94 |
| 1:A:499:HIS:HB2 | 1:A:500:ALA:HB3 | 1.51 | 0.93 |
| 1:C:42:ASP:HB2 | 1:C:142:PHE:HB3 | 1.50 | 0.92 |
| 4:N:148:LYS:HA | 4:N:181:THR:HG22 | 1.53 | 0.90 |
| 3:Q:134:VAL:HG21 | 4:R:129:LEU:HD13 | 1.51 | 0.90 |
| 3:Q:91:HIS:HE2 | 3:Q:98:SER:HG | 1.11 | 0.89 |
| 1:C:131:GLN:OE1 | 4:N:52:ASN:ND2 | 2.06 | 0.89 |
| 1:C:90:TYR:HA | 1:C:118:LYS:HA | 1.56 | 0.88 |
| 1:C:187:THR:HB | 1:C:290:LYS:HB2 | 1.53 | 0.88 |
| 1:E:48:ILE:HB | 1:E:280:LEU:HB2 | 1.56 | 0.87 |
| 1:A:457:SER:OG | 2:B:24:LYS:NZ | 2.08 | 0.87 |
| 1:A:355:VAL:H | 1:A:374:MET:HA | 1.41 | 0.85 |
| 1:E:53:LEU:HD22 | 1:E:130:ILE:HA | 1.56 | 0.84 |
| 3:M:4:LEU:HD11 | 3:M:91:HIS:H | 1.41 | 0.84 |
| 1:E:90:TYR:HA | 1:E:118:LYS:HA | 1.57 | 0.84 |
| 1:E:3:CYS:HB3 | 1:E:9:ARG:HG3 | 1.58 | 0.84 |
| 1:E:2:ASN:ND2 | 1:E:152:HIS:O | 2.10 | 0.84 |
| 3:M:80:GLU:H | 3:M:83:ASP:HB2 | 1.41 | 0.84 |
| 1:C:355:VAL:H | 1:C:374:MET:HA | 1.41 | 0.84 |
| 1:C:123:SER:HA | 3:M:28:SER:HA | 1.60 | 0.83 |
| 1:A:127:GLY:HA2 | 1:A:204:MET:HA | 1.61 | 0.83 |
| 1:E:189:ASP:HB2 | 1:E:288:ARG:HB3 | 1.58 | 0.82 |
| 3:M:48:LEU:HA | 3:M:59:VAL:HG11 | 1.60 | 0.82 |
| 1:A:42:ASP:HB2 | 1:A:142:PHE:HB3 | 1.61 | 0.82 |
| 1:A:90:TYR:HA | 1:A:118:LYS:HA | 1.62 | 0.81 |
| 1:A:2:ASN:ND2 | 1:A:152:HIS:O | 2.13 | 0.81 |
| 1:A:193:ARG:NH2 | 1:E:381:SER:O | 2.14 | 0.81 |
| 1:A:193:ARG:HD3 | 1:E:397:HIS:HB2 | 1.60 | 0.81 |
| 1:E:499:HIS:HB2 | 1:E:500:ALA:HB3 | 1.61 | 0.80 |
| 1:C:12:ILE:HB | 1:C:33:ILE:HA | 1.62 | 0.80 |
| 2:D:57:ASN:OD1 | 2:D:58:GLY:N | 2.14 | 0.80 |
| 4:N:58:PRO:HB3 | 4:N:70:PHE:HB2 | 1.62 | 0.80 |
| 3:Q:97:ARG:HH22 | 4:R:104:GLY:HA2 | 1.43 | 0.80 |
| 1:A:228:PRO:HD3 | 1:C:79:GLU:HB3 | 1.64 | 0.80 |
| 2:B:57:ASN:OD1 | 2:B:58:GLY:N | 2.15 | 0.80 |
| 3:M:99:GLU:HG3 | 4:N:45:LEU:HB2 | 1.62 | 0.80 |
| 3:M:186:GLU:HA | 3:M:189:ARG:HG2 | 1.62 | 0.79 |
| 4:R:140:MET:HA | 4:R:189:PRO:HA | 1.62 | 0.79 |
| 1:C:58:SER:HB2 | 1:C:226:THR:HB | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:121:CYS:O | 3:Q:27:GLN:NE2 | 2.15 | 0.79 |
| 3:Q:150:LYS:HB2 | 3:Q:194:THR:HB | 1.65 | 0.79 |
| 1:A:197:ASN:HB3 | 1:A:200:ALA:HB2 | 1.63 | 0.79 |
| 1:E:55:GLU:HG2 | 1:E:128:ARG:HG2 | 1.65 | 0.78 |
| 1:C:2:ASN:ND2 | 1:C:152:HIS:O | 2.15 | 0.78 |
| 1:C:499:HIS:HB2 | 1:C:500:ALA:HB3 | 1.66 | 0.78 |
| 1:C:189:ASP:HB2 | 1:C:288:ARG:HB3 | 1.64 | 0.78 |
| 3:Q:137:LEU:O | 3:Q:176:MET:N | 2.14 | 0.78 |
| 1:E:224:PRO:HB3 | 1:E:236:ARG:HA | 1.63 | 0.78 |
| 1:A:338:PRO:HB2 | 1:A:386:GLY:HA2 | 1.66 | 0.77 |
| 1:E:158:GLN:NE2 | 1:E:163:GLN:OE1 | 2.17 | 0.77 |
| 2:F:57:ASN:OD1 | 2:F:58:GLY:N | 2.17 | 0.77 |
| 1:E:305:THR:N | 1:E:332:ASP:OD2 | 2.17 | 0.77 |
| 3:M:133:VAL:HB | 3:M:180:LEU:HB3 | 1.66 | 0.77 |
| 1:E:217:TRP:NE1 | 2:F:5:GLN:O | 2.17 | 0.77 |
| 1:E:342:VAL:HG23 | 1:E:382:TYR:HB2 | 1.66 | 0.77 |
| 4:N:157:VAL:HG21 | 4:N:182:LEU:HD11 | 1.65 | 0.77 |
| 1:A:79:GLU:HB3 | 1:C:228:PRO:HD3 | 1.64 | 0.77 |
| 1:E:471:MET:HB3 | 1:E:483:ALA:HB1 | 1.67 | 0.77 |
| 3:M:64:SER:N | 3:M:75:ASN:O | 2.17 | 0.77 |
| 4:R:127:TYR:HB2 | 4:R:146:LEU:HB3 | 1.65 | 0.76 |
| 1:A:40:THR:HB | 1:A:144:HIS:HB2 | 1.65 | 0.76 |
| 1:C:40:THR:OG1 | 1:C:355:VAL:O | 2.02 | 0.76 |
| 4:N:18:VAL:HG12 | 4:N:86:LEU:HD21 | 1.66 | 0.76 |
| 1:E:204:MET:N | 1:E:211:PHE:O | 2.16 | 0.76 |
| 4:R:58:PRO:HB3 | 4:R:70:PHE:HB2 | 1.67 | 0.76 |
| 1:A:30:CYS:HA | 1:A:44:ARG:HB3 | 1.67 | 0.76 |
| 3:Q:186:GLU:HA | 3:Q:189:ARG:HG2 | 1.66 | 0.76 |
| 1:E:89:SER:O | 1:E:119:PHE:N | 2.19 | 0.76 |
| 1:C:40:THR:HB | 1:C:144:HIS:HB2 | 1.67 | 0.76 |
| 1:C:314:PRO:HA | 1:C:324:ILE:HG22 | 1.68 | 0.75 |
| 3:Q:80:GLU:H | 3:Q:83:ASP:HB2 | 1.51 | 0.75 |
| 3:M:161:LEU:HD13 | 4:N:176:GLN:HE21 | 1.51 | 0.75 |
| 4:N:140:MET:HA | 4:N:189:PRO:HA | 1.68 | 0.75 |
| 1:C:205:THR:HA | 1:C:210:SER:HA | 1.68 | 0.75 |
| 1:A:58:SER:HB2 | 1:A:226:THR:HB | 1.69 | 0.75 |
| 1:A:297:LYS:O | 1:A:358:ASN:ND2 | 2.20 | 0.75 |
| 1:E:33:ILE:HB | 1:E:41:LEU:HB2 | 1.69 | 0.75 |
| 1:E:128:ARG:N | 1:E:203:VAL:O | 2.18 | 0.75 |
| 1:E:40:THR:HB | 1:E:144:HIS:HB2 | 1.69 | 0.74 |
| 3:M:120:PRO:O | 4:N:218:ARG:NH2 | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:41:LEU:HD23 | 1:A:143:VAL:HB | 1.69 | 0.74 |
| 3:M:150:LYS:HA | 3:M:155:GLU:HA | 1.69 | 0.74 |
| 1:A:180:LEU:N | 1:A:184:GLY:O | 2.19 | 0.74 |
| 1:A:258:GLN:HB3 | 2:B:2:VAL:HG21 | 1.68 | 0.74 |
| 3:M:16:GLY:N | 3:M:79:VAL:O | 2.20 | 0.74 |
| 1:A:142:PHE:HE1 | 1:A:158:GLN:HE21 | 1.33 | 0.74 |
| 1:E:128:ARG:NH1 | 1:E:205:THR:OG1 | 2.21 | 0.74 |
| 4:N:176:GLN:NE2 | 4:N:181:THR:OG1 | 2.21 | 0.74 |
| 1:E:214:HIS:O | 1:E:218:PHE:N | 2.19 | 0.73 |
| 1:A:62:HIS:HB3 | 1:A:123:SER:HB2 | 1.70 | 0.73 |
| 4:R:22:CYS:O | 4:R:79:ALA:N | 2.15 | 0.73 |
| 1:C:73:ARG:HD3 | 1:C:80:ALA:HA | 1.70 | 0.73 |
| 3:M:111:ASP:HB3 | 3:M:201:THR:HG22 | 1.70 | 0.73 |
| 3:M:119:PHE:HB2 | 3:M:134:VAL:HG23 | 1.68 | 0.73 |
| 3:Q:5:THR:HG23 | 3:Q:24:ARG:HH11 | 1.51 | 0.73 |
| 1:A:312:LYS:HB2 | 1:A:325:GLU:H | 1.54 | 0.73 |
| 1:C:35:ALA:HB3 | 1:C:38:LYS:HB2 | 1.71 | 0.73 |
| 1:E:97:THR:HB | 1:E:99:ARG:HH12 | 1.53 | 0.73 |
| 1:E:46:ILE:N | 1:E:138:GLU:O | 2.16 | 0.73 |
| 4:R:130:ALA:HB3 | 4:R:218:ARG:HG3 | 1.70 | 0.73 |
| 1:C:127:GLY:HA2 | 1:C:204:MET:HA | 1.70 | 0.73 |
| 3:Q:50:TYR:N | 3:Q:54:ASN:O | 2.21 | 0.73 |
| 3:Q:55:LEU:HD11 | 3:Q:61:SER:HA | 1.69 | 0.73 |
| 4:R:98:ARG:NH2 | 4:R:106:ASP:OD2 | 2.22 | 0.73 |
| 1:A:40:THR:O | 1:A:144:HIS:N | 2.20 | 0.72 |
| 1:A:213:VAL:HA | 2:B:7:HIS:CE1 | 2.24 | 0.72 |
| 1:E:48:ILE:HD11 | 1:E:283:GLY:HA2 | 1.71 | 0.72 |
| 4:R:51:ILE:HA | 4:R:58:PRO:HA | 1.70 | 0.72 |
| 1:A:41:LEU:HA | 1:A:143:VAL:HA | 1.72 | 0.72 |
| 1:E:40:THR:OG1 | 1:E:355:VAL:O | 2.05 | 0.72 |
| 4:N:61:ALA:HB3 | 4:N:64:PHE:HD2 | 1.52 | 0.72 |
| 3:Q:150:LYS:HA | 3:Q:155:GLU:HA | 1.72 | 0.72 |
| 1:E:412:LYS:HG2 | 1:E:416:ARG:HG3 | 1.71 | 0.72 |
| 1:E:190:CYS:HA | 1:E:287:CYS:HA | 1.72 | 0.71 |
| 3:M:115:THR:HB | 3:M:138:ASN:HB2 | 1.72 | 0.71 |
| 1:E:73:ARG:HB2 | 1:E:112:SER:HB3 | 1.72 | 0.71 |
| 3:M:64:SER:HB3 | 3:M:75:ASN:HB3 | 1.70 | 0.71 |
| 1:A:12:ILE:N | 1:A:32:THR:O | 2.18 | 0.71 |
| 1:A:89:SER:O | 1:A:119:PHE:N | 2.23 | 0.71 |
| 1:C:65:VAL:HG23 | 1:C:254:ALA:HB2 | 1.72 | 0.71 |
| 1:E:65:VAL:HG23 | 1:E:254:ALA:HB2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:62:HIS:HB3 | 1:C:123:SER:HB2 | 1.71 | 0.71 |
| 1:E:212:LEU:HB2 | 1:E:270:ILE:HD13 | 1.72 | 0.71 |
| 1:A:131:GLN:OE1 | 4:R:52:ASN:ND2 | 2.23 | 0.71 |
| 1:A:342:VAL:HG21 | 1:A:384:VAL:HG23 | 1.71 | 0.71 |
| 1:A:123:SER:HA | 3:Q:28:SER:HA | 1.73 | 0.71 |
| 1:A:142:PHE:HD1 | 1:A:164:ALA:HB2 | 1.55 | 0.71 |
| 1:C:226:THR:HG23 | 1:C:233:TRP:HE1 | 1.56 | 0.71 |
| 3:Q:35:HIS:ND1 | 3:Q:50:TYR:HA | 2.06 | 0.71 |
| 4:R:67:ARG:NH1 | 4:R:85:ASN:O | 2.24 | 0.71 |
| 1:A:73:ARG:HD3 | 1:A:80:ALA:HA | 1.71 | 0.70 |
| 1:C:42:ASP:N | 1:C:142:PHE:O | 2.24 | 0.70 |
| 1:C:52:GLN:NE2 | 4:N:52:ASN:HA | 2.07 | 0.70 |
| 4:R:145:CYS:N | 4:R:184:SER:O | 2.22 | 0.70 |
| 4:R:168:VAL:HA | 4:R:186:VAL:HA | 1.74 | 0.70 |
| 1:E:147:THR:HB | 1:E:152:HIS:HB2 | 1.71 | 0.70 |
| 1:E:151:ASN:OD1 | 1:E:152:HIS:N | 2.25 | 0.70 |
| 1:E:338:PRO:HB2 | 1:E:386:GLY:HA2 | 1.74 | 0.70 |
| 1:A:412:LYS:O | 1:A:416:ARG:N | 2.25 | 0.70 |
| 1:C:56:VAL:HG21 | 1:C:202:TYR:CZ | 2.26 | 0.70 |
| 1:E:243:GLU:H | 1:E:250:GLN:HE21 | 1.38 | 0.70 |
| 2:F:4:VAL:HG12 | 2:F:5:GLN:H | 1.56 | 0.70 |
| 4:N:69:ALA:HB3 | 4:N:82:GLN:HB3 | 1.74 | 0.70 |
| 3:Q:164:TRP:HB3 | 3:Q:176:MET:HG3 | 1.74 | 0.70 |
| 1:E:136:LYS:HA | 1:E:170:THR:HG22 | 1.73 | 0.70 |
| 3:M:133:VAL:N | 3:M:180:LEU:O | 2.20 | 0.70 |
| 3:Q:121:PRO:HD3 | 3:Q:133:VAL:HG22 | 1.73 | 0.70 |
| 3:Q:184:LYS:HA | 3:Q:187:TYR:HB3 | 1.74 | 0.70 |
| 1:E:241:GLU:N | 1:E:253:VAL:O | 2.24 | 0.70 |
| 4:N:161:SER:N | 4:N:201:ASN:OD1 | 2.22 | 0.70 |
| 1:A:190:CYS:HA | 1:A:287:CYS:HA | 1.74 | 0.69 |
| 1:E:38:LYS:NZ | 1:E:294:LEU:O | 2.25 | 0.69 |
| 3:M:151:ILE:HD11 | 3:M:180:LEU:HD21 | 1.75 | 0.69 |
| 1:A:9:ARG:H | 1:A:319:HIS:CE1 | 2.10 | 0.69 |
| 4:N:153:GLU:HG3 | 4:N:180:TYR:CD2 | 2.27 | 0.69 |
| 1:E:457:SER:N | 1:E:460:THR:OG1 | 2.26 | 0.69 |
| 4:R:157:VAL:HG21 | 4:R:182:LEU:HD11 | 1.72 | 0.69 |
| 1:A:68:ILE:HD13 | 1:A:252:VAL:H | 1.58 | 0.69 |
| 1:E:92:CYS:HA | 1:E:116:CYS:HA | 1.74 | 0.69 |
| 4:N:155:VAL:HG12 | 4:N:204:HIS:HB2 | 1.75 | 0.69 |
| 1:A:52:GLN:HE22 | 4:R:53:THR:H | 1.38 | 0.69 |
| 1:E:476:ARG:HB2 | 1:E:479:SER:HB3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:98:ARG:NH2 | 4:N:106:ASP:OD2 | 2.20 | 0.69 |
| 3:Q:4:LEU:HD11 | 3:Q:91:HIS:H | 1.58 | 0.69 |
| 3:Q:151:ILE:HG12 | 3:Q:193:TYR:HD1 | 1.57 | 0.69 |
| 4:R:149:GLY:H | 4:R:181:THR:HG22 | 1.57 | 0.69 |
| 4:N:157:VAL:HG22 | 4:N:202:VAL:HG22 | 1.74 | 0.69 |
| 2:B:33:GLU:HA | 2:B:36:ILE:HG22 | 1.74 | 0.68 |
| 1:C:146:THR:HG21 | 1:C:362:ALA:HB2 | 1.75 | 0.68 |
| 1:E:12:ILE:N | 1:E:32:THR:O | 2.22 | 0.68 |
| 4:R:176:GLN:NE2 | 4:R:181:THR:OG1 | 2.26 | 0.68 |
| 1:E:60:CYS:HB3 | 1:E:224:PRO:HB2 | 1.73 | 0.68 |
| 4:N:6:GLU:HA | 4:N:22:CYS:HA | 1.75 | 0.68 |
| 1:A:42:ASP:N | 1:A:142:PHE:O | 2.20 | 0.68 |
| 1:A:212:LEU:HD12 | 1:A:270:ILE:HD13 | 1.73 | 0.68 |
| 1:C:27:GLY:HA2 | 1:C:45:MET:HB3 | 1.75 | 0.68 |
| 1:C:147:THR:HB | 1:C:152:HIS:HB2 | 1.74 | 0.68 |
| 1:E:66:THR:O | 1:E:118:LYS:N | 2.26 | 0.68 |
| 1:E:213:VAL:HA | 2:F:7:HIS:CE1 | 2.29 | 0.68 |
| 3:M:109:ARG:NH1 | 3:M:110:ALA:O | 2.26 | 0.68 |
| 3:Q:36:TRP:CD2 | 3:Q:74:LEU:HB2 | 2.28 | 0.68 |
| 4:R:12:LYS:N | 4:R:115:THR:O | 2.23 | 0.68 |
| 4:R:18:VAL:HG12 | 4:R:86:LEU:HD21 | 1.75 | 0.68 |
| 1:A:147:THR:HB | 1:A:152:HIS:HB2 | 1.75 | 0.68 |
| 1:E:3:CYS:SG | 1:E:32:THR:OG1 | 2.51 | 0.68 |
| 4:R:5:MET:HG3 | 4:R:23:LYS:HB3 | 1.74 | 0.68 |
| 1:A:226:THR:HG23 | 1:A:233:TRP:HE1 | 1.57 | 0.68 |
| 4:R:147:VAL:HG11 | 4:R:155:VAL:HG21 | 1.76 | 0.68 |
| 1:E:35:ALA:HB3 | 1:E:38:LYS:HB2 | 1.76 | 0.68 |
| 3:M:77:HIS:CG | 3:M:78:PRO:HD3 | 2.28 | 0.68 |
| 1:E:16:SER:OG | 1:E:36:ASN:ND2 | 2.20 | 0.68 |
| 1:E:52:GLN:O | 1:E:134:ASN:ND2 | 2.27 | 0.68 |
| 4:N:20:ILE:HD12 | 4:N:81:LEU:HD23 | 1.75 | 0.68 |
| 1:A:304:CYS:H | 1:A:338:PRO:HD3 | 1.58 | 0.68 |
| 1:C:151:ASN:OD1 | 1:C:152:HIS:N | 2.27 | 0.68 |
| 3:Q:34:MET:O | 3:Q:52:VAL:N | 2.26 | 0.68 |
| 1:A:442:HIS:HA | 1:A:445:PHE:HB3 | 1.76 | 0.67 |
| 4:N:106:ASP:OD1 | 4:N:107:TYR:N | 2.27 | 0.67 |
| 1:E:42:ASP:N | 1:E:142:PHE:O | 2.27 | 0.67 |
| 3:Q:109:ARG:NH1 | 3:Q:110:ALA:O | 2.27 | 0.67 |
| 4:R:123:PRO:HB3 | 4:R:209:THR:HG21 | 1.74 | 0.67 |
| 1:C:121:CYS:O | 3:M:27:GLN:NE2 | 2.19 | 0.67 |
| 1:C:243:GLU:H | 1:C:250:GLN:HE21 | 1.41 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:35:HIS:NE2 | 4:R:103:TYR:O | 2.27 | 0.67 |
| 3:Q:168:ASP:N | 3:Q:173:THR:O | 2.27 | 0.67 |
| 3:Q:4:LEU:HG | 3:Q:91:HIS:HD2 | 1.60 | 0.67 |
| 3:Q:132:SER:HA | 3:Q:181:THR:HA | 1.77 | 0.67 |
| 1:E:261:GLY:O | 1:E:265:ALA:N | 2.24 | 0.67 |
| 3:M:66:SER:O | 3:M:73:THR:N | 2.24 | 0.67 |
| 1:C:92:CYS:HA | 1:C:116:CYS:HA | 1.77 | 0.67 |
| 1:C:142:PHE:HE1 | 1:C:158:GLN:HE21 | 1.41 | 0.67 |
| 4:N:51:ILE:HA | 4:N:58:PRO:HA | 1.75 | 0.67 |
| 4:R:69:ALA:HB3 | 4:R:82:GLN:HB3 | 1.76 | 0.67 |
| 1:A:189:ASP:HB2 | 1:A:288:ARG:HB3 | 1.76 | 0.67 |
| 1:A:49:GLU:O | 1:A:136:LYS:N | 2.22 | 0.67 |
| 1:C:46:ILE:N | 1:C:138:GLU:O | 2.23 | 0.67 |
| 2:D:3:SER:HB2 | 2:F:3:SER:HB2 | 1.76 | 0.67 |
| 1:A:126:ILE:O | 1:A:205:THR:N | 2.27 | 0.66 |
| 1:C:52:GLN:O | 1:C:134:ASN:ND2 | 2.27 | 0.66 |
| 4:N:22:CYS:O | 4:N:79:ALA:N | 2.28 | 0.66 |
| 3:Q:140:PHE:N | 3:Q:174:TYR:O | 2.23 | 0.66 |
| 4:R:38:LYS:HG3 | 4:R:94:TYR:HE1 | 1.60 | 0.66 |
| 1:A:60:CYS:HB3 | 1:A:224:PRO:HB2 | 1.76 | 0.66 |
| 1:C:132:PRO:HD3 | 1:C:198:THR:HG21 | 1.78 | 0.66 |
| 2:D:69:LEU:HD22 | 2:F:70:VAL:HG13 | 1.76 | 0.66 |
| 3:M:168:ASP:N | 3:M:173:THR:O | 2.28 | 0.66 |
| 1:A:48:ILE:O | 1:A:280:LEU:N | 2.26 | 0.66 |
| 1:A:60:CYS:HA | 1:A:124:LYS:HA | 1.77 | 0.66 |
| 1:E:82:ASN:ND2 | 1:E:116:CYS:SG | 2.69 | 0.66 |
| 1:C:40:THR:O | 1:C:144:HIS:N | 2.24 | 0.66 |
| 4:N:19:LYS:HA | 4:N:82:GLN:HA | 1.78 | 0.66 |
| 3:Q:151:ILE:HG12 | 3:Q:193:TYR:CD1 | 2.31 | 0.66 |
| 3:M:5:THR:HG23 | 3:M:24:ARG:HH11 | 1.61 | 0.66 |
| 4:N:53:THR:HA | 4:N:72:LEU:HD11 | 1.78 | 0.65 |
| 3:Q:135:CYS:N | 3:Q:178:SER:O | 2.23 | 0.65 |
| 1:A:46:ILE:N | 1:A:138:GLU:O | 2.22 | 0.65 |
| 1:C:413:GLY:O | 1:C:417:LEU:N | 2.27 | 0.65 |
| 1:E:492:LEU:O | 1:E:496:THR:N | 2.26 | 0.65 |
| 1:A:52:GLN:O | 1:A:134:ASN:ND2 | 2.29 | 0.65 |
| 1:C:55:GLU:HA | 1:C:128:ARG:HG2 | 1.78 | 0.65 |
| 3:Q:35:HIS:HB3 | 3:Q:47:LEU:HD11 | 1.77 | 0.65 |
| 3:Q:137:LEU:N | 3:Q:176:MET:O | 2.30 | 0.65 |
| 4:R:22:CYS:HB3 | 4:R:79:ALA:HB3 | 1.78 | 0.65 |
| 1:A:457:SER:N | 1:A:460:THR:OG1 | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:77:HIS:CG | 3:Q:78:PRO:HD3 | 2.31 | 0.65 |
| 1:E:416:ARG:HB3 | 1:E:427:PHE:CE2 | 2.32 | 0.65 |
| 1:A:274:TYR:OH | 4:R:101:GLY:HA3 | 1.96 | 0.65 |
| 4:N:16:GLU:HB2 | 4:N:86:LEU:HD12 | 1.78 | 0.65 |
| 3:Q:13:VAL:O | 3:Q:108:LYS:N | 2.26 | 0.65 |
| 1:C:48:ILE:O | 1:C:280:LEU:N | 2.30 | 0.65 |
| 4:N:35:HIS:ND1 | 4:N:50:TRP:HB3 | 2.11 | 0.65 |
| 3:Q:131:ALA:O | 3:Q:182:LEU:N | 2.26 | 0.65 |
| 1:A:149:SER:OG | 1:A:325:GLU:OE1 | 2.14 | 0.65 |
| 1:E:31:LEU:O | 1:E:43:VAL:N | 2.29 | 0.65 |
| 1:E:75:PRO:HD3 | 1:E:111:GLY:HA2 | 1.77 | 0.65 |
| 1:E:297:LYS:O | 1:E:358:ASN:ND2 | 2.30 | 0.65 |
| 1:A:322:VAL:HG23 | 1:A:376:PRO:HG3 | 1.77 | 0.65 |
| 2:D:33:GLU:HA | 2:D:36:ILE:HG22 | 1.79 | 0.65 |
| 1:E:131:GLN:OE1 | 1:E:134:ASN:ND2 | 2.30 | 0.65 |
| 3:M:91:HIS:NE2 | 3:M:98:SER:OG | 2.22 | 0.65 |
| 4:N:38:LYS:HG3 | 4:N:94:TYR:HE1 | 1.62 | 0.65 |
| 3:Q:133:VAL:N | 3:Q:180:LEU:O | 2.22 | 0.65 |
| 1:A:69:SER:O | 1:A:116:CYS:N | 2.27 | 0.65 |
| 1:E:342:VAL:HG21 | 1:E:384:VAL:HG23 | 1.78 | 0.65 |
| 1:E:324:ILE:HD12 | 1:E:326:LEU:HD21 | 1.80 | 0.64 |
| 1:A:432:GLY:HA2 | 1:A:436:SER:HB2 | 1.77 | 0.64 |
| 1:A:205:THR:HA | 1:A:210:SER:HA | 1.77 | 0.64 |
| 1:C:23:LEU:N | 1:C:287:CYS:O | 2.23 | 0.64 |
| 1:C:142:PHE:HD1 | 1:C:164:ALA:HB2 | 1.62 | 0.64 |
| 1:C:230:SER:OG | 1:C:231:THR:HG23 | 1.96 | 0.64 |
| 1:E:142:PHE:HD1 | 1:E:164:ALA:HB2 | 1.60 | 0.64 |
| 3:M:97:ARG:HH12 | 4:N:101:GLY:HA2 | 1.61 | 0.64 |
| 1:E:75:PRO:HB3 | 1:E:110:LYS:HB2 | 1.80 | 0.64 |
| 4:N:12:LYS:N | 4:N:115:THR:O | 2.23 | 0.64 |
| 3:Q:135:CYS:HB3 | 3:Q:178:SER:HB3 | 1.77 | 0.64 |
| 3:M:27:GLN:HE21 | 3:M:28:SER:H | 1.44 | 0.64 |
| 3:M:132:SER:HA | 3:M:181:THR:HA | 1.80 | 0.64 |
| 4:N:5:MET:HG3 | 4:N:23:LYS:HB3 | 1.78 | 0.64 |
| 4:R:155:VAL:HG12 | 4:R:204:HIS:HB2 | 1.79 | 0.64 |
| 1:C:242:PHE:HB3 | 1:C:250:GLN:HE21 | 1.63 | 0.64 |
| 1:E:71:VAL:O | 1:E:114:ASP:N | 2.26 | 0.64 |
| 1:E:170:THR:OG1 | 1:E:173:ALA:N | 2.31 | 0.64 |
| 3:Q:36:TRP:HD1 | 3:Q:49:ILE:HB | 1.61 | 0.64 |
| 1:E:57:ARG:HA | 1:E:228:PRO:HA | 1.80 | 0.64 |
| 3:M:23:CYS:N | 3:M:72:PHE:O | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:274:TYR:OH | 4:N:101:GLY:HA3 | 1.98 | 0.64 |
| 1:A:158:GLN:HA | 1:A:161:ALA:HB3 | 1.80 | 0.63 |
| 1:A:230:SER:OG | 1:A:231:THR:HG23 | 1.96 | 0.63 |
| 3:M:35:HIS:CE1 | 3:M:51:LEU:H | 2.16 | 0.63 |
| 3:M:156:ARG:NH1 | 3:M:186:GLU:OE2 | 2.31 | 0.63 |
| 1:A:59:TYR:CD1 | 1:A:225:TRP:HB3 | 2.33 | 0.63 |
| 1:A:73:ARG:HB2 | 1:A:112:SER:HB3 | 1.80 | 0.63 |
| 4:R:119:PRO:HG3 | 4:R:178:ASP:HB3 | 1.80 | 0.63 |
| 4:N:33:SER:OG | 4:N:99:GLY:HA3 | 1.98 | 0.63 |
| 4:R:51:ILE:HB | 4:R:70:PHE:HB3 | 1.81 | 0.63 |
| 1:A:4:LEU:HB2 | 1:A:152:HIS:NE2 | 2.14 | 0.63 |
| 1:A:128:ARG:NH2 | 3:Q:93:ARG:O | 2.31 | 0.63 |
| 1:E:59:TYR:N | 1:E:125:ALA:O | 2.22 | 0.63 |
| 4:N:48:MET:HG2 | 4:N:64:PHE:CE1 | 2.33 | 0.63 |
| 3:Q:137:LEU:HB2 | 3:Q:176:MET:HB3 | 1.80 | 0.63 |
| 1:C:463:LEU:O | 1:C:467:LEU:N | 2.32 | 0.63 |
| 3:Q:36:TRP:HA | 3:Q:88:TYR:O | 1.98 | 0.63 |
| 1:A:308:PHE:HZ | 1:A:338:PRO:HD2 | 1.63 | 0.63 |
| 1:C:388:GLY:O | 1:C:391:GLN:N | 2.18 | 0.63 |
| 1:C:158:GLN:HA | 1:C:161:ALA:HB3 | 1.80 | 0.63 |
| 2:D:19:TRP:CD1 | 2:D:20:LEU:HG | 2.33 | 0.63 |
| 1:E:298:GLY:HA2 | 1:E:301:TYR:HD2 | 1.64 | 0.63 |
| 1:C:128:ARG:NH2 | 3:M:93:ARG:O | 2.32 | 0.63 |
| 1:E:226:THR:HG22 | 1:E:227:PRO:O | 1.99 | 0.63 |
| 3:M:62:ARG:HB2 | 3:M:78:PRO:HD2 | 1.81 | 0.63 |
| 1:E:189:ASP:O | 1:E:288:ARG:N | 2.30 | 0.63 |
| 3:Q:36:TRP:CE2 | 3:Q:74:LEU:HB2 | 2.33 | 0.63 |
| 4:R:35:HIS:ND1 | 4:R:50:TRP:HB3 | 2.14 | 0.63 |
| 2:D:56:ASN:HD22 | 2:D:59:GLN:NE2 | 1.96 | 0.62 |
| 3:M:34:MET:O | 3:M:52:VAL:N | 2.32 | 0.62 |
| 3:Q:76:ILE:HB | 3:Q:79:VAL:HG12 | 1.81 | 0.62 |
| 3:Q:177:SER:HG | 4:R:183:SER:HG | 1.45 | 0.62 |
| 1:A:9:ARG:HB3 | 1:A:319:HIS:CD2 | 2.34 | 0.62 |
| 2:B:56:ASN:HB2 | 2:B:59:GLN:HG2 | 1.79 | 0.62 |
| 3:Q:140:PHE:O | 3:Q:174:TYR:N | 2.31 | 0.62 |
| 4:R:22:CYS:N | 4:R:79:ALA:O | 2.29 | 0.62 |
| 1:C:158:GLN:NE2 | 1:C:163:GLN:OE1 | 2.32 | 0.62 |
| 1:C:183:TYR:O | 1:C:295:ALA:N | 2.28 | 0.62 |
| 1:C:322:VAL:HG23 | 1:C:376:PRO:HG3 | 1.81 | 0.62 |
| 1:E:56:VAL:HG13 | 1:E:57:ARG:HG2 | 1.81 | 0.62 |
| 1:E:146:THR:OG1 | 1:E:360:PHE:O | 2.13 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:489:GLY:C | 1:A:491:LEU:H | 2.02 | 0.62 |
| 1:C:459:ILE:O | 1:C:463:LEU:N | 2.19 | 0.62 |
| 1:C:60:CYS:HA | 1:C:124:LYS:HA | 1.81 | 0.62 |
| 1:C:492:LEU:O | 1:C:496:THR:N | 2.30 | 0.62 |
| 3:Q:116:VAL:O | 3:Q:208:LYS:NZ | 2.25 | 0.62 |
| 1:A:356:THR:HB | 1:A:372:VAL:HG13 | 1.81 | 0.62 |
| 1:A:492:LEU:O | 1:A:496:THR:N | 2.28 | 0.62 |
| 1:C:226:THR:HG22 | 1:C:227:PRO:O | 1.99 | 0.62 |
| 3:M:140:PHE:N | 3:M:174:TYR:O | 2.28 | 0.62 |
| 1:A:40:THR:OG1 | 1:A:355:VAL:O | 2.09 | 0.62 |
| 1:A:226:THR:HG22 | 1:A:227:PRO:O | 2.00 | 0.62 |
| 1:A:261:GLY:HA3 | 2:B:2:VAL:HG23 | 1.80 | 0.62 |
| 3:M:13:VAL:HG11 | 3:M:105:LEU:HD11 | 1.82 | 0.62 |
| 3:Q:151:ILE:HD11 | 3:Q:180:LEU:HD21 | 1.80 | 0.62 |
| 1:A:12:ILE:HB | 1:A:33:ILE:HA | 1.81 | 0.62 |
| 1:A:132:PRO:HD3 | 1:A:198:THR:HG21 | 1.82 | 0.62 |
| 1:A:339:ILE:HG22 | 1:A:359:PRO:HG3 | 1.82 | 0.62 |
| 4:R:19:LYS:HA | 4:R:82:GLN:HA | 1.80 | 0.62 |
| 4:R:101:GLY:O | 4:R:104:GLY:N | 2.22 | 0.62 |
| 1:A:3:CYS:SG | 1:A:32:THR:OG1 | 2.57 | 0.62 |
| 1:A:193:ARG:NH1 | 1:E:380:ASP:HA | 2.14 | 0.62 |
| 1:E:328:TYR:OH | 1:E:332:ASP:OD2 | 2.17 | 0.62 |
| 3:M:2:ILE:HG23 | 3:M:91:HIS:CE1 | 2.35 | 0.62 |
| 1:A:188:LEU:HA | 1:A:288:ARG:O | 2.00 | 0.61 |
| 1:C:284:HIS:HB2 | 2:D:13:VAL:HG13 | 1.82 | 0.61 |
| 1:C:458:TRP:HD1 | 1:C:498:VAL:HG13 | 1.63 | 0.61 |
| 1:E:9:ARG:HB3 | 1:E:319:HIS:CD2 | 2.35 | 0.61 |
| 1:E:440:ALA:HA | 1:E:443:GLN:HB2 | 1.81 | 0.61 |
| 3:M:7:SER:OG | 3:M:22:SER:OG | 2.13 | 0.61 |
| 3:M:34:MET:HA | 3:M:90:GLN:O | 2.01 | 0.61 |
| 3:M:136:PHE:CD1 | 4:N:185:SER:HB3 | 2.35 | 0.61 |
| 1:A:93:LYS:N | 1:A:115:THR:O | 2.32 | 0.61 |
| 1:C:426:ASP:O | 1:C:429:SER:OG | 2.15 | 0.61 |
| 1:E:388:GLY:O | 1:E:391:GLN:HG2 | 2.00 | 0.61 |
| 3:M:91:HIS:ND1 | 3:M:91:HIS:O | 2.34 | 0.61 |
| 3:Q:133:VAL:HB | 3:Q:180:LEU:HB3 | 1.82 | 0.61 |
| 4:R:24:ALA:HB3 | 4:R:77:SER:HB3 | 1.83 | 0.61 |
| 1:E:9:ARG:H | 1:E:319:HIS:CE1 | 2.17 | 0.61 |
| 3:Q:97:ARG:HB2 | 4:R:47:TRP:CD2 | 2.35 | 0.61 |
| 1:A:61:TYR:CZ | 1:A:123:SER:HB3 | 2.36 | 0.61 |
| 1:E:265:ALA:HB2 | 2:F:2:VAL:HA | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:343:ALA:HB2 | 1:E:351:VAL:HG11 | 1.83 | 0.61 |
| 1:E:359:PRO:HB3 | 1:E:372:VAL:HG11 | 1.81 | 0.61 |
| 3:Q:99:GLU:HG3 | 4:R:45:LEU:HB2 | 1.82 | 0.61 |
| 4:R:161:SER:N | 4:R:201:ASN:OD1 | 2.22 | 0.61 |
| 1:A:3:CYS:HB3 | 1:A:9:ARG:HG3 | 1.81 | 0.61 |
| 1:A:74:CYS:O | 1:A:77:THR:OG1 | 2.17 | 0.61 |
| 1:C:304:CYS:H | 1:C:338:PRO:HD3 | 1.65 | 0.61 |
| 4:N:68:PHE:HE1 | 4:N:83:ILE:HG23 | 1.66 | 0.61 |
| 1:A:59:TYR:O | 1:A:125:ALA:N | 2.27 | 0.61 |
| 3:Q:13:VAL:HG11 | 3:Q:105:LEU:HD11 | 1.83 | 0.61 |
| 4:R:150:TYR:O | 4:R:180:TYR:N | 2.31 | 0.61 |
| 1:C:190:CYS:HA | 1:C:287:CYS:HA | 1.81 | 0.61 |
| 2:D:38:ARG:HD2 | 1:E:216:GLU:OE2 | 2.00 | 0.61 |
| 3:M:134:VAL:HG21 | 4:N:129:LEU:HD13 | 1.83 | 0.61 |
| 3:Q:38:GLN:HG3 | 3:Q:46:ARG:HB3 | 1.81 | 0.61 |
| 1:A:56:VAL:HG21 | 1:A:202:TYR:CZ | 2.36 | 0.61 |
| 3:M:37:TYR:HB2 | 3:M:88:TYR:HB2 | 1.81 | 0.61 |
| 3:M:135:CYS:N | 3:M:178:SER:O | 2.24 | 0.61 |
| 1:E:325:GLU:HA | 1:E:371:LEU:HA | 1.83 | 0.61 |
| 3:M:36:TRP:CD2 | 3:M:74:LEU:HB2 | 2.36 | 0.61 |
| 4:N:11:LEU:HD23 | 4:N:115:THR:HB | 1.82 | 0.61 |
| 4:R:160:ASN:ND2 | 4:R:197:THR:O | 2.32 | 0.61 |
| 1:C:180:LEU:HD12 | 1:C:294:LEU:HD13 | 1.82 | 0.60 |
| 1:E:49:GLU:HB3 | 1:E:136:LYS:HB2 | 1.82 | 0.60 |
| 1:E:68:ILE:HD13 | 1:E:252:VAL:H | 1.66 | 0.60 |
| 3:Q:16:GLY:N | 3:Q:79:VAL:O | 2.21 | 0.60 |
| 3:M:137:LEU:O | 3:M:176:MET:N | 2.21 | 0.60 |
| 1:A:202:TYR:CE2 | 1:A:215:ARG:HB2 | 2.37 | 0.60 |
| 1:A:437:ILE:HG13 | 1:A:441:VAL:HG23 | 1.82 | 0.60 |
| 4:R:143:LEU:HD21 | 4:R:193:TRP:CD1 | 2.36 | 0.60 |
| 1:A:284:HIS:HB2 | 2:B:13:VAL:HG13 | 1.82 | 0.60 |
| 1:A:1:PHE:HA | 1:A:140:GLY:HA3 | 1.84 | 0.60 |
| 1:A:298:GLY:HA2 | 1:A:301:TYR:HD2 | 1.66 | 0.60 |
| 1:C:59:TYR:CD2 | 1:C:225:TRP:HB3 | 2.36 | 0.60 |
| 4:N:203:ALA:HA | 4:N:210:LYS:HA | 1.83 | 0.60 |
| 3:Q:147:VAL:HG21 | 3:Q:162:ASN:HD21 | 1.65 | 0.60 |
| 1:A:265:ALA:HB2 | 2:B:2:VAL:O | 2.02 | 0.60 |
| 1:E:1:PHE:H1 | 1:E:44:ARG:HH11 | 1.49 | 0.60 |
| 1:E:19:THR:O | 1:E:291:MET:N | 2.33 | 0.60 |
| 3:M:149:TRP:CD2 | 3:M:180:LEU:HB2 | 2.36 | 0.60 |
| 1:A:267:ALA:HB3 | 2:B:8:GLY:HA3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:35:TRP:CE3 | 2:B:72:PRO:HG3 | 2.37 | 0.60 |
| 1:C:407:PHE:O | 1:C:411:LEU:N | 2.34 | 0.60 |
| 3:M:184:LYS:HA | 3:M:187:TYR:HB3 | 1.84 | 0.60 |
| 4:N:12:LYS:HB2 | 4:N:116:VAL:HG22 | 1.84 | 0.60 |
| 3:Q:48:LEU:HA | 3:Q:59:VAL:HG11 | 1.83 | 0.60 |
| 1:A:274:TYR:CD2 | 4:R:102:LEU:HB2 | 2.36 | 0.60 |
| 1:C:177:THR:HA | 1:C:187:THR:HA | 1.82 | 0.60 |
| 1:E:72:ALA:HA | 1:E:113:ILE:HA | 1.82 | 0.60 |
| 1:E:489:GLY:C | 1:E:491:LEU:H | 2.04 | 0.60 |
| 4:N:147:VAL:HG11 | 4:N:155:VAL:HG21 | 1.84 | 0.60 |
| 1:A:59:TYR:HA | 1:A:225:TRP:HA | 1.83 | 0.59 |
| 1:A:381:SER:N | 1:A:396:TRP:O | 2.34 | 0.59 |
| 1:E:61:TYR:CE2 | 1:E:259:GLU:HB2 | 2.37 | 0.59 |
| 3:Q:156:ARG:HG2 | 3:Q:158:ASN:H | 1.67 | 0.59 |
| 1:E:417:LEU:HA | 1:E:424:ALA:HB1 | 1.83 | 0.59 |
| 4:N:101:GLY:O | 4:N:104:GLY:N | 2.27 | 0.59 |
| 4:N:127:TYR:HB2 | 4:N:146:LEU:HB3 | 1.84 | 0.59 |
| 4:R:16:GLU:HB2 | 4:R:86:LEU:HD12 | 1.83 | 0.59 |
| 1:C:468:LEU:HB3 | 1:C:487:THR:HG22 | 1.84 | 0.59 |
| 1:E:34:MET:SD | 1:E:355:VAL:HA | 2.43 | 0.59 |
| 3:M:187:TYR:O | 3:M:193:TYR:OH | 2.20 | 0.59 |
| 3:Q:97:ARG:NH2 | 4:R:104:GLY:HA2 | 2.17 | 0.59 |
| 1:A:121:CYS:HB2 | 1:A:233:TRP:CZ3 | 2.37 | 0.59 |
| 1:C:179:LYS:HA | 1:C:185:GLU:HA | 1.84 | 0.59 |
| 1:C:298:GLY:HA2 | 1:C:301:TYR:CD1 | 2.37 | 0.59 |
| 1:E:32:THR:HA | 1:E:41:LEU:O | 2.01 | 0.59 |
| 1:E:342:VAL:O | 1:E:382:TYR:N | 2.21 | 0.59 |
| 3:M:164:TRP:HA | 3:M:176:MET:HA | 1.84 | 0.59 |
| 1:C:128:ARG:O | 1:C:203:VAL:N | 2.23 | 0.59 |
| 1:C:130:ILE:O | 1:C:198:THR:OG1 | 2.20 | 0.59 |
| 3:M:97:ARG:HD2 | 4:N:47:TRP:CE2 | 2.37 | 0.59 |
| 3:M:109:ARG:NE | 3:M:171:ASP:O | 2.35 | 0.59 |
| 4:R:48:MET:HG2 | 4:R:64:PHE:CE1 | 2.38 | 0.59 |
| 4:R:91:THR:HG23 | 4:R:115:THR:HA | 1.84 | 0.59 |
| 1:A:20:TRP:HA | 1:A:290:LYS:HA | 1.85 | 0.59 |
| 1:C:63:ALA:HA | 1:C:122:THR:H | 1.67 | 0.59 |
| 1:E:223:LEU:HG | 1:E:224:PRO:HD2 | 1.84 | 0.59 |
| 4:N:170:THR:HA | 4:N:184:SER:HA | 1.85 | 0.59 |
| 2:B:14:ASN:HD21 | 2:B:18:THR:HG22 | 1.67 | 0.59 |
| 1:E:239:LEU:O | 1:E:255:LEU:N | 2.33 | 0.59 |
| 4:N:29:PHE:O | 4:N:53:THR:HG21 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:7:SER:OG | 3:Q:22:SER:OG | 2.19 | 0.59 |
| 1:E:205:THR:HA | 1:E:210:SER:HA | 1.85 | 0.59 |
| 3:Q:66:SER:O | 3:Q:73:THR:N | 2.27 | 0.59 |
| 4:R:4:LEU:HD11 | 4:R:98:ARG:HB2 | 1.84 | 0.59 |
| 1:C:73:ARG:N | 1:C:112:SER:O | 2.28 | 0.59 |
| 1:C:379:GLY:N | 1:C:398:LYS:O | 2.36 | 0.59 |
| 3:M:4:LEU:HG | 3:M:91:HIS:HD2 | 1.67 | 0.59 |
| 3:M:13:VAL:O | 3:M:108:LYS:N | 2.24 | 0.59 |
| 3:M:24:ARG:HA | 3:M:71:ASP:HA | 1.84 | 0.59 |
| 1:A:57:ARG:HG2 | 1:A:218:PHE:HE2 | 1.68 | 0.59 |
| 1:C:304:CYS:HB3 | 1:C:328:TYR:CZ | 2.38 | 0.59 |
| 1:E:243:GLU:O | 1:E:250:GLN:NE2 | 2.35 | 0.59 |
| 4:N:174:VAL:HG23 | 4:N:176:GLN:HE22 | 1.68 | 0.59 |
| 1:C:439:LYS:O | 1:C:443:GLN:N | 2.34 | 0.58 |
| 1:E:60:CYS:HB2 | 1:E:233:TRP:CZ3 | 2.38 | 0.58 |
| 3:M:27:GLN:NE2 | 3:M:28:SER:H | 2.00 | 0.58 |
| 3:M:36:TRP:O | 3:M:48:LEU:N | 2.26 | 0.58 |
| 3:M:118:ILE:HB | 3:M:195:CYS:SG | 2.43 | 0.58 |
| 3:M:182:LEU:HD12 | 3:M:187:TYR:HD1 | 1.68 | 0.58 |
| 3:Q:121:PRO:HG2 | 3:Q:131:ALA:HB1 | 1.85 | 0.58 |
| 1:C:4:LEU:HB2 | 1:C:152:HIS:NE2 | 2.18 | 0.58 |
| 3:Q:27:GLN:HE21 | 3:Q:28:SER:H | 1.50 | 0.58 |
| 4:R:2:VAL:HG13 | 4:R:27:TYR:CD1 | 2.38 | 0.58 |
| 4:R:6:GLU:N | 4:R:110:GLN:OE1 | 2.33 | 0.58 |
| 1:E:220:ASP:HB3 | 2:F:5:GLN:NE2 | 2.18 | 0.58 |
| 3:Q:91:HIS:ND1 | 3:Q:91:HIS:O | 2.35 | 0.58 |
| 4:R:46:LYS:NZ | 4:R:63:ASP:OD2 | 2.28 | 0.58 |
| 1:A:458:TRP:CE3 | 1:A:459:ILE:HB | 2.38 | 0.58 |
| 1:C:1:PHE:HA | 1:C:140:GLY:HA3 | 1.84 | 0.58 |
| 1:C:121:CYS:HB2 | 1:C:233:TRP:HZ3 | 1.68 | 0.58 |
| 1:C:460:THR:OG1 | 1:C:461:GLN:OE1 | 2.21 | 0.58 |
| 3:Q:118:ILE:HB | 3:Q:195:CYS:SG | 2.44 | 0.58 |
| 4:R:51:ILE:HD13 | 4:R:72:LEU:HG | 1.85 | 0.58 |
| 1:A:412:LYS:HG2 | 1:A:416:ARG:HG3 | 1.85 | 0.58 |
| 1:C:261:GLY:HA3 | 2:D:2:VAL:HB | 1.84 | 0.58 |
| 1:E:58:SER:H | 1:E:226:THR:HB | 1.68 | 0.58 |
| 1:E:187:THR:HB | 1:E:290:LYS:HB2 | 1.85 | 0.58 |
| 3:Q:115:THR:O | 3:Q:138:ASN:N | 2.35 | 0.58 |
| 3:M:137:LEU:N | 3:M:176:MET:O | 2.32 | 0.58 |
| 3:Q:6:GLN:HE21 | 3:Q:21:ILE:HG21 | 1.67 | 0.58 |
| 3:Q:111:ASP:HB3 | 3:Q:201:THR:HG22 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:182:ASP:HB3 | 1:C:297:LYS:HD3 | 1.85 | 0.58 |
| 1:C:394:HIS:ND1 | 1:C:395:HIS:O | 2.37 | 0.58 |
| 1:A:73:ARG:N | 1:A:112:SER:O | 2.26 | 0.58 |
| 1:A:493:PHE:O | 1:A:497:ASN:N | 2.23 | 0.58 |
| 1:C:128:ARG:N | 1:C:203:VAL:O | 2.36 | 0.58 |
| 1:C:261:GLY:O | 1:C:265:ALA:N | 2.30 | 0.58 |
| 3:M:62:ARG:NE | 3:M:83:ASP:OD1 | 2.37 | 0.58 |
| 4:R:33:SER:O | 4:R:99:GLY:N | 2.30 | 0.58 |
| 1:A:56:VAL:O | 1:A:228:PRO:HG3 | 2.04 | 0.58 |
| 1:E:46:ILE:HD11 | 1:E:166:LYS:HB3 | 1.85 | 0.58 |
| 1:E:298:GLY:HA2 | 1:E:301:TYR:CD2 | 2.38 | 0.58 |
| 1:E:412:LYS:O | 1:E:416:ARG:N | 2.33 | 0.58 |
| 3:M:160:VAL:HA | 3:M:179:THR:O | 2.04 | 0.58 |
| 1:A:212:LEU:HD13 | 2:B:12:LEU:HD11 | 1.86 | 0.57 |
| 3:Q:149:TRP:NE1 | 3:Q:178:SER:OG | 2.30 | 0.57 |
| 1:A:151:ASN:OD1 | 1:A:152:HIS:N | 2.36 | 0.57 |
| 3:Q:10:SER:HA | 3:Q:104:TRP:H | 1.69 | 0.57 |
| 1:A:48:ILE:HB | 1:A:280:LEU:HB2 | 1.85 | 0.57 |
| 1:C:432:GLY:HA2 | 1:C:436:SER:HB2 | 1.86 | 0.57 |
| 2:D:70:VAL:HG21 | 2:F:66:LEU:HD21 | 1.86 | 0.57 |
| 1:E:1:PHE:HB3 | 1:E:166:LYS:HE3 | 1.87 | 0.57 |
| 1:E:100:GLY:N | 1:E:103:ASN:OD1 | 2.37 | 0.57 |
| 3:M:177:SER:HB2 | 4:N:171:PHE:CD2 | 2.39 | 0.57 |
| 3:M:211:ASN:HB3 | 3:M:214:GLU:HG2 | 1.86 | 0.57 |
| 3:Q:109:ARG:NE | 3:Q:171:ASP:O | 2.37 | 0.57 |
| 4:R:61:ALA:HB3 | 4:R:64:PHE:HD2 | 1.69 | 0.57 |
| 4:R:152:PRO:O | 4:R:204:HIS:NE2 | 2.37 | 0.57 |
| 1:E:146:THR:HG21 | 1:E:362:ALA:HB2 | 1.85 | 0.57 |
| 1:E:158:GLN:O | 1:E:163:GLN:N | 2.35 | 0.57 |
| 4:N:156:THR:HB | 4:N:203:ALA:HB3 | 1.85 | 0.57 |
| 3:Q:39:GLN:NE2 | 4:R:39:GLN:OE1 | 2.37 | 0.57 |
| 3:Q:119:PHE:HB2 | 3:Q:134:VAL:HG23 | 1.84 | 0.57 |
| 4:R:11:LEU:HD11 | 4:R:152:PRO:HG3 | 1.87 | 0.57 |
| 2:D:54:GLY:HA2 | 2:F:59:GLN:HE22 | 1.69 | 0.57 |
| 1:E:217:TRP:HA | 1:E:220:ASP:HB2 | 1.86 | 0.57 |
| 4:N:23:LYS:NZ | 4:N:76:ALA:O | 2.35 | 0.57 |
| 1:E:87:ASP:HB3 | 1:E:90:TYR:HD2 | 1.69 | 0.57 |
| 1:E:180:LEU:N | 1:E:184:GLY:O | 2.31 | 0.57 |
| 1:E:323:VAL:HA | 1:E:373:GLU:HA | 1.87 | 0.57 |
| 3:M:131:ALA:O | 3:M:182:LEU:N | 2.19 | 0.57 |
| 4:N:143:LEU:HD21 | 4:N:193:TRP:CD1 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:128:PRO:HB2 | 4:R:215:ILE:HA | 1.87 | 0.57 |
| 1:E:147:THR:OG1 | 1:E:371:LEU:O | 2.21 | 0.57 |
| 1:E:481:ALA:O | 1:E:485:LEU:N | 2.37 | 0.57 |
| 3:Q:6:GLN:HB3 | 3:Q:101:GLY:O | 2.04 | 0.57 |
| 3:Q:33:TYR:HB3 | 3:Q:92:ILE:HB | 1.86 | 0.57 |
| 1:C:93:LYS:N | 1:C:115:THR:O | 2.34 | 0.57 |
| 1:E:327:SER:HB2 | 1:E:369:LYS:HG2 | 1.86 | 0.57 |
| 3:M:67:GLY:HA3 | 3:M:72:PHE:HA | 1.86 | 0.57 |
| 4:R:73:GLU:HB3 | 4:R:78:THR:OG1 | 2.04 | 0.57 |
| 1:C:212:LEU:HD12 | 1:C:270:ILE:HD13 | 1.86 | 0.57 |
| 1:E:127:GLY:HA2 | 1:E:204:MET:HA | 1.86 | 0.57 |
| 1:E:475:ALA:HB3 | 1:E:480:ILE:HA | 1.86 | 0.57 |
| 4:N:37:VAL:HG22 | 4:N:47:TRP:HD1 | 1.70 | 0.57 |
| 3:Q:4:LEU:HD11 | 3:Q:91:HIS:N | 2.19 | 0.57 |
| 1:C:121:CYS:HB2 | 1:C:233:TRP:CZ3 | 2.40 | 0.57 |
| 3:M:107:ILE:O | 3:M:167:GLN:NE2 | 2.38 | 0.57 |
| 3:Q:168:ASP:O | 3:Q:172:SER:N | 2.34 | 0.57 |
| 1:A:124:LYS:HG2 | 3:Q:28:SER:CB | 2.34 | 0.56 |
| 1:C:177:THR:HG22 | 1:C:187:THR:HG23 | 1.87 | 0.56 |
| 1:C:202:TYR:CZ | 1:C:215:ARG:HB2 | 2.40 | 0.56 |
| 1:E:39:PRO:HG3 | 1:E:296:LEU:HD23 | 1.87 | 0.56 |
| 1:A:129:THR:OG1 | 1:A:215:ARG:NH2 | 2.37 | 0.56 |
| 1:C:356:THR:HB | 1:C:372:VAL:HG13 | 1.87 | 0.56 |
| 1:E:62:HIS:HB3 | 1:E:123:SER:HB2 | 1.87 | 0.56 |
| 1:E:180:LEU:HD11 | 1:E:186:VAL:HG13 | 1.87 | 0.56 |
| 1:A:128:ARG:O | 1:A:203:VAL:N | 2.28 | 0.56 |
| 2:B:19:TRP:CD1 | 2:B:20:LEU:HG | 2.40 | 0.56 |
| 1:C:457:SER:N | 1:C:460:THR:OG1 | 2.38 | 0.56 |
| 2:D:13:VAL:HG12 | 2:D:14:ASN:H | 1.69 | 0.56 |
| 1:E:128:ARG:HB2 | 1:E:203:VAL:HB | 1.87 | 0.56 |
| 3:M:121:PRO:HG2 | 3:M:131:ALA:HB1 | 1.87 | 0.56 |
| 1:A:180:LEU:HD13 | 1:A:294:LEU:HD13 | 1.87 | 0.56 |
| 1:A:304:CYS:HB3 | 1:A:328:TYR:CZ | 2.41 | 0.56 |
| 1:E:8:ASN:HB3 | 1:E:29:SER:HA | 1.86 | 0.56 |
| 1:E:310:PHE:CE2 | 1:E:392:ILE:HD12 | 2.41 | 0.56 |
| 3:M:136:PHE:CG | 4:N:185:SER:HB3 | 2.40 | 0.56 |
| 4:N:68:PHE:CE1 | 4:N:83:ILE:HG23 | 2.41 | 0.56 |
| 1:A:341:SER:O | 1:A:351:VAL:N | 2.32 | 0.56 |
| 1:A:439:LYS:O | 1:A:443:GLN:N | 2.38 | 0.56 |
| 1:C:242:PHE:HB3 | 1:C:250:GLN:NE2 | 2.20 | 0.56 |
| 3:Q:23:CYS:O | 3:Q:72:PHE:N | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:120:PRO:O | 4:R:218:ARG:NH2 | 2.39 | 0.56 |
| 4:R:158:THR:OG1 | 4:R:201:ASN:HB2 | 2.06 | 0.56 |
| 1:C:96:PHE:N | 1:C:113:ILE:HG12 | 2.21 | 0.56 |
| 3:Q:137:LEU:HD23 | 3:Q:145:ILE:HD11 | 1.87 | 0.56 |
| 1:A:28:ASP:OD1 | 1:A:29:SER:N | 2.38 | 0.56 |
| 4:N:51:ILE:HD13 | 4:N:72:LEU:HG | 1.86 | 0.56 |
| 1:E:40:THR:O | 1:E:144:HIS:N | 2.38 | 0.56 |
| 2:F:33:GLU:O | 2:F:37:ILE:N | 2.28 | 0.56 |
| 1:A:456:MET:HB3 | 1:A:461:GLN:HB3 | 1.86 | 0.56 |
| 1:A:468:LEU:HB3 | 1:A:487:THR:HG22 | 1.87 | 0.56 |
| 1:C:38:LYS:NZ | 1:C:294:LEU:O | 2.33 | 0.56 |
| 1:C:175:SER:OG | 1:C:189:ASP:OD1 | 2.14 | 0.56 |
| 1:E:59:TYR:O | 1:E:125:ALA:N | 2.32 | 0.56 |
| 1:E:360:PHE:CE2 | 1:E:362:ALA:HA | 2.41 | 0.56 |
| 1:A:202:TYR:CZ | 1:A:215:ARG:HB2 | 2.41 | 0.56 |
| 1:C:61:TYR:CE2 | 1:C:259:GLU:HB2 | 2.41 | 0.56 |
| 2:F:19:TRP:CD1 | 2:F:20:LEU:HG | 2.41 | 0.56 |
| 4:R:127:TYR:HD2 | 4:R:146:LEU:HD23 | 1.71 | 0.56 |
| 1:A:158:GLN:NE2 | 1:A:163:GLN:OE1 | 2.39 | 0.55 |
| 3:M:149:TRP:NE1 | 3:M:178:SER:OG | 2.39 | 0.55 |
| 4:R:29:PHE:HZ | 4:R:72:LEU:HD22 | 1.72 | 0.55 |
| 1:A:383:ILE:O | 1:A:393:ASN:HA | 2.06 | 0.55 |
| 1:C:12:ILE:HG13 | 1:C:33:ILE:HG13 | 1.87 | 0.55 |
| 1:C:180:LEU:N | 1:C:184:GLY:O | 2.27 | 0.55 |
| 1:C:308:PHE:HZ | 1:C:338:PRO:HD2 | 1.71 | 0.55 |
| 3:M:135:CYS:O | 3:M:178:SER:N | 2.29 | 0.55 |
| 3:Q:4:LEU:HD21 | 3:Q:91:HIS:HB3 | 1.88 | 0.55 |
| 4:R:2:VAL:HG22 | 4:R:27:TYR:HB3 | 1.88 | 0.55 |
| 3:M:116:VAL:O | 3:M:208:LYS:NZ | 2.30 | 0.55 |
| 1:A:458:TRP:O | 1:A:462:GLY:N | 2.40 | 0.55 |
| 3:M:114:PRO:HB3 | 3:M:140:PHE:CD2 | 2.41 | 0.55 |
| 1:C:100:GLY:N | 1:C:103:ASN:OD1 | 2.35 | 0.55 |
| 1:A:61:TYR:CE2 | 1:A:259:GLU:HB2 | 2.42 | 0.55 |
| 1:A:199:GLU:HA | 1:A:215:ARG:NH2 | 2.21 | 0.55 |
| 1:A:268:GLY:HA3 | 2:B:10:SER:H | 1.71 | 0.55 |
| 2:B:57:ASN:H | 2:B:60:ARG:NH1 | 2.05 | 0.55 |
| 1:E:4:LEU:HB2 | 1:E:152:HIS:NE2 | 2.22 | 0.55 |
| 3:M:38:GLN:HB3 | 3:M:48:LEU:HD11 | 1.88 | 0.55 |
| 1:A:92:CYS:HA | 1:A:116:CYS:HA | 1.88 | 0.55 |
| 1:E:233:TRP:H | 1:E:236:ARG:HD3 | 1.70 | 0.55 |
| 3:M:120:PRO:HG2 | 4:N:218:ARG:NE | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:119:PRO:HG3 | 4:N:178:ASP:HB3 | 1.88 | 0.55 |
| 1:A:52:GLN:H | 1:A:134:ASN:HB3 | 1.71 | 0.55 |
| 1:A:202:TYR:N | 1:A:213:VAL:O | 2.34 | 0.55 |
| 1:C:197:ASN:HB3 | 1:C:200:ALA:HB2 | 1.87 | 0.55 |
| 3:M:38:GLN:O | 3:M:46:ARG:N | 2.27 | 0.55 |
| 3:Q:23:CYS:N | 3:Q:72:PHE:O | 2.34 | 0.55 |
| 3:Q:64:SER:N | 3:Q:75:ASN:O | 2.28 | 0.55 |
| 3:Q:184:LYS:NZ | 3:Q:188:GLU:OE2 | 2.26 | 0.55 |
| 1:A:325:GLU:HA | 1:A:371:LEU:HA | 1.88 | 0.55 |
| 1:C:322:VAL:O | 1:C:373:GLU:HG3 | 2.05 | 0.55 |
| 1:E:202:TYR:CE2 | 1:E:215:ARG:HB2 | 2.42 | 0.55 |
| 3:M:77:HIS:CD2 | 3:M:78:PRO:HD3 | 2.41 | 0.55 |
| 4:N:23:LYS:HA | 4:N:78:THR:HA | 1.88 | 0.55 |
| 3:Q:191:ASN:HB3 | 3:Q:211:ASN:OD1 | 2.07 | 0.55 |
| 1:A:321:THR:HA | 1:A:376:PRO:HD2 | 1.89 | 0.55 |
| 1:E:215:ARG:HA | 1:E:218:PHE:HB3 | 1.89 | 0.55 |
| 3:M:79:VAL:HB | 3:M:105:LEU:HD21 | 1.89 | 0.55 |
| 3:M:116:VAL:HG22 | 3:M:137:LEU:HG | 1.89 | 0.55 |
| 3:M:151:ILE:HG12 | 3:M:193:TYR:HD1 | 1.72 | 0.55 |
| 3:Q:4:LEU:HB2 | 3:Q:100:ALA:HB2 | 1.88 | 0.55 |
| 1:C:73:ARG:HB2 | 1:C:112:SER:HB3 | 1.89 | 0.54 |
| 1:E:226:THR:HG23 | 1:E:233:TRP:NE1 | 2.21 | 0.54 |
| 1:E:385:VAL:O | 1:E:391:GLN:HA | 2.07 | 0.54 |
| 1:E:11:PHE:HD1 | 1:E:32:THR:HB | 1.73 | 0.54 |
| 1:E:73:ARG:HH21 | 1:E:77:THR:HB | 1.72 | 0.54 |
| 1:E:80:ALA:O | 1:E:94:GLN:NE2 | 2.41 | 0.54 |
| 2:F:30:MET:O | 2:F:34:ASN:N | 2.20 | 0.54 |
| 3:Q:136:PHE:CD1 | 4:R:185:SER:HB3 | 2.42 | 0.54 |
| 1:A:183:TYR:HB3 | 1:A:294:LEU:HD12 | 1.89 | 0.54 |
| 1:C:2:ASN:HB2 | 1:C:152:HIS:CE1 | 2.42 | 0.54 |
| 1:C:16:SER:OG | 1:C:36:ASN:ND2 | 2.38 | 0.54 |
| 2:D:23:THR:O | 2:D:27:ARG:HG2 | 2.08 | 0.54 |
| 1:E:48:ILE:HG12 | 1:E:137:TYR:HD1 | 1.71 | 0.54 |
| 4:N:91:THR:HG23 | 4:N:115:THR:HA | 1.89 | 0.54 |
| 3:Q:88:TYR:CE1 | 3:Q:102:PRO:HB3 | 2.43 | 0.54 |
| 3:Q:91:HIS:NE2 | 3:Q:98:SER:OG | 2.16 | 0.54 |
| 4:R:160:ASN:OD1 | 4:R:199:THR:N | 2.36 | 0.54 |
| 1:A:4:LEU:HB2 | 1:A:152:HIS:CD2 | 2.43 | 0.54 |
| 1:C:298:GLY:HA2 | 1:C:301:TYR:HD1 | 1.72 | 0.54 |
| 1:E:59:TYR:OH | 1:E:218:PHE:O | 2.17 | 0.54 |
| 1:E:73:ARG:NH2 | 1:E:77:THR:HB | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:84:LYS:HB3 | 1:E:90:TYR:HB3 | 1.88 | 0.54 |
| 1:E:304:CYS:HB3 | 1:E:328:TYR:CZ | 2.42 | 0.54 |
| 2:F:56:ASN:HD22 | 2:F:59:GLN:NE2 | 2.05 | 0.54 |
| 3:M:6:GLN:HE21 | 3:M:21:ILE:HG21 | 1.73 | 0.54 |
| 4:N:20:ILE:N | 4:N:81:LEU:O | 2.35 | 0.54 |
| 3:Q:40:LYS:HB2 | 3:Q:43:GLN:CD | 2.28 | 0.54 |
| 3:Q:45:PRO:HB2 | 4:R:108:TRP:CE2 | 2.42 | 0.54 |
| 3:Q:67:GLY:HA3 | 3:Q:72:PHE:HA | 1.89 | 0.54 |
| 1:A:96:PHE:N | 1:A:113:ILE:HG12 | 2.23 | 0.54 |
| 1:A:128:ARG:N | 1:A:203:VAL:O | 2.40 | 0.54 |
| 1:A:142:PHE:HA | 1:A:164:ALA:HA | 1.90 | 0.54 |
| 1:C:41:LEU:HD23 | 1:C:143:VAL:HB | 1.90 | 0.54 |
| 1:E:119:PHE:CD2 | 1:E:236:ARG:HD2 | 2.43 | 0.54 |
| 2:F:65:ILE:HD12 | 2:F:68:LEU:HD22 | 1.90 | 0.54 |
| 3:Q:35:HIS:HE2 | 4:R:103:TYR:C | 2.11 | 0.54 |
| 1:A:61:TYR:HA | 1:A:223:LEU:HD11 | 1.90 | 0.54 |
| 1:A:121:CYS:HB2 | 1:A:233:TRP:HZ3 | 1.71 | 0.54 |
| 1:C:42:ASP:O | 1:C:142:PHE:N | 2.32 | 0.54 |
| 1:C:412:LYS:HE2 | 1:C:416:ARG:HD3 | 1.90 | 0.54 |
| 1:C:437:ILE:HD12 | 1:C:440:ALA:HB3 | 1.88 | 0.54 |
| 1:C:449:PHE:O | 1:C:452:LEU:N | 2.41 | 0.54 |
| 2:F:23:THR:HB | 2:F:27:ARG:HH12 | 1.73 | 0.54 |
| 3:Q:19:ALA:HB3 | 3:Q:79:VAL:HG11 | 1.90 | 0.54 |
| 3:Q:62:ARG:HB2 | 3:Q:78:PRO:HD2 | 1.89 | 0.54 |
| 1:A:65:VAL:HG23 | 1:A:254:ALA:HB2 | 1.87 | 0.54 |
| 1:C:256:GLY:H | 1:E:263:HIS:CD2 | 2.26 | 0.54 |
| 1:E:482:LEU:HA | 1:E:485:LEU:HG | 1.90 | 0.54 |
| 3:Q:17:GLN:O | 3:Q:79:VAL:HG22 | 2.08 | 0.54 |
| 4:R:29:PHE:O | 4:R:53:THR:HG21 | 2.07 | 0.54 |
| 1:C:449:PHE:H | 1:C:452:LEU:HD12 | 1.73 | 0.54 |
| 1:E:142:PHE:HA | 1:E:164:ALA:HA | 1.89 | 0.54 |
| 3:M:163:SER:O | 3:M:177:SER:N | 2.38 | 0.54 |
| 4:N:202:VAL:O | 4:N:211:VAL:N | 2.25 | 0.54 |
| 1:A:223:LEU:HG | 1:A:224:PRO:HD2 | 1.90 | 0.54 |
| 1:C:179:LYS:HG2 | 1:C:185:GLU:HB2 | 1.89 | 0.54 |
| 3:M:76:ILE:HB | 3:M:79:VAL:HG12 | 1.90 | 0.54 |
| 4:R:38:LYS:HG3 | 4:R:94:TYR:CE1 | 2.42 | 0.54 |
| 1:C:316:ASP:HA | 1:C:322:VAL:HA | 1.89 | 0.54 |
| 1:E:4:LEU:HB2 | 1:E:152:HIS:CD2 | 2.42 | 0.54 |
| 1:E:49:GLU:O | 1:E:136:LYS:N | 2.40 | 0.54 |
| 1:E:59:TYR:CD1 | 1:E:225:TRP:HB3 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:5:MET:O | 4:R:23:LYS:N | 2.31 | 0.54 |
| 1:A:9:ARG:HG2 | 1:A:11:PHE:HE1 | 1.73 | 0.53 |
| 1:C:53:LEU:HD22 | 1:C:130:ILE:HG12 | 1.90 | 0.53 |
| 1:E:130:ILE:O | 1:E:198:THR:OG1 | 2.17 | 0.53 |
| 3:M:50:TYR:HB3 | 3:M:56:GLU:OE2 | 2.08 | 0.53 |
| 1:C:52:GLN:H | 1:C:134:ASN:HB3 | 1.72 | 0.53 |
| 4:N:36:TRP:CH2 | 4:N:96:CYS:HB3 | 2.44 | 0.53 |
| 3:Q:133:VAL:O | 3:Q:180:LEU:N | 2.31 | 0.53 |
| 1:A:58:SER:O | 1:A:226:THR:N | 2.41 | 0.53 |
| 1:C:41:LEU:HA | 1:C:143:VAL:HA | 1.91 | 0.53 |
| 3:M:17:GLN:O | 3:M:79:VAL:HG22 | 2.07 | 0.53 |
| 3:M:36:TRP:O | 3:M:47:LEU:HD12 | 2.08 | 0.53 |
| 4:N:8:GLY:O | 4:N:10:GLU:HG3 | 2.08 | 0.53 |
| 3:Q:44:PRO:HB3 | 4:R:109:GLY:O | 2.08 | 0.53 |
| 4:R:37:VAL:HG22 | 4:R:47:TRP:HD1 | 1.73 | 0.53 |
| 4:R:93:SER:HA | 4:R:113:SER:HA | 1.89 | 0.53 |
| 3:M:168:ASP:O | 3:M:172:SER:N | 2.36 | 0.53 |
| 4:N:47:TRP:HZ2 | 4:N:50:TRP:HD1 | 1.57 | 0.53 |
| 3:Q:62:ARG:O | 3:Q:76:ILE:HA | 2.08 | 0.53 |
| 1:A:27:GLY:N | 1:A:45:MET:HB3 | 2.24 | 0.53 |
| 1:A:50:ALA:HA | 1:A:135:ILE:HA | 1.91 | 0.53 |
| 1:A:378:PHE:CD2 | 1:A:402:THR:HG22 | 2.43 | 0.53 |
| 1:C:481:ALA:HA | 1:C:484:PHE:HB3 | 1.89 | 0.53 |
| 3:M:117:SER:O | 3:M:135:CYS:HA | 2.09 | 0.53 |
| 3:Q:95:LEU:HD23 | 3:Q:97:ARG:HG3 | 1.90 | 0.53 |
| 3:Q:177:SER:HB2 | 4:R:171:PHE:CD2 | 2.43 | 0.53 |
| 4:R:38:LYS:N | 4:R:46:LYS:O | 2.41 | 0.53 |
| 4:R:125:SER:HB2 | 4:R:148:LYS:HB3 | 1.91 | 0.53 |
| 1:A:93:LYS:O | 1:A:115:THR:N | 2.31 | 0.53 |
| 3:M:121:PRO:HD3 | 3:M:133:VAL:HG22 | 1.91 | 0.53 |
| 3:Q:23:CYS:HB3 | 3:Q:72:PHE:HB2 | 1.91 | 0.53 |
| 4:R:141:VAL:HG13 | 4:R:190:SER:HB3 | 1.89 | 0.53 |
| 1:E:416:ARG:HB3 | 1:E:427:PHE:HE2 | 1.73 | 0.53 |
| 3:M:125:GLN:HG2 | 3:M:130:GLY:O | 2.09 | 0.53 |
| 4:N:33:SER:OG | 4:N:35:HIS:NE2 | 2.35 | 0.53 |
| 4:N:38:LYS:N | 4:N:46:LYS:O | 2.41 | 0.53 |
| 3:Q:27:GLN:NE2 | 3:Q:28:SER:H | 2.06 | 0.53 |
| 2:B:1:SER:OG | 2:B:2:VAL:N | 2.40 | 0.53 |
| 3:M:135:CYS:HB3 | 3:M:178:SER:HB3 | 1.91 | 0.53 |
| 1:A:494:LEU:O | 1:A:498:VAL:HG12 | 2.09 | 0.53 |
| 3:M:92:ILE:HG21 | 4:N:101:GLY:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:160:ASN:ND2 | 4:N:197:THR:O | 2.36 | 0.53 |
| 4:R:38:LYS:N | 4:R:48:MET:HG3 | 2.24 | 0.53 |
| 4:R:199:THR:HA | 4:R:214:LYS:HA | 1.91 | 0.53 |
| 4:R:203:ALA:HA | 4:R:210:LYS:HA | 1.91 | 0.53 |
| 1:A:370:VAL:HG12 | 1:A:372:VAL:HG23 | 1.92 | 0.53 |
| 1:C:124:LYS:HG2 | 3:M:28:SER:CB | 2.38 | 0.53 |
| 1:C:311:ALA:N | 1:C:325:GLU:O | 2.39 | 0.53 |
| 2:D:57:ASN:O | 2:D:60:ARG:N | 2.38 | 0.53 |
| 1:E:304:CYS:H | 1:E:338:PRO:HD3 | 1.74 | 0.53 |
| 3:M:2:ILE:O | 3:M:91:HIS:NE2 | 2.41 | 0.53 |
| 3:M:55:LEU:HD11 | 3:M:61:SER:HA | 1.89 | 0.53 |
| 3:M:188:GLU:HA | 3:M:212:ARG:CZ | 2.39 | 0.53 |
| 4:N:150:TYR:O | 4:N:180:TYR:N | 2.42 | 0.53 |
| 1:C:456:MET:HB2 | 1:C:461:GLN:HB3 | 1.91 | 0.52 |
| 1:E:20:TRP:HA | 1:E:289:LEU:O | 2.09 | 0.52 |
| 1:E:460:THR:O | 1:E:464:MET:HG2 | 2.09 | 0.52 |
| 4:N:5:MET:O | 4:N:23:LYS:N | 2.37 | 0.52 |
| 1:A:61:TYR:CG | 1:A:262:LEU:HD11 | 2.44 | 0.52 |
| 1:C:38:LYS:HD2 | 1:C:294:LEU:HD23 | 1.90 | 0.52 |
| 1:C:39:PRO:HG2 | 1:C:183:TYR:CD1 | 2.44 | 0.52 |
| 1:C:489:GLY:C | 1:C:491:LEU:H | 2.13 | 0.52 |
| 1:E:60:CYS:HB2 | 1:E:233:TRP:CE3 | 2.44 | 0.52 |
| 1:E:155:TYR:CE1 | 1:E:166:LYS:HG3 | 2.44 | 0.52 |
| 1:E:178:LEU:C | 1:E:185:GLU:HG3 | 2.29 | 0.52 |
| 1:A:242:PHE:HB3 | 1:A:250:GLN:HE21 | 1.74 | 0.52 |
| 1:C:149:SER:OG | 1:C:325:GLU:OE1 | 2.16 | 0.52 |
| 3:M:120:PRO:HG2 | 4:N:218:ARG:CZ | 2.39 | 0.52 |
| 3:Q:197:ALA:O | 3:Q:206:ILE:N | 2.32 | 0.52 |
| 1:A:31:LEU:N | 1:A:43:VAL:O | 2.38 | 0.52 |
| 1:E:432:GLY:H | 1:E:436:SER:H | 1.57 | 0.52 |
| 1:E:479:SER:HA | 1:E:482:LEU:HD13 | 1.91 | 0.52 |
| 3:M:6:GLN:HG2 | 3:M:103:SER:OG | 2.09 | 0.52 |
| 4:R:156:THR:N | 4:R:203:ALA:O | 2.27 | 0.52 |
| 1:C:4:LEU:HB2 | 1:C:152:HIS:CD2 | 2.44 | 0.52 |
| 1:E:88:SER:O | 1:E:236:ARG:NH2 | 2.43 | 0.52 |
| 1:E:465:GLY:HA3 | 1:E:492:LEU:HD11 | 1.91 | 0.52 |
| 3:M:156:ARG:HG2 | 3:M:158:ASN:H | 1.73 | 0.52 |
| 4:N:64:PHE:HD1 | 4:N:68:PHE:CE2 | 2.28 | 0.52 |
| 1:A:242:PHE:HB3 | 1:A:250:GLN:NE2 | 2.24 | 0.52 |
| 1:C:243:GLU:CD | 1:C:251:SER:HB3 | 2.30 | 0.52 |
| 1:E:97:THR:O | 1:E:99:ARG:NH1 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:206:VAL:N | 1:E:209:LYS:O | 2.36 | 0.52 |
| 3:M:145:ILE:HB | 3:M:199:HIS:HD2 | 1.74 | 0.52 |
| 4:R:91:THR:OG1 | 4:R:116:VAL:N | 2.32 | 0.52 |
| 4:R:144:GLY:HA2 | 4:R:185:SER:HA | 1.90 | 0.52 |
| 1:A:38:LYS:NZ | 1:A:294:LEU:O | 2.32 | 0.52 |
| 1:C:167:PHE:HZ | 1:C:188:LEU:HD22 | 1.75 | 0.52 |
| 1:C:263:HIS:CD2 | 1:E:256:GLY:H | 2.28 | 0.52 |
| 1:E:167:PHE:HZ | 1:E:188:LEU:HD22 | 1.75 | 0.52 |
| 3:M:36:TRP:HD1 | 3:M:49:ILE:HB | 1.74 | 0.52 |
| 4:N:158:THR:OG1 | 4:N:201:ASN:HB2 | 2.09 | 0.52 |
| 1:A:207:GLY:O | 3:Q:93:ARG:NH1 | 2.26 | 0.52 |
| 1:C:463:LEU:HA | 1:C:466:ALA:HB3 | 1.91 | 0.52 |
| 1:E:12:ILE:HB | 1:E:33:ILE:HA | 1.91 | 0.52 |
| 1:E:16:SER:HG | 1:E:36:ASN:HD22 | 1.52 | 0.52 |
| 3:M:13:VAL:N | 3:M:106:GLU:O | 2.41 | 0.52 |
| 4:N:72:LEU:HD23 | 4:N:79:ALA:HA | 1.92 | 0.52 |
| 3:Q:187:TYR:O | 3:Q:212:ARG:NE | 2.43 | 0.52 |
| 1:A:489:GLY:O | 1:A:491:LEU:N | 2.43 | 0.52 |
| 1:E:147:THR:O | 1:E:371:LEU:N | 2.31 | 0.52 |
| 4:N:150:TYR:HE1 | 4:N:153:GLU:HA | 1.74 | 0.52 |
| 4:N:164:LEU:O | 4:N:168:VAL:HG21 | 2.10 | 0.52 |
| 3:Q:163:SER:O | 3:Q:177:SER:N | 2.39 | 0.52 |
| 4:R:97:ALA:HB1 | 4:R:105:VAL:HB | 1.92 | 0.52 |
| 2:B:55:SER:HA | 2:B:60:ARG:HH11 | 1.74 | 0.51 |
| 1:E:258:GLN:O | 1:E:262:LEU:N | 2.39 | 0.51 |
| 4:N:152:PRO:HA | 4:N:180:TYR:HE2 | 1.76 | 0.51 |
| 3:Q:38:GLN:N | 3:Q:46:ARG:O | 2.43 | 0.51 |
| 1:A:337:ILE:HB | 1:A:359:PRO:HB2 | 1.92 | 0.51 |
| 1:E:137:TYR:HB2 | 1:E:169:VAL:HG23 | 1.91 | 0.51 |
| 2:F:41:GLY:HA2 | 2:F:44:PHE:HD2 | 1.75 | 0.51 |
| 4:N:141:VAL:N | 4:N:188:VAL:O | 2.43 | 0.51 |
| 3:Q:77:HIS:CD2 | 3:Q:78:PRO:HD3 | 2.45 | 0.51 |
| 3:Q:149:TRP:CD2 | 3:Q:180:LEU:HB2 | 2.46 | 0.51 |
| 1:A:226:THR:HA | 1:A:233:TRP:CD1 | 2.46 | 0.51 |
| 1:A:434:PHE:O | 1:A:438:GLY:N | 2.39 | 0.51 |
| 1:C:202:TYR:CE2 | 1:C:215:ARG:HB2 | 2.46 | 0.51 |
| 4:N:47:TRP:CZ2 | 4:N:50:TRP:HD1 | 2.27 | 0.51 |
| 1:A:243:GLU:CD | 1:A:251:SER:HB3 | 2.31 | 0.51 |
| 1:C:207:GLY:O | 3:M:93:ARG:NH1 | 2.35 | 0.51 |
| 1:C:241:GLU:HB2 | 1:C:253:VAL:HG23 | 1.92 | 0.51 |
| 1:E:460:THR:OG1 | 1:E:461:GLN:OE1 | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:48:MET:HA | 4:N:64:PHE:CD2 | 2.44 | 0.51 |
| 3:Q:48:LEU:HD23 | 3:Q:59:VAL:HG11 | 1.92 | 0.51 |
| 1:C:8:ASN:HD22 | 1:C:29:SER:HB3 | 1.75 | 0.51 |
| 1:C:126:ILE:O | 1:C:205:THR:N | 2.37 | 0.51 |
| 1:C:301:TYR:CE2 | 1:C:334:PRO:HB2 | 2.46 | 0.51 |
| 1:E:458:TRP:O | 1:E:462:GLY:N | 2.40 | 0.51 |
| 3:M:120:PRO:HB3 | 3:M:210:PHE:CZ | 2.46 | 0.51 |
| 4:N:171:PHE:O | 4:N:182:LEU:HB2 | 2.11 | 0.51 |
| 1:A:193:ARG:NE | 1:E:395:HIS:CE1 | 2.79 | 0.51 |
| 1:C:89:SER:O | 1:C:119:PHE:N | 2.43 | 0.51 |
| 1:E:1:PHE:HA | 1:E:140:GLY:HA3 | 1.91 | 0.51 |
| 1:E:12:ILE:HD11 | 1:E:31:LEU:HB3 | 1.92 | 0.51 |
| 1:E:50:ALA:HA | 1:E:134:ASN:O | 2.11 | 0.51 |
| 1:E:442:HIS:HA | 1:E:445:PHE:HB3 | 1.92 | 0.51 |
| 3:M:116:VAL:O | 3:M:208:LYS:HG3 | 2.11 | 0.51 |
| 1:A:137:TYR:CG | 1:A:285:LEU:HD22 | 2.46 | 0.51 |
| 1:A:269:ALA:HB2 | 2:B:7:HIS:HD1 | 1.76 | 0.51 |
| 3:Q:97:ARG:HD2 | 4:R:47:TRP:CE2 | 2.46 | 0.51 |
| 1:A:342:VAL:O | 1:A:381:SER:HB2 | 2.09 | 0.51 |
| 1:C:1:PHE:CD1 | 1:C:155:TYR:HB2 | 2.46 | 0.51 |
| 1:C:56:VAL:O | 1:C:228:PRO:HG3 | 2.10 | 0.51 |
| 1:C:100:GLY:HA2 | 1:C:108:PHE:CD1 | 2.45 | 0.51 |
| 1:C:489:GLY:HA2 | 1:C:493:PHE:HB2 | 1.92 | 0.51 |
| 1:E:91:VAL:HG11 | 1:E:237:GLU:CG | 2.41 | 0.51 |
| 1:E:237:GLU:O | 1:E:240:MET:N | 2.42 | 0.51 |
| 3:M:23:CYS:HB2 | 3:M:36:TRP:CH2 | 2.46 | 0.51 |
| 4:N:73:GLU:HB3 | 4:N:78:THR:OG1 | 2.11 | 0.51 |
| 4:R:56:GLY:HA2 | 4:R:72:LEU:HD12 | 1.93 | 0.51 |
| 1:E:214:HIS:H | 2:F:7:HIS:CD2 | 2.29 | 0.51 |
| 1:E:225:TRP:O | 1:E:233:TRP:HB3 | 2.11 | 0.51 |
| 4:N:186:VAL:HG22 | 4:N:188:VAL:HG13 | 1.93 | 0.51 |
| 3:Q:161:LEU:N | 3:Q:179:THR:O | 2.40 | 0.51 |
| 3:Q:194:THR:HG23 | 3:Q:209:SER:HB2 | 1.93 | 0.51 |
| 4:R:127:TYR:HE2 | 4:R:148:LYS:HD3 | 1.75 | 0.51 |
| 4:R:160:ASN:HD21 | 4:R:198:VAL:HA | 1.75 | 0.51 |
| 1:A:143:VAL:N | 1:A:163:GLN:O | 2.43 | 0.51 |
| 1:C:43:VAL:HG22 | 1:C:141:ILE:HG13 | 1.93 | 0.51 |
| 1:C:201:PHE:CE1 | 1:C:212:LEU:HD22 | 2.46 | 0.51 |
| 1:E:301:TYR:CE1 | 1:E:334:PRO:HB2 | 2.46 | 0.51 |
| 1:E:303:MET:HB3 | 1:E:338:PRO:HG3 | 1.91 | 0.51 |
| 1:E:322:VAL:C | 1:E:373:GLU:HG3 | 2.32 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:334:PRO:HB3 | 1:E:360:PHE:CZ | 2.46 | 0.51 |
| 1:E:376:PRO:HG2 | 1:E:398:LYS:HB2 | 1.93 | 0.51 |
| 4:N:129:LEU:HD11 | 4:N:146:LEU:HB2 | 1.92 | 0.51 |
| 1:A:363:THR:HG23 | 1:A:365:SER:H | 1.75 | 0.50 |
| 2:B:15:LYS:O | 2:B:16:THR:HG23 | 2.11 | 0.50 |
| 4:N:2:VAL:HG13 | 4:N:27:TYR:CD1 | 2.46 | 0.50 |
| 3:Q:34:MET:HA | 3:Q:90:GLN:O | 2.11 | 0.50 |
| 1:A:53:LEU:HD22 | 1:A:130:ILE:HG12 | 1.92 | 0.50 |
| 1:A:187:THR:HB | 1:A:290:LYS:HD3 | 1.93 | 0.50 |
| 1:A:272:VAL:HB | 1:A:278:VAL:HG23 | 1.93 | 0.50 |
| 1:E:39:PRO:HD2 | 1:E:294:LEU:HD11 | 1.92 | 0.50 |
| 1:E:213:VAL:HA | 2:F:7:HIS:ND1 | 2.26 | 0.50 |
| 1:E:345:LEU:HD21 | 1:E:393:ASN:HD21 | 1.76 | 0.50 |
| 3:M:60:PRO:HG2 | 3:M:62:ARG:NH1 | 2.26 | 0.50 |
| 4:N:125:SER:HB2 | 4:N:148:LYS:HB3 | 1.94 | 0.50 |
| 1:A:437:ILE:HD12 | 1:A:440:ALA:HB3 | 1.93 | 0.50 |
| 1:C:204:MET:O | 1:C:211:PHE:N | 2.44 | 0.50 |
| 1:C:274:TYR:HE2 | 4:N:100:VAL:O | 1.95 | 0.50 |
| 1:C:402:THR:O | 1:C:406:ALA:N | 2.34 | 0.50 |
| 1:C:450:ARG:HD3 | 1:C:490:VAL:HG13 | 1.93 | 0.50 |
| 3:M:197:ALA:O | 3:M:206:ILE:N | 2.31 | 0.50 |
| 4:R:106:ASP:OD1 | 4:R:107:TYR:N | 2.42 | 0.50 |
| 1:A:458:TRP:H | 1:A:461:GLN:HE22 | 1.59 | 0.50 |
| 1:C:107:LEU:HD23 | 1:C:108:PHE:H | 1.76 | 0.50 |
| 1:C:382:TYR:CD1 | 1:C:395:HIS:HA | 2.47 | 0.50 |
| 1:E:101:TRP:NE1 | 1:E:106:GLY:O | 2.43 | 0.50 |
| 1:E:235:ASN:HB3 | 1:E:238:LEU:HG | 1.92 | 0.50 |
| 2:F:57:ASN:H | 2:F:60:ARG:NH1 | 2.09 | 0.50 |
| 3:M:51:LEU:C | 3:M:53:SER:H | 2.15 | 0.50 |
| 3:M:134:VAL:HG11 | 4:N:146:LEU:HD13 | 1.94 | 0.50 |
| 1:A:193:ARG:HG3 | 1:A:194:SER:N | 2.25 | 0.50 |
| 1:A:460:THR:HG1 | 1:A:461:GLN:H | 1.59 | 0.50 |
| 1:E:24:VAL:HA | 1:E:285:LEU:O | 2.10 | 0.50 |
| 1:E:87:ASP:HB3 | 1:E:90:TYR:CD2 | 2.46 | 0.50 |
| 1:E:214:HIS:CD2 | 2:F:7:HIS:CD2 | 3.00 | 0.50 |
| 1:E:351:VAL:HG23 | 1:E:352:GLY:H | 1.76 | 0.50 |
| 3:M:190:HIS:O | 3:M:212:ARG:NH2 | 2.35 | 0.50 |
| 4:R:48:MET:HA | 4:R:64:PHE:CD2 | 2.47 | 0.50 |
| 1:C:237:GLU:OE1 | 1:C:237:GLU:N | 2.41 | 0.50 |
| 1:C:453:PHE:HB3 | 2:F:45:LEU:HD21 | 1.94 | 0.50 |
| 3:Q:141:TYR:HB2 | 3:Q:173:THR:HA | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:165:THR:N | 3:Q:175:SER:O | 2.43 | 0.50 |
| 1:A:207:GLY:HA2 | 3:Q:31:THR:HG21 | 1.94 | 0.50 |
| 1:C:258:GLN:HB3 | 2:D:2:VAL:HG11 | 1.93 | 0.50 |
| 1:E:306:GLY:O | 1:E:328:TYR:HE1 | 1.94 | 0.50 |
| 4:N:86:LEU:HD22 | 4:N:116:VAL:HG21 | 1.94 | 0.50 |
| 3:Q:49:ILE:HG21 | 3:Q:65:GLY:HA3 | 1.94 | 0.50 |
| 3:Q:147:VAL:HG11 | 3:Q:178:SER:HB2 | 1.94 | 0.50 |
| 1:A:204:MET:N | 1:A:211:PHE:O | 2.26 | 0.50 |
| 1:C:370:VAL:HG12 | 1:C:372:VAL:HG23 | 1.94 | 0.50 |
| 1:E:70:THR:HA | 1:E:115:THR:HA | 1.93 | 0.50 |
| 1:E:487:THR:OG1 | 1:E:488:GLY:N | 2.44 | 0.50 |
| 3:M:151:ILE:HG12 | 3:M:193:TYR:CD1 | 2.47 | 0.50 |
| 4:N:10:GLU:HB3 | 4:N:12:LYS:HE2 | 1.94 | 0.50 |
| 4:N:21:SER:HA | 4:N:80:TYR:CD1 | 2.47 | 0.50 |
| 3:Q:114:PRO:CA | 3:Q:140:PHE:HB3 | 2.42 | 0.50 |
| 4:R:171:PHE:O | 4:R:182:LEU:HB2 | 2.12 | 0.50 |
| 1:A:60:CYS:N | 1:A:224:PRO:O | 2.33 | 0.50 |
| 1:A:75:PRO:HB3 | 1:A:110:LYS:HB2 | 1.94 | 0.50 |
| 1:A:183:TYR:O | 1:A:294:LEU:HA | 2.12 | 0.50 |
| 1:A:311:ALA:N | 1:A:325:GLU:O | 2.43 | 0.50 |
| 1:A:499:HIS:N | 1:A:500:ALA:O | 2.37 | 0.50 |
| 1:C:88:SER:O | 1:C:236:ARG:NH2 | 2.45 | 0.50 |
| 1:C:147:THR:OG1 | 1:C:371:LEU:O | 2.30 | 0.50 |
| 1:C:224:PRO:HB3 | 1:C:236:ARG:HA | 1.94 | 0.50 |
| 1:E:387:ARG:CA | 1:E:391:GLN:HB3 | 2.41 | 0.50 |
| 4:N:2:VAL:HG21 | 4:N:98:ARG:HH12 | 1.77 | 0.50 |
| 4:N:156:THR:N | 4:N:203:ALA:O | 2.27 | 0.50 |
| 3:Q:33:TYR:H | 3:Q:51:LEU:HA | 1.77 | 0.50 |
| 1:A:19:THR:O | 1:A:291:MET:N | 2.42 | 0.49 |
| 1:E:117:ALA:HB2 | 1:E:252:VAL:HG21 | 1.94 | 0.49 |
| 1:E:197:ASN:HD22 | 1:E:200:ALA:HB2 | 1.77 | 0.49 |
| 4:N:174:VAL:HG23 | 4:N:176:GLN:NE2 | 2.25 | 0.49 |
| 4:R:167:GLY:C | 4:R:187:THR:H | 2.15 | 0.49 |
| 1:A:39:PRO:HB2 | 1:A:143:VAL:CG2 | 2.42 | 0.49 |
| 1:A:52:GLN:NE2 | 4:R:53:THR:H | 2.08 | 0.49 |
| 1:C:32:THR:HA | 1:C:41:LEU:O | 2.12 | 0.49 |
| 4:N:193:TRP:CZ2 | 4:N:215:ILE:HG22 | 2.48 | 0.49 |
| 4:R:149:GLY:N | 4:R:181:THR:HG22 | 2.27 | 0.49 |
| 1:A:20:TRP:HA | 1:A:289:LEU:O | 2.12 | 0.49 |
| 1:A:183:TYR:HA | 1:A:295:ALA:HB3 | 1.94 | 0.49 |
| 1:C:210:SER:O | 1:C:272:VAL:HG22 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:336:LYS:O | 1:C:338:PRO:HD3 | 2.13 | 0.49 |
| 1:E:73:ARG:N | 1:E:112:SER:O | 2.33 | 0.49 |
| 1:E:437:ILE:HD12 | 1:E:440:ALA:HB3 | 1.94 | 0.49 |
| 2:F:33:GLU:HA | 2:F:36:ILE:HG22 | 1.94 | 0.49 |
| 3:Q:24:ARG:HA | 3:Q:71:ASP:HA | 1.94 | 0.49 |
| 3:Q:33:TYR:O | 3:Q:92:ILE:N | 2.33 | 0.49 |
| 3:Q:39:GLN:NE2 | 3:Q:43:GLN:O | 2.45 | 0.49 |
| 1:A:55:GLU:HA | 1:A:128:ARG:HG2 | 1.94 | 0.49 |
| 1:A:172:ASN:HA | 1:E:394:HIS:CD2 | 2.47 | 0.49 |
| 1:A:417:LEU:HA | 1:A:424:ALA:HB1 | 1.92 | 0.49 |
| 1:C:284:HIS:CE1 | 1:C:423:THR:HG21 | 2.47 | 0.49 |
| 1:C:458:TRP:N | 1:C:461:GLN:HE22 | 2.11 | 0.49 |
| 1:E:175:SER:OG | 1:E:189:ASP:OD1 | 2.25 | 0.49 |
| 1:E:243:GLU:HB2 | 1:E:250:GLN:HG3 | 1.93 | 0.49 |
| 3:M:37:TYR:CE2 | 3:M:47:LEU:HD13 | 2.47 | 0.49 |
| 1:C:90:TYR:O | 1:C:236:ARG:NH2 | 2.42 | 0.49 |
| 1:C:337:ILE:HG12 | 1:C:361:VAL:HG23 | 1.93 | 0.49 |
| 1:E:405:LYS:O | 1:E:409:THR:N | 2.40 | 0.49 |
| 3:M:34:MET:SD | 3:M:89:CYS:HB2 | 2.52 | 0.49 |
| 4:N:124:PRO:HA | 4:N:150:TYR:HB3 | 1.95 | 0.49 |
| 3:Q:37:TYR:CZ | 3:Q:47:LEU:HD13 | 2.47 | 0.49 |
| 3:Q:115:THR:HB | 3:Q:138:ASN:HB2 | 1.94 | 0.49 |
| 4:R:68:PHE:CD1 | 4:R:83:ILE:HG12 | 2.47 | 0.49 |
| 1:A:119:PHE:CD2 | 1:A:236:ARG:HD2 | 2.48 | 0.49 |
| 1:C:18:ALA:HB1 | 1:C:20:TRP:CD1 | 2.47 | 0.49 |
| 1:C:59:TYR:HA | 1:C:225:TRP:HA | 1.93 | 0.49 |
| 1:C:189:ASP:O | 1:C:288:ARG:N | 2.46 | 0.49 |
| 1:E:51:SER:H | 1:E:134:ASN:HB3 | 1.77 | 0.49 |
| 1:E:54:ALA:O | 1:E:129:THR:N | 2.38 | 0.49 |
| 1:E:84:LYS:O | 1:E:90:TYR:HB2 | 2.13 | 0.49 |
| 4:N:91:THR:OG1 | 4:N:116:VAL:N | 2.31 | 0.49 |
| 4:R:35:HIS:HD1 | 4:R:50:TRP:HB3 | 1.78 | 0.49 |
| 1:A:308:PHE:CD2 | 1:A:385:VAL:HG12 | 2.48 | 0.49 |
| 1:C:9:ARG:HB3 | 1:C:319:HIS:CD2 | 2.48 | 0.49 |
| 1:C:209:LYS:HE2 | 1:C:211:PHE:HZ | 1.77 | 0.49 |
| 1:C:311:ALA:HB3 | 1:C:325:GLU:HG2 | 1.95 | 0.49 |
| 1:C:466:ALA:HA | 1:C:469:LEU:HG | 1.94 | 0.49 |
| 1:E:155:TYR:OH | 1:E:166:LYS:N | 2.42 | 0.49 |
| 1:E:222:ALA:H | 2:F:1:SER:H1 | 1.60 | 0.49 |
| 1:E:284:HIS:HE2 | 1:E:423:THR:HG21 | 1.77 | 0.49 |
| 2:F:12:LEU:O | 2:F:12:LEU:HD12 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:M:165:THR:N | 3:M:175:SER:O | 2.44 | 0.49 |
| 4:N:46:LYS:NZ | 4:N:63:ASP:OD2 | 2.35 | 0.49 |
| 3:Q:143:LYS:HB3 | 3:Q:174:TYR:CE2 | 2.48 | 0.49 |
| 4:R:23:LYS:HA | 4:R:78:THR:HA | 1.94 | 0.49 |
| 4:R:23:LYS:NZ | 4:R:76:ALA:O | 2.45 | 0.49 |
| 4:R:68:PHE:HE1 | 4:R:83:ILE:HG23 | 1.77 | 0.49 |
| 1:A:193:ARG:NH1 | 1:E:397:HIS:HA | 2.27 | 0.49 |
| 1:C:100:GLY:HA3 | 1:E:5:GLY:HA3 | 1.95 | 0.49 |
| 1:C:454:GLY:O | 2:F:39:ASN:ND2 | 2.45 | 0.49 |
| 1:E:261:GLY:C | 2:F:2:VAL:HB | 2.33 | 0.49 |
| 4:R:52:ASN:HD22 | 4:R:55:THR:HB | 1.77 | 0.49 |
| 1:A:121:CYS:HB3 | 3:Q:27:GLN:NE2 | 2.27 | 0.49 |
| 1:A:130:ILE:O | 1:A:198:THR:OG1 | 2.29 | 0.49 |
| 1:A:484:PHE:O | 1:A:487:THR:OG1 | 2.21 | 0.49 |
| 1:C:72:ALA:HA | 1:C:113:ILE:HA | 1.93 | 0.49 |
| 1:C:126:ILE:HD12 | 3:M:93:ARG:O | 2.13 | 0.49 |
| 1:E:32:THR:CG2 | 1:E:40:THR:HG22 | 2.42 | 0.49 |
| 1:E:70:THR:HG21 | 1:E:248:THR:O | 2.13 | 0.49 |
| 1:E:99:ARG:NH2 | 1:E:248:THR:HG22 | 2.28 | 0.49 |
| 4:N:122:THR:N | 4:N:151:PHE:O | 2.34 | 0.49 |
| 3:Q:97:ARG:O | 4:R:47:TRP:HB3 | 2.13 | 0.49 |
| 4:R:64:PHE:HD1 | 4:R:68:PHE:CE2 | 2.30 | 0.49 |
| 1:A:39:PRO:HB2 | 1:A:143:VAL:HG22 | 1.93 | 0.49 |
| 1:A:137:TYR:O | 1:A:168:THR:HA | 2.13 | 0.49 |
| 1:A:193:ARG:HH12 | 1:E:380:ASP:HA | 1.76 | 0.49 |
| 1:A:231:THR:O | 1:A:233:TRP:CD1 | 2.66 | 0.49 |
| 1:A:310:PHE:HA | 1:A:326:LEU:HD23 | 1.94 | 0.49 |
| 1:C:60:CYS:N | 1:C:224:PRO:O | 2.35 | 0.49 |
| 1:C:188:LEU:HA | 1:C:288:ARG:O | 2.12 | 0.49 |
| 1:C:201:PHE:HA | 1:C:215:ARG:H | 1.77 | 0.49 |
| 1:E:206:VAL:HG21 | 1:E:266:LEU:HD11 | 1.95 | 0.49 |
| 1:E:345:LEU:HD21 | 1:E:393:ASN:ND2 | 2.28 | 0.49 |
| 3:Q:23:CYS:HB2 | 3:Q:36:TRP:CH2 | 2.48 | 0.49 |
| 4:R:71:SER:OG | 4:R:80:TYR:HB2 | 2.13 | 0.49 |
| 1:A:310:PHE:HB3 | 1:A:312:LYS:O | 2.13 | 0.48 |
| 1:A:334:PRO:HB3 | 1:A:360:PHE:CZ | 2.48 | 0.48 |
| 1:E:129:THR:HB | 1:E:202:TYR:CE1 | 2.47 | 0.48 |
| 1:E:201:PHE:CE1 | 1:E:212:LEU:HD22 | 2.48 | 0.48 |
| 3:M:45:PRO:HG2 | 4:N:45:LEU:HD11 | 1.95 | 0.48 |
| 3:Q:119:PHE:HB2 | 3:Q:134:VAL:CG2 | 2.43 | 0.48 |
| 2:B:29:LEU:O | 2:B:32:THR:OG1 | 2.24 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:12:ILE:N | 1:C:32:THR:O | 2.46 | 0.48 |
| 1:C:107:LEU:HD23 | 1:C:108:PHE:N | 2.28 | 0.48 |
| 1:C:199:GLU:HA | 1:C:215:ARG:CZ | 2.42 | 0.48 |
| 1:C:214:HIS:O | 1:C:218:PHE:N | 2.44 | 0.48 |
| 4:N:61:ALA:O | 4:N:65:LYS:HG3 | 2.13 | 0.48 |
| 3:Q:109:ARG:HD2 | 3:Q:172:SER:HB2 | 1.95 | 0.48 |
| 4:R:164:LEU:HD13 | 4:R:186:VAL:HG21 | 1.94 | 0.48 |
| 1:A:351:VAL:HG23 | 1:A:352:GLY:H | 1.77 | 0.48 |
| 1:A:396:TRP:CG | 1:A:397:HIS:N | 2.81 | 0.48 |
| 2:F:8:GLY:HA2 | 2:F:9:GLU:HA | 1.54 | 0.48 |
| 3:M:4:LEU:HD21 | 3:M:91:HIS:HB3 | 1.95 | 0.48 |
| 1:C:327:SER:HB2 | 1:C:369:LYS:HG2 | 1.95 | 0.48 |
| 1:E:126:ILE:O | 1:E:205:THR:N | 2.46 | 0.48 |
| 1:E:149:SER:OG | 1:E:325:GLU:OE1 | 2.24 | 0.48 |
| 4:N:36:TRP:O | 4:N:48:MET:N | 2.46 | 0.48 |
| 4:N:37:VAL:HA | 4:N:47:TRP:HA | 1.95 | 0.48 |
| 4:N:141:VAL:HG13 | 4:N:190:SER:HB3 | 1.94 | 0.48 |
| 4:R:67:ARG:CZ | 4:R:87:LYS:HD3 | 2.43 | 0.48 |
| 1:A:63:ALA:HA | 1:A:122:THR:H | 1.77 | 0.48 |
| 1:A:225:TRP:CZ2 | 1:A:234:ARG:HG3 | 2.48 | 0.48 |
| 1:C:351:VAL:HG23 | 1:C:352:GLY:H | 1.78 | 0.48 |
| 1:E:91:VAL:HG11 | 1:E:237:GLU:HG2 | 1.96 | 0.48 |
| 1:E:245:ALA:HB2 | 1:E:250:GLN:HB2 | 1.96 | 0.48 |
| 3:M:162:ASN:HD22 | 3:M:178:SER:HA | 1.78 | 0.48 |
| 4:R:36:TRP:N | 4:R:49:GLY:O | 2.36 | 0.48 |
| 1:A:187:THR:HB | 1:A:290:LYS:HB2 | 1.95 | 0.48 |
| 1:A:487:THR:O | 1:A:492:LEU:HD13 | 2.13 | 0.48 |
| 1:C:123:SER:HA | 3:M:28:SER:CA | 2.38 | 0.48 |
| 1:C:457:SER:HB3 | 2:D:28:TYR:OH | 2.14 | 0.48 |
| 1:E:148:THR:HG22 | 1:E:369:LYS:O | 2.13 | 0.48 |
| 1:E:214:HIS:HE1 | 2:F:12:LEU:HD23 | 1.78 | 0.48 |
| 1:E:308:PHE:CZ | 1:E:337:ILE:HG23 | 2.48 | 0.48 |
| 1:A:8:ASN:ND2 | 1:A:29:SER:HB3 | 2.29 | 0.48 |
| 1:C:19:THR:HG21 | 1:C:292:ASP:HA | 1.95 | 0.48 |
| 1:C:49:GLU:O | 1:C:136:LYS:N | 2.41 | 0.48 |
| 1:C:231:THR:O | 1:C:233:TRP:CD1 | 2.66 | 0.48 |
| 1:C:275:SER:N | 1:C:277:SER:O | 2.43 | 0.48 |
| 4:N:168:VAL:HA | 4:N:186:VAL:HA | 1.95 | 0.48 |
| 4:R:68:PHE:CE1 | 4:R:83:ILE:HG23 | 2.49 | 0.48 |
| 1:A:206:VAL:HB | 1:A:211:PHE:CE2 | 2.49 | 0.48 |
| 1:A:339:ILE:HA | 1:A:385:VAL:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:84:LYS:HD2 | 1:C:90:TYR:CE1 | 2.49 | 0.48 |
| 1:C:137:TYR:HE2 | 1:C:192:PRO:HB3 | 1.78 | 0.48 |
| 1:E:119:PHE:CE1 | 1:E:236:ARG:HB2 | 2.49 | 0.48 |
| 3:M:114:PRO:N | 3:M:140:PHE:HB3 | 2.29 | 0.48 |
| 3:M:141:TYR:CD1 | 3:M:142:PRO:HA | 2.49 | 0.48 |
| 4:N:24:ALA:HB1 | 4:N:27:TYR:CE1 | 2.49 | 0.48 |
| 4:N:123:PRO:HB3 | 4:N:209:THR:HG21 | 1.96 | 0.48 |
| 4:R:122:THR:HB | 4:R:151:PHE:H | 1.77 | 0.48 |
| 1:C:129:THR:OG1 | 1:C:215:ARG:NH2 | 2.46 | 0.48 |
| 1:C:183:TYR:O | 1:C:294:LEU:HD12 | 2.14 | 0.48 |
| 1:E:91:VAL:O | 1:E:117:ALA:N | 2.31 | 0.48 |
| 4:N:127:TYR:HD2 | 4:N:146:LEU:HD23 | 1.78 | 0.48 |
| 3:Q:188:GLU:HA | 3:Q:212:ARG:CZ | 2.44 | 0.48 |
| 1:A:35:ALA:HB3 | 1:A:38:LYS:HB2 | 1.94 | 0.48 |
| 1:A:199:GLU:HA | 1:A:215:ARG:CZ | 2.44 | 0.48 |
| 1:A:265:ALA:O | 2:B:7:HIS:N | 2.42 | 0.48 |
| 1:C:19:THR:O | 1:C:291:MET:N | 2.39 | 0.48 |
| 2:D:32:THR:HG22 | 2:D:72:PRO:HB2 | 1.96 | 0.48 |
| 1:E:298:GLY:HA3 | 1:E:358:ASN:HD21 | 1.78 | 0.48 |
| 3:M:48:LEU:O | 3:M:59:VAL:HG21 | 2.14 | 0.48 |
| 3:Q:38:GLN:O | 3:Q:46:ARG:N | 2.43 | 0.48 |
| 3:Q:133:VAL:HG13 | 3:Q:210:PHE:HE1 | 1.79 | 0.48 |
| 1:A:59:TYR:HB3 | 1:A:223:LEU:CD2 | 2.44 | 0.47 |
| 1:A:70:THR:HA | 1:A:115:THR:HA | 1.96 | 0.47 |
| 1:C:68:ILE:HG21 | 1:C:251:SER:HA | 1.96 | 0.47 |
| 3:Q:115:THR:N | 3:Q:138:ASN:O | 2.25 | 0.47 |
| 4:R:61:ALA:O | 4:R:65:LYS:HG3 | 2.14 | 0.47 |
| 4:R:132:VAL:HG22 | 4:R:135:ASP:OD2 | 2.14 | 0.47 |
| 1:A:475:ALA:HB3 | 1:A:480:ILE:HG12 | 1.94 | 0.47 |
| 1:C:59:TYR:O | 1:C:125:ALA:N | 2.29 | 0.47 |
| 1:C:99:ARG:HD2 | 1:C:103:ASN:O | 2.14 | 0.47 |
| 1:E:142:PHE:HE1 | 1:E:158:GLN:HE21 | 1.62 | 0.47 |
| 1:E:493:PHE:O | 1:E:497:ASN:N | 2.43 | 0.47 |
| 3:M:114:PRO:CA | 3:M:140:PHE:HB3 | 2.43 | 0.47 |
| 3:M:133:VAL:O | 3:M:180:LEU:N | 2.25 | 0.47 |
| 3:M:164:TRP:HB3 | 3:M:176:MET:HG3 | 1.95 | 0.47 |
| 4:N:173:ALA:HB2 | 4:N:182:LEU:HB3 | 1.96 | 0.47 |
| 3:Q:117:SER:HB3 | 3:Q:119:PHE:CE1 | 2.48 | 0.47 |
| 3:Q:146:ASN:HB3 | 3:Q:198:THR:HG22 | 1.95 | 0.47 |
| 4:R:33:SER:OG | 4:R:35:HIS:NE2 | 2.32 | 0.47 |
| 1:A:132:PRO:HA | 1:A:135:ILE:HD12 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:460:THR:O | 1:A:464:MET:HG2 | 2.14 | 0.47 |
| 1:C:52:GLN:HB3 | 1:C:134:ASN:ND2 | 2.29 | 0.47 |
| 1:E:93:LYS:O | 1:E:115:THR:N | 2.43 | 0.47 |
| 1:E:308:PHE:CE2 | 1:E:337:ILE:HG23 | 2.49 | 0.47 |
| 1:E:341:SER:O | 1:E:350:PRO:HA | 2.14 | 0.47 |
| 1:E:448:ALA:HA | 1:E:452:LEU:HG | 1.95 | 0.47 |
| 1:E:494:LEU:O | 1:E:498:VAL:HG12 | 2.15 | 0.47 |
| 4:N:97:ALA:HB1 | 4:N:105:VAL:HB | 1.97 | 0.47 |
| 1:A:73:ARG:HB3 | 1:A:77:THR:OG1 | 2.15 | 0.47 |
| 1:A:360:PHE:CE2 | 1:A:362:ALA:HA | 2.49 | 0.47 |
| 1:C:339:ILE:HG13 | 1:C:385:VAL:HG22 | 1.97 | 0.47 |
| 3:M:15:LEU:HB2 | 3:M:80:GLU:HA | 1.97 | 0.47 |
| 3:M:37:TYR:O | 3:M:88:TYR:N | 2.45 | 0.47 |
| 4:N:35:HIS:HB2 | 4:N:97:ALA:HB3 | 1.96 | 0.47 |
| 4:N:191:SER:O | 4:N:195:SER:OG | 2.18 | 0.47 |
| 4:R:8:GLY:O | 4:R:10:GLU:HG3 | 2.15 | 0.47 |
| 1:C:305:THR:N | 1:C:332:ASP:OD2 | 2.37 | 0.47 |
| 2:D:1:SER:OG | 2:D:2:VAL:N | 2.47 | 0.47 |
| 1:E:26:GLU:HB2 | 1:E:29:SER:OG | 2.15 | 0.47 |
| 3:M:121:PRO:HG3 | 3:M:132:SER:N | 2.30 | 0.47 |
| 3:Q:51:LEU:C | 3:Q:53:SER:H | 2.16 | 0.47 |
| 4:R:35:HIS:CD2 | 4:R:105:VAL:HG12 | 2.49 | 0.47 |
| 1:A:193:ARG:NH2 | 1:E:396:TRP:O | 2.48 | 0.47 |
| 1:C:51:SER:HA | 1:C:277:SER:HB2 | 1.96 | 0.47 |
| 1:C:61:TYR:CG | 1:C:262:LEU:HD11 | 2.49 | 0.47 |
| 1:C:99:ARG:NE | 1:C:105:CYS:SG | 2.87 | 0.47 |
| 1:C:354:LEU:HB3 | 1:C:356:THR:O | 2.15 | 0.47 |
| 1:C:461:GLN:OE1 | 1:C:461:GLN:N | 2.31 | 0.47 |
| 3:Q:118:ILE:N | 4:R:135:ASP:OD1 | 2.47 | 0.47 |
| 4:R:33:SER:OG | 4:R:99:GLY:HA3 | 2.14 | 0.47 |
| 4:R:35:HIS:HA | 4:R:50:TRP:HA | 1.96 | 0.47 |
| 4:R:70:PHE:HE1 | 4:R:81:LEU:HD13 | 1.79 | 0.47 |
| 1:A:52:GLN:NE2 | 4:R:52:ASN:HA | 2.30 | 0.47 |
| 1:A:334:PRO:HB3 | 1:A:360:PHE:HZ | 1.79 | 0.47 |
| 1:A:380:ASP:OD1 | 1:A:397:HIS:ND1 | 2.47 | 0.47 |
| 1:C:30:CYS:HA | 1:C:44:ARG:HB3 | 1.96 | 0.47 |
| 1:C:66:THR:O | 1:C:118:LYS:N | 2.47 | 0.47 |
| 1:C:226:THR:HG23 | 1:C:233:TRP:NE1 | 2.26 | 0.47 |
| 1:E:183:TYR:CZ | 1:E:297:LYS:HG2 | 2.50 | 0.47 |
| 3:M:36:TRP:CE3 | 3:M:74:LEU:HB2 | 2.50 | 0.47 |
| 4:N:28:THR:OG1 | 4:N:31:ASP:OD2 | 2.26 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:52:ASN:HB3 | 4:N:57:GLU:H | 1.79 | 0.47 |
| 4:N:130:ALA:HB3 | 4:N:218:ARG:HG3 | 1.97 | 0.47 |
| 3:Q:60:PRO:HG2 | 3:Q:62:ARG:NH1 | 2.29 | 0.47 |
| 3:Q:118:ILE:HG22 | 3:Q:208:LYS:HB3 | 1.96 | 0.47 |
| 3:Q:164:TRP:HA | 3:Q:176:MET:HA | 1.96 | 0.47 |
| 4:R:48:MET:HA | 4:R:64:PHE:CE2 | 2.50 | 0.47 |
| 4:R:119:PRO:CG | 4:R:178:ASP:HB3 | 2.45 | 0.47 |
| 4:R:139:SER:O | 4:R:190:SER:N | 2.34 | 0.47 |
| 1:A:301:TYR:CE1 | 1:A:334:PRO:HB2 | 2.50 | 0.47 |
| 1:A:355:VAL:HG21 | 1:A:373:GLU:HG2 | 1.97 | 0.47 |
| 1:E:1:PHE:CD1 | 1:E:155:TYR:HB2 | 2.50 | 0.47 |
| 1:E:46:ILE:HD12 | 1:E:138:GLU:HB3 | 1.97 | 0.47 |
| 1:E:494:LEU:HA | 1:E:497:ASN:HB3 | 1.96 | 0.47 |
| 4:R:148:LYS:HA | 4:R:181:THR:HG22 | 1.95 | 0.47 |
| 1:A:9:ARG:HB3 | 1:A:319:HIS:NE2 | 2.28 | 0.47 |
| 1:C:199:GLU:HA | 1:C:215:ARG:NH2 | 2.30 | 0.47 |
| 1:E:81:HIS:CE1 | 1:E:85:ARG:HB2 | 2.49 | 0.47 |
| 1:E:450:ARG:HA | 1:E:453:PHE:CZ | 2.49 | 0.47 |
| 3:M:97:ARG:HB2 | 4:N:47:TRP:CD2 | 2.50 | 0.47 |
| 4:N:27:TYR:CE2 | 4:N:29:PHE:HA | 2.49 | 0.47 |
| 4:N:128:PRO:HD3 | 4:N:213:LYS:HB3 | 1.97 | 0.47 |
| 3:Q:66:SER:N | 3:Q:73:THR:O | 2.42 | 0.47 |
| 3:Q:142:PRO:O | 3:Q:199:HIS:NE2 | 2.46 | 0.47 |
| 4:R:37:VAL:HA | 4:R:47:TRP:HA | 1.96 | 0.47 |
| 4:R:64:PHE:HB3 | 4:R:68:PHE:HD2 | 1.80 | 0.47 |
| 1:A:56:VAL:HG21 | 1:A:202:TYR:CE2 | 2.50 | 0.47 |
| 1:A:308:PHE:HB2 | 1:A:392:ILE:HG12 | 1.97 | 0.47 |
| 1:C:274:TYR:CD2 | 4:N:102:LEU:HB2 | 2.49 | 0.47 |
| 1:C:464:MET:O | 1:C:468:LEU:N | 2.47 | 0.47 |
| 1:E:99:ARG:O | 1:E:108:PHE:HA | 2.14 | 0.47 |
| 3:M:6:GLN:HB3 | 3:M:101:GLY:O | 2.15 | 0.47 |
| 3:Q:97:ARG:HD2 | 4:R:47:TRP:CZ2 | 2.50 | 0.47 |
| 3:Q:140:PHE:CE1 | 3:Q:174:TYR:HB2 | 2.50 | 0.47 |
| 1:A:174:PRO:HB2 | 1:E:382:TYR:HE2 | 1.80 | 0.46 |
| 1:C:150:GLU:O | 1:C:154:ASN:N | 2.49 | 0.46 |
| 1:E:167:PHE:CZ | 1:E:188:LEU:HD22 | 2.50 | 0.46 |
| 4:N:38:LYS:HG3 | 4:N:94:TYR:CE1 | 2.44 | 0.46 |
| 4:R:5:MET:CG | 4:R:23:LYS:HB3 | 2.45 | 0.46 |
| 4:R:18:VAL:HB | 4:R:86:LEU:HD11 | 1.97 | 0.46 |
| 1:A:448:ALA:HA | 1:A:452:LEU:HG | 1.97 | 0.46 |
| 1:A:478:ARG:O | 1:A:482:LEU:HD13 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:487:THR:OG1 | 1:A:488:GLY:N | 2.48 | 0.46 |
| 1:C:45:MET:HE3 | 1:C:137:TYR:HD1 | 1.80 | 0.46 |
| 1:C:121:CYS:HB3 | 3:M:27:GLN:NE2 | 2.30 | 0.46 |
| 1:C:214:HIS:H | 2:D:7:HIS:CD2 | 2.33 | 0.46 |
| 2:D:15:LYS:O | 2:D:16:THR:HG23 | 2.15 | 0.46 |
| 1:E:38:LYS:HG3 | 1:E:291:MET:SD | 2.55 | 0.46 |
| 1:E:339:ILE:HG13 | 1:E:385:VAL:HA | 1.96 | 0.46 |
| 3:M:112:ALA:N | 3:M:141:TYR:O | 2.46 | 0.46 |
| 1:A:80:ALA:HB2 | 1:A:112:SER:OG | 2.16 | 0.46 |
| 1:A:201:PHE:CE1 | 1:A:212:LEU:HD22 | 2.51 | 0.46 |
| 1:E:84:LYS:HB2 | 1:E:92:CYS:SG | 2.55 | 0.46 |
| 4:R:18:VAL:HG12 | 4:R:83:ILE:HB | 1.97 | 0.46 |
| 1:A:241:GLU:O | 1:A:252:VAL:HG13 | 2.16 | 0.46 |
| 1:A:322:VAL:C | 1:A:373:GLU:HG3 | 2.36 | 0.46 |
| 1:C:65:VAL:HG21 | 1:C:252:VAL:HG12 | 1.98 | 0.46 |
| 1:C:341:SER:HB2 | 1:C:374:MET:SD | 2.55 | 0.46 |
| 1:E:2:ASN:HD21 | 1:E:153:GLY:HA2 | 1.80 | 0.46 |
| 1:E:304:CYS:HB3 | 1:E:328:TYR:OH | 2.16 | 0.46 |
| 1:E:344:SER:HA | 1:E:382:TYR:CE1 | 2.50 | 0.46 |
| 1:E:476:ARG:O | 1:E:480:ILE:N | 2.48 | 0.46 |
| 3:M:36:TRP:HA | 3:M:88:TYR:O | 2.14 | 0.46 |
| 3:M:121:PRO:HD2 | 3:M:187:TYR:CZ | 2.51 | 0.46 |
| 3:M:135:CYS:HB2 | 3:M:149:TRP:CH2 | 2.50 | 0.46 |
| 4:N:37:VAL:HG11 | 4:N:45:LEU:HB3 | 1.96 | 0.46 |
| 3:Q:21:ILE:O | 3:Q:74:LEU:N | 2.25 | 0.46 |
| 1:A:183:TYR:CZ | 1:A:297:LYS:HG2 | 2.50 | 0.46 |
| 1:A:225:TRP:HZ3 | 1:C:79:GLU:OE1 | 1.98 | 0.46 |
| 1:C:213:VAL:HG21 | 1:C:218:PHE:CD1 | 2.51 | 0.46 |
| 1:E:178:LEU:O | 1:E:185:GLU:HG3 | 2.15 | 0.46 |
| 4:N:4:LEU:O | 4:N:109:GLY:HA2 | 2.15 | 0.46 |
| 3:Q:197:ALA:O | 3:Q:206:ILE:HD12 | 2.15 | 0.46 |
| 1:A:52:GLN:NE2 | 4:R:52:ASN:OD1 | 2.48 | 0.46 |
| 1:A:84:LYS:HD2 | 1:A:90:TYR:CE1 | 2.51 | 0.46 |
| 1:C:73:ARG:HE | 1:C:77:THR:HB | 1.81 | 0.46 |
| 1:E:341:SER:O | 1:E:351:VAL:HG22 | 2.15 | 0.46 |
| 3:M:15:LEU:HD23 | 3:M:107:ILE:HD12 | 1.96 | 0.46 |
| 3:M:185:ASP:O | 3:M:189:ARG:N | 2.48 | 0.46 |
| 4:N:152:PRO:O | 4:N:204:HIS:NE2 | 2.48 | 0.46 |
| 3:Q:135:CYS:HB2 | 3:Q:149:TRP:CH2 | 2.51 | 0.46 |
| 4:R:141:VAL:N | 4:R:188:VAL:O | 2.48 | 0.46 |
| 1:A:145:GLY:HA3 | 1:A:163:GLN:NE2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:268:GLY:HA3 | 2:D:10:SER:H | 1.80 | 0.46 |
| 1:C:308:PHE:CE2 | 1:C:337:ILE:HG23 | 2.50 | 0.46 |
| 1:E:71:VAL:HB | 1:E:114:ASP:HB3 | 1.98 | 0.46 |
| 1:E:92:CYS:HB3 | 1:E:114:ASP:OD1 | 2.15 | 0.46 |
| 1:E:128:ARG:O | 1:E:203:VAL:N | 2.49 | 0.46 |
| 1:E:129:THR:HB | 1:E:202:TYR:HE1 | 1.81 | 0.46 |
| 4:R:53:THR:HA | 4:R:72:LEU:CD1 | 2.46 | 0.46 |
| 1:A:266:LEU:HB3 | 1:A:269:ALA:HB3 | 1.98 | 0.46 |
| 1:C:450:ARG:HA | 1:C:453:PHE:CZ | 2.51 | 0.46 |
| 1:E:141:ILE:O | 1:E:165:ALA:N | 2.34 | 0.46 |
| 1:E:328:TYR:O | 1:E:367:ASN:N | 2.47 | 0.46 |
| 4:R:6:GLU:OE2 | 4:R:96:CYS:N | 2.31 | 0.46 |
| 4:R:11:LEU:HD23 | 4:R:115:THR:HB | 1.97 | 0.46 |
| 1:C:84:LYS:HB2 | 1:C:116:CYS:SG | 2.56 | 0.46 |
| 1:E:183:TYR:CE1 | 1:E:297:LYS:HG2 | 2.51 | 0.46 |
| 1:E:389:ASP:OD1 | 1:E:390:LYS:N | 2.49 | 0.46 |
| 1:E:458:TRP:CE3 | 1:E:459:ILE:HB | 2.51 | 0.46 |
| 3:M:115:THR:O | 3:M:138:ASN:N | 2.45 | 0.46 |
| 3:M:140:PHE:O | 3:M:174:TYR:N | 2.40 | 0.46 |
| 3:Q:162:ASN:HD22 | 3:Q:178:SER:HA | 1.80 | 0.46 |
| 4:R:32:TYR:CD2 | 4:R:98:ARG:HD2 | 2.51 | 0.46 |
| 4:R:72:LEU:HD23 | 4:R:79:ALA:HA | 1.97 | 0.46 |
| 1:A:52:GLN:NE2 | 4:R:33:SER:HA | 2.31 | 0.46 |
| 1:A:206:VAL:HB | 1:A:211:PHE:HE2 | 1.81 | 0.46 |
| 1:C:26:GLU:OE2 | 2:D:15:LYS:NZ | 2.39 | 0.46 |
| 1:E:61:TYR:CD1 | 1:E:262:LEU:HD11 | 2.51 | 0.46 |
| 1:E:127:GLY:HA3 | 1:E:218:PHE:CZ | 2.51 | 0.46 |
| 1:E:201:PHE:HA | 1:E:215:ARG:N | 2.31 | 0.46 |
| 2:F:14:ASN:OD1 | 2:F:16:THR:OG1 | 2.34 | 0.46 |
| 2:F:15:LYS:O | 2:F:16:THR:HG23 | 2.16 | 0.46 |
| 4:N:38:LYS:N | 4:N:48:MET:HG3 | 2.31 | 0.46 |
| 4:N:124:PRO:CA | 4:N:150:TYR:HB3 | 2.45 | 0.46 |
| 1:A:380:ASP:HA | 1:A:397:HIS:HA | 1.98 | 0.45 |
| 1:C:70:THR:HA | 1:C:115:THR:HA | 1.99 | 0.45 |
| 1:C:292:ASP:OD1 | 1:C:293:LYS:N | 2.49 | 0.45 |
| 1:E:240:MET:HA | 1:E:254:ALA:HA | 1.97 | 0.45 |
| 1:E:322:VAL:O | 1:E:373:GLU:HG3 | 2.16 | 0.45 |
| 1:E:337:ILE:HB | 1:E:359:PRO:HB2 | 1.98 | 0.45 |
| 3:M:40:LYS:HB2 | 3:M:43:GLN:CD | 2.37 | 0.45 |
| 1:A:224:PRO:HB3 | 1:A:236:ARG:HA | 1.99 | 0.45 |
| 1:A:458:TRP:N | 1:A:461:GLN:HE22 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:62:HIS:CG | 1:C:257:SER:HA | 2.50 | 0.45 |
| 1:C:155:TYR:O | 1:C:159:VAL:HG23 | 2.16 | 0.45 |
| 1:C:412:LYS:O | 1:C:416:ARG:N | 2.39 | 0.45 |
| 1:E:39:PRO:HB2 | 1:E:143:VAL:CG2 | 2.46 | 0.45 |
| 1:E:45:MET:HA | 1:E:139:VAL:HA | 1.97 | 0.45 |
| 1:E:50:ALA:O | 1:E:278:VAL:HG12 | 2.15 | 0.45 |
| 1:E:68:ILE:HG21 | 1:E:251:SER:HA | 1.98 | 0.45 |
| 1:E:421:GLY:HA2 | 1:E:442:HIS:CE1 | 2.51 | 0.45 |
| 3:M:136:PHE:HD1 | 4:N:171:PHE:CE2 | 2.34 | 0.45 |
| 1:C:52:GLN:NE2 | 4:N:33:SER:HA | 2.31 | 0.45 |
| 1:C:55:GLU:HG2 | 1:C:128:ARG:NE | 2.31 | 0.45 |
| 1:C:380:ASP:OD1 | 1:C:397:HIS:ND1 | 2.48 | 0.45 |
| 1:C:407:PHE:HB3 | 1:C:411:LEU:HD12 | 1.97 | 0.45 |
| 2:D:57:ASN:H | 2:D:60:ARG:NH1 | 2.14 | 0.45 |
| 1:E:227:PRO:HD2 | 1:E:233:TRP:CD1 | 2.51 | 0.45 |
| 1:E:437:ILE:O | 1:E:441:VAL:HG23 | 2.15 | 0.45 |
| 4:N:2:VAL:HG22 | 4:N:27:TYR:HB3 | 1.99 | 0.45 |
| 3:Q:146:ASN:OD1 | 3:Q:147:VAL:N | 2.49 | 0.45 |
| 1:A:214:HIS:O | 1:A:218:PHE:N | 2.45 | 0.45 |
| 1:A:256:GLY:O | 1:A:258:GLN:NE2 | 2.50 | 0.45 |
| 1:C:223:LEU:HG | 1:C:224:PRO:HD2 | 1.99 | 0.45 |
| 1:C:226:THR:HA | 1:C:233:TRP:CD1 | 2.50 | 0.45 |
| 1:E:332:ASP:OD1 | 1:E:332:ASP:N | 2.47 | 0.45 |
| 3:M:55:LEU:HD21 | 3:M:63:PHE:O | 2.16 | 0.45 |
| 4:N:6:GLU:HG2 | 4:N:22:CYS:HB2 | 1.98 | 0.45 |
| 3:Q:135:CYS:O | 3:Q:178:SER:N | 2.27 | 0.45 |
| 4:R:20:ILE:HD11 | 4:R:114:VAL:HG23 | 1.97 | 0.45 |
| 4:R:36:TRP:CH2 | 4:R:96:CYS:HB3 | 2.51 | 0.45 |
| 4:R:37:VAL:HG22 | 4:R:47:TRP:CD1 | 2.51 | 0.45 |
| 1:A:61:TYR:CB | 1:A:262:LEU:HD11 | 2.46 | 0.45 |
| 1:C:61:TYR:CZ | 1:C:123:SER:HB3 | 2.51 | 0.45 |
| 1:C:137:TYR:CZ | 1:C:285:LEU:HD13 | 2.51 | 0.45 |
| 1:C:198:THR:HG23 | 1:C:199:GLU:HG3 | 1.99 | 0.45 |
| 1:E:27:GLY:N | 1:E:45:MET:HB3 | 2.32 | 0.45 |
| 1:E:61:TYR:OH | 1:E:123:SER:HB3 | 2.16 | 0.45 |
| 1:E:328:TYR:CD2 | 1:E:361:VAL:HG21 | 2.52 | 0.45 |
| 4:N:204:HIS:NE2 | 4:N:206:ALA:HB3 | 2.32 | 0.45 |
| 4:R:169:HIS:N | 4:R:185:SER:O | 2.30 | 0.45 |
| 1:A:389:ASP:OD1 | 1:A:390:LYS:N | 2.49 | 0.45 |
| 1:C:28:ASP:OD1 | 1:C:29:SER:N | 2.50 | 0.45 |
| 1:C:33:ILE:N | 1:C:41:LEU:O | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:23:LEU:N | 1:E:287:CYS:O | 2.43 | 0.45 |
| 1:E:355:VAL:N | 1:E:374:MET:HA | 2.12 | 0.45 |
| 1:E:432:GLY:H | 1:E:436:SER:N | 2.14 | 0.45 |
| 4:N:39:GLN:O | 4:N:92:ALA:HB1 | 2.17 | 0.45 |
| 1:A:85:ARG:NH2 | 1:A:94:GLN:HG2 | 2.32 | 0.45 |
| 1:A:193:ARG:HG2 | 1:E:395:HIS:CE1 | 2.52 | 0.45 |
| 1:A:243:GLU:O | 1:A:250:GLN:NE2 | 2.49 | 0.45 |
| 1:A:304:CYS:HB3 | 1:A:328:TYR:OH | 2.16 | 0.45 |
| 1:A:355:VAL:HB | 1:A:373:GLU:C | 2.37 | 0.45 |
| 1:E:41:LEU:HD23 | 1:E:143:VAL:HB | 1.98 | 0.45 |
| 1:E:137:TYR:CE2 | 1:E:285:LEU:HD13 | 2.52 | 0.45 |
| 1:E:220:ASP:HB3 | 2:F:5:GLN:HE21 | 1.79 | 0.45 |
| 1:E:465:GLY:O | 1:E:469:LEU:HG | 2.17 | 0.45 |
| 2:F:7:HIS:CE1 | 2:F:10:SER:HB2 | 2.52 | 0.45 |
| 3:M:150:LYS:HB2 | 3:M:194:THR:HB | 1.99 | 0.45 |
| 4:N:61:ALA:HB3 | 4:N:64:PHE:CD2 | 2.43 | 0.45 |
| 3:Q:119:PHE:N | 3:Q:134:VAL:O | 2.42 | 0.45 |
| 3:Q:147:VAL:HG21 | 3:Q:162:ASN:ND2 | 2.32 | 0.45 |
| 4:R:23:LYS:HG3 | 4:R:78:THR:HG22 | 1.98 | 0.45 |
| 4:R:37:VAL:HA | 4:R:48:MET:H | 1.80 | 0.45 |
| 4:R:191:SER:O | 4:R:195:SER:OG | 2.23 | 0.45 |
| 1:A:310:PHE:CE2 | 1:A:392:ILE:HD12 | 2.51 | 0.45 |
| 1:A:326:LEU:O | 1:A:370:VAL:N | 2.46 | 0.45 |
| 1:C:74:CYS:HA | 1:C:105:CYS:SG | 2.57 | 0.45 |
| 1:C:475:ALA:HB3 | 1:C:480:ILE:HG12 | 1.99 | 0.45 |
| 2:D:50:GLY:HA3 | 2:D:64:THR:HG23 | 1.98 | 0.45 |
| 1:A:99:ARG:HH22 | 1:A:248:THR:HG22 | 1.82 | 0.45 |
| 1:A:272:VAL:HB | 1:A:278:VAL:CG2 | 2.47 | 0.45 |
| 1:C:20:TRP:CH2 | 1:C:430:ILE:HG22 | 2.52 | 0.45 |
| 1:C:492:LEU:HA | 1:C:495:ALA:HB3 | 1.98 | 0.45 |
| 2:D:1:SER:HB2 | 2:F:31:LYS:HZ1 | 1.82 | 0.45 |
| 4:R:53:THR:HA | 4:R:72:LEU:HD13 | 1.99 | 0.45 |
| 4:R:137:THR:N | 4:R:140:MET:O | 2.46 | 0.45 |
| 4:R:204:HIS:O | 4:R:208:SER:N | 2.50 | 0.45 |
| 1:A:73:ARG:NE | 1:A:77:THR:HB | 2.31 | 0.45 |
| 1:A:142:PHE:HE2 | 1:A:144:HIS:ND1 | 2.15 | 0.45 |
| 1:A:458:TRP:HE3 | 2:B:28:TYR:HD2 | 1.65 | 0.45 |
| 1:A:476:ARG:O | 1:A:480:ILE:N | 2.46 | 0.45 |
| 1:C:52:GLN:HE22 | 4:N:52:ASN:HA | 1.79 | 0.45 |
| 1:E:148:THR:HG23 | 1:E:151:ASN:HD21 | 1.82 | 0.45 |
| 3:M:36:TRP:CE2 | 3:M:74:LEU:HB2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:51:ILE:HB | 4:N:70:PHE:HB3 | 1.99 | 0.45 |
| 4:R:127:TYR:N | 4:R:146:LEU:O | 2.47 | 0.45 |
| 4:R:128:PRO:HD3 | 4:R:213:LYS:HB3 | 1.97 | 0.45 |
| 1:A:45:MET:HA | 1:A:139:VAL:HA | 1.99 | 0.44 |
| 1:A:72:ALA:HB1 | 1:A:99:ARG:NH2 | 2.32 | 0.44 |
| 1:A:100:GLY:N | 1:A:103:ASN:OD1 | 2.46 | 0.44 |
| 1:A:489:GLY:C | 1:A:491:LEU:N | 2.69 | 0.44 |
| 1:C:65:VAL:HG22 | 1:C:240:MET:SD | 2.57 | 0.44 |
| 1:C:82:ASN:N | 1:C:114:ASP:OD2 | 2.46 | 0.44 |
| 1:C:437:ILE:O | 1:C:441:VAL:HG23 | 2.17 | 0.44 |
| 1:E:1:PHE:H2 | 1:E:44:ARG:HD3 | 1.81 | 0.44 |
| 1:E:284:HIS:NE2 | 1:E:423:THR:HG21 | 2.32 | 0.44 |
| 1:E:476:ARG:O | 1:E:480:ILE:HG13 | 2.15 | 0.44 |
| 1:E:489:GLY:HA2 | 1:E:493:PHE:HB2 | 1.99 | 0.44 |
| 1:E:492:LEU:HA | 1:E:495:ALA:HB3 | 1.99 | 0.44 |
| 3:M:151:ILE:HA | 3:M:192:SER:O | 2.16 | 0.44 |
| 4:N:152:PRO:HA | 4:N:180:TYR:CE2 | 2.52 | 0.44 |
| 3:Q:92:ILE:HG23 | 3:Q:97:ARG:NH2 | 2.31 | 0.44 |
| 4:R:2:VAL:HG13 | 4:R:27:TYR:HD1 | 1.83 | 0.44 |
| 4:R:4:LEU:HD21 | 4:R:98:ARG:N | 2.33 | 0.44 |
| 4:R:157:VAL:HG22 | 4:R:202:VAL:HG22 | 1.98 | 0.44 |
| 1:C:59:TYR:HB3 | 1:C:223:LEU:HD22 | 1.98 | 0.44 |
| 1:C:87:ASP:HB3 | 1:C:90:TYR:HD1 | 1.81 | 0.44 |
| 1:E:143:VAL:O | 1:E:163:GLN:HB3 | 2.16 | 0.44 |
| 3:M:112:ALA:C | 3:M:201:THR:HG21 | 2.36 | 0.44 |
| 3:Q:114:PRO:HB3 | 3:Q:140:PHE:CD2 | 2.53 | 0.44 |
| 3:Q:211:ASN:HB3 | 3:Q:214:GLU:HG2 | 1.98 | 0.44 |
| 2:B:13:VAL:HG12 | 2:B:14:ASN:H | 1.81 | 0.44 |
| 1:C:26:GLU:HG2 | 1:C:283:GLY:O | 2.17 | 0.44 |
| 1:E:59:TYR:HB3 | 1:E:223:LEU:CD2 | 2.48 | 0.44 |
| 1:E:468:LEU:HB3 | 1:E:487:THR:HG22 | 2.00 | 0.44 |
| 3:M:13:VAL:HG12 | 3:M:106:GLU:O | 2.17 | 0.44 |
| 4:N:37:VAL:HG22 | 4:N:47:TRP:CD1 | 2.50 | 0.44 |
| 3:Q:23:CYS:HB2 | 3:Q:36:TRP:HH2 | 1.83 | 0.44 |
| 3:Q:190:HIS:O | 3:Q:212:ARG:NH2 | 2.40 | 0.44 |
| 4:R:4:LEU:O | 4:R:109:GLY:HA2 | 2.17 | 0.44 |
| 1:C:321:THR:HG22 | 1:C:375:GLU:HG3 | 1.99 | 0.44 |
| 2:F:35:TRP:CE3 | 2:F:72:PRO:HG3 | 2.53 | 0.44 |
| 2:F:59:GLN:HA | 2:F:62:VAL:HG23 | 1.99 | 0.44 |
| 2:F:71:ALA:HB3 | 2:F:72:PRO:HD3 | 1.98 | 0.44 |
| 3:M:49:ILE:HG21 | 3:M:65:GLY:HA3 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:N:155:VAL:HG12 | 4:N:204:HIS:CB | 2.47 | 0.44 |
| 3:Q:21:ILE:HD12 | 3:Q:87:TYR:HD2 | 1.83 | 0.44 |
| 3:Q:60:PRO:HG2 | 3:Q:62:ARG:HH12 | 1.82 | 0.44 |
| 4:R:52:ASN:ND2 | 4:R:55:THR:H | 2.15 | 0.44 |
| 1:A:271:VAL:HG22 | 2:B:19:TRP:HE3 | 1.82 | 0.44 |
| 1:C:50:ALA:HA | 1:C:135:ILE:HA | 2.00 | 0.44 |
| 1:C:99:ARG:O | 1:C:109:GLY:N | 2.41 | 0.44 |
| 1:E:214:HIS:HB2 | 1:E:217:TRP:HB3 | 1.99 | 0.44 |
| 3:M:109:ARG:HH12 | 3:M:112:ALA:HB2 | 1.83 | 0.44 |
| 4:N:92:ALA:HB3 | 4:N:94:TYR:CE1 | 2.52 | 0.44 |
| 1:A:39:PRO:HD2 | 1:A:294:LEU:HD11 | 2.00 | 0.44 |
| 1:C:316:ASP:O | 1:E:108:PHE:HB2 | 2.18 | 0.44 |
| 1:E:75:PRO:HD2 | 1:E:105:CYS:SG | 2.58 | 0.44 |
| 1:E:201:PHE:O | 1:E:215:ARG:NH2 | 2.33 | 0.44 |
| 3:M:149:TRP:O | 3:M:156:ARG:N | 2.48 | 0.44 |
| 3:Q:39:GLN:O | 3:Q:86:THR:HB | 2.17 | 0.44 |
| 1:C:227:PRO:HD2 | 1:C:233:TRP:CD1 | 2.53 | 0.44 |
| 1:E:137:TYR:CD2 | 1:E:285:LEU:HD22 | 2.53 | 0.44 |
| 1:E:211:PHE:HE1 | 1:E:271:VAL:HG22 | 1.82 | 0.44 |
| 1:E:322:VAL:HG21 | 1:E:396:TRP:CD1 | 2.53 | 0.44 |
| 1:E:437:ILE:O | 1:E:441:VAL:N | 2.49 | 0.44 |
| 3:M:149:TRP:HA | 3:M:194:THR:O | 2.18 | 0.44 |
| 4:N:92:ALA:O | 4:N:113:SER:HA | 2.17 | 0.44 |
| 1:A:58:SER:OG | 1:A:126:ILE:HG12 | 2.18 | 0.44 |
| 1:A:227:PRO:HD3 | 1:A:232:ALA:O | 2.17 | 0.44 |
| 1:C:101:TRP:HB3 | 1:E:312:LYS:NZ | 2.33 | 0.44 |
| 1:C:201:PHE:HA | 1:C:214:HIS:HA | 2.00 | 0.44 |
| 1:C:241:GLU:O | 1:C:252:VAL:HG13 | 2.18 | 0.44 |
| 1:E:387:ARG:HA | 1:E:391:GLN:HB3 | 2.00 | 0.44 |
| 4:N:93:SER:HA | 4:N:113:SER:HA | 1.99 | 0.44 |
| 4:R:2:VAL:HA | 4:R:25:SER:O | 2.18 | 0.44 |
| 4:R:86:LEU:HD23 | 4:R:86:LEU:HA | 1.83 | 0.44 |
| 4:R:91:THR:HA | 4:R:114:VAL:O | 2.18 | 0.44 |
| 1:A:2:ASN:HD21 | 1:A:153:GLY:HA2 | 1.83 | 0.44 |
| 1:A:30:CYS:HB2 | 1:A:44:ARG:HD2 | 2.00 | 0.44 |
| 1:A:99:ARG:HA | 1:A:103:ASN:HD21 | 1.83 | 0.44 |
| 1:A:167:PHE:HZ | 1:A:188:LEU:HD22 | 1.83 | 0.44 |
| 1:A:180:LEU:CD1 | 1:A:294:LEU:HD13 | 2.48 | 0.44 |
| 1:E:334:PRO:HB3 | 1:E:360:PHE:HZ | 1.82 | 0.44 |
| 4:N:167:GLY:O | 4:N:187:THR:N | 2.50 | 0.44 |
| 3:Q:21:ILE:HB | 3:Q:74:LEU:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:107:ILE:O | 3:Q:167:GLN:NE2 | 2.49 | 0.44 |
| 3:Q:151:ILE:HD12 | 3:Q:156:ARG:HB3 | 2.00 | 0.44 |
| 1:A:265:ALA:HA | 2:B:6:THR:HG22 | 2.00 | 0.43 |
| 2:D:69:LEU:HD21 | 2:F:74:TYR:C | 2.39 | 0.43 |
| 1:E:128:ARG:NH1 | 1:E:205:THR:HG1 | 2.15 | 0.43 |
| 4:N:159:TRP:CZ3 | 4:N:200:CYS:HB3 | 2.52 | 0.43 |
| 3:Q:36:TRP:CG | 3:Q:74:LEU:HD13 | 2.53 | 0.43 |
| 3:Q:121:PRO:HD2 | 3:Q:187:TYR:CZ | 2.52 | 0.43 |
| 1:A:196:LEU:HD23 | 2:B:13:VAL:HG21 | 2.00 | 0.43 |
| 1:A:328:TYR:CD2 | 1:A:361:VAL:HG21 | 2.53 | 0.43 |
| 2:D:66:LEU:O | 2:D:70:VAL:HG23 | 2.18 | 0.43 |
| 1:E:439:LYS:NZ | 1:E:443:GLN:OE1 | 2.48 | 0.43 |
| 3:M:83:ASP:O | 3:M:87:TYR:OH | 2.19 | 0.43 |
| 4:R:68:PHE:HB3 | 4:R:81:LEU:HD11 | 2.00 | 0.43 |
| 4:R:87:LYS:HB3 | 4:R:89:GLU:OE1 | 2.17 | 0.43 |
| 1:A:142:PHE:CG | 1:A:143:VAL:N | 2.86 | 0.43 |
| 1:A:260:GLY:O | 1:A:264:GLN:HG2 | 2.18 | 0.43 |
| 1:A:449:PHE:H | 1:A:452:LEU:HD12 | 1.83 | 0.43 |
| 1:C:39:PRO:HB2 | 1:C:143:VAL:CG2 | 2.49 | 0.43 |
| 1:C:425:TRP:CD1 | 1:C:439:LYS:HA | 2.53 | 0.43 |
| 2:D:55:SER:HA | 2:D:60:ARG:HD3 | 1.99 | 0.43 |
| 1:E:62:HIS:CE1 | 1:E:122:THR:HG21 | 2.54 | 0.43 |
| 1:E:202:TYR:O | 1:E:212:LEU:HA | 2.18 | 0.43 |
| 3:M:25:ALA:N | 3:M:70:THR:O | 2.48 | 0.43 |
| 3:M:140:PHE:CZ | 3:M:176:MET:HB2 | 2.54 | 0.43 |
| 4:N:91:THR:HA | 4:N:114:VAL:O | 2.18 | 0.43 |
| 3:Q:35:HIS:HE2 | 3:Q:92:ILE:HG13 | 1.84 | 0.43 |
| 4:R:21:SER:HA | 4:R:80:TYR:CD1 | 2.52 | 0.43 |
| 2:B:37:ILE:O | 2:B:40:PRO:HD3 | 2.19 | 0.43 |
| 1:C:67:ASP:OD2 | 1:C:90:TYR:HE2 | 2.01 | 0.43 |
| 1:E:68:ILE:HA | 1:E:116:CYS:O | 2.18 | 0.43 |
| 1:E:339:ILE:HD12 | 1:E:385:VAL:HG13 | 2.00 | 0.43 |
| 3:M:122:SER:HA | 4:N:218:ARG:HH12 | 1.82 | 0.43 |
| 4:N:175:LEU:HG | 4:N:180:TYR:HE1 | 1.83 | 0.43 |
| 1:A:394:HIS:ND1 | 1:A:395:HIS:O | 2.49 | 0.43 |
| 1:C:20:TRP:HA | 1:C:290:LYS:HA | 1.99 | 0.43 |
| 1:C:46:ILE:HD12 | 1:C:138:GLU:HB3 | 2.01 | 0.43 |
| 1:E:341:SER:O | 1:E:351:VAL:N | 2.41 | 0.43 |
| 4:N:159:TRP:HZ3 | 4:N:215:ILE:HD13 | 1.84 | 0.43 |
| 3:Q:36:TRP:O | 3:Q:47:LEU:HD12 | 2.18 | 0.43 |
| 3:Q:36:TRP:CD1 | 3:Q:49:ILE:HB | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:119:PHE:HE1 | 4:R:135:ASP:HB3 | 1.83 | 0.43 |
| 3:Q:151:ILE:HA | 3:Q:192:SER:O | 2.18 | 0.43 |
| 4:R:204:HIS:NE2 | 4:R:206:ALA:HB3 | 2.34 | 0.43 |
| 1:A:206:VAL:N | 1:A:209:LYS:O | 2.51 | 0.43 |
| 1:A:292:ASP:OD1 | 1:A:293:LYS:N | 2.49 | 0.43 |
| 1:C:36:ASN:C | 1:C:38:LYS:H | 2.21 | 0.43 |
| 1:C:57:ARG:HD2 | 1:C:59:TYR:CE1 | 2.54 | 0.43 |
| 1:C:359:PRO:HB3 | 1:C:372:VAL:HG11 | 2.00 | 0.43 |
| 1:E:461:GLN:HG3 | 1:E:494:LEU:HD11 | 1.99 | 0.43 |
| 2:F:4:VAL:HG12 | 2:F:5:GLN:N | 2.30 | 0.43 |
| 3:M:133:VAL:HG13 | 3:M:210:PHE:HE2 | 1.83 | 0.43 |
| 3:M:143:LYS:HB3 | 3:M:174:TYR:CE2 | 2.54 | 0.43 |
| 4:N:159:TRP:NE1 | 4:N:184:SER:OG | 2.38 | 0.43 |
| 3:Q:37:TYR:CE2 | 3:Q:47:LEU:HD13 | 2.53 | 0.43 |
| 4:R:145:CYS:O | 4:R:184:SER:N | 2.43 | 0.43 |
| 4:R:203:ALA:CB | 4:R:210:LYS:HG2 | 2.48 | 0.43 |
| 1:C:39:PRO:HG3 | 1:C:296:LEU:HD23 | 2.01 | 0.43 |
| 1:C:309:SER:OG | 1:C:327:SER:O | 2.20 | 0.43 |
| 1:C:326:LEU:O | 1:C:370:VAL:N | 2.38 | 0.43 |
| 1:E:31:LEU:N | 1:E:43:VAL:O | 2.47 | 0.43 |
| 1:E:151:ASN:O | 1:E:158:GLN:HG2 | 2.18 | 0.43 |
| 1:E:225:TRP:CE2 | 1:E:234:ARG:HB2 | 2.53 | 0.43 |
| 1:E:487:THR:O | 1:E:492:LEU:HD13 | 2.19 | 0.43 |
| 3:Q:21:ILE:N | 3:Q:74:LEU:O | 2.30 | 0.43 |
| 4:R:143:LEU:HG | 4:R:215:ILE:HG21 | 2.00 | 0.43 |
| 1:A:40:THR:HG22 | 1:A:144:HIS:HD2 | 1.83 | 0.43 |
| 1:A:57:ARG:HD2 | 1:A:59:TYR:CE2 | 2.53 | 0.43 |
| 1:A:171:PRO:N | 1:A:192:PRO:HB2 | 2.34 | 0.43 |
| 1:C:208:SER:OG | 3:M:31:THR:HB | 2.19 | 0.43 |
| 1:C:227:PRO:HD3 | 1:C:232:ALA:O | 2.19 | 0.43 |
| 1:E:232:ALA:C | 1:E:233:TRP:HD1 | 2.22 | 0.43 |
| 3:Q:2:ILE:HG23 | 3:Q:91:HIS:CE1 | 2.53 | 0.43 |
| 3:Q:4:LEU:CB | 3:Q:100:ALA:HB2 | 2.48 | 0.43 |
| 3:Q:125:GLN:HG2 | 3:Q:130:GLY:O | 2.19 | 0.43 |
| 4:R:29:PHE:CZ | 4:R:72:LEU:HD22 | 2.50 | 0.43 |
| 1:A:193:ARG:NE | 1:E:395:HIS:ND1 | 2.67 | 0.43 |
| 1:C:20:TRP:HA | 1:C:289:LEU:O | 2.18 | 0.43 |
| 1:C:243:GLU:HB2 | 1:C:250:GLN:HG3 | 2.01 | 0.43 |
| 1:E:291:MET:O | 1:E:294:LEU:HB3 | 2.19 | 0.43 |
| 4:N:7:SER:N | 4:N:21:SER:O | 2.51 | 0.43 |
| 3:Q:114:PRO:N | 3:Q:140:PHE:HB3 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:140:PHE:HB2 | 3:Q:199:HIS:NE2 | 2.34 | 0.43 |
| 3:Q:148:LYS:HB2 | 3:Q:196:GLU:HG2 | 2.01 | 0.43 |
| 3:Q:151:ILE:HD12 | 3:Q:156:ARG:CB | 2.48 | 0.43 |
| 4:R:100:VAL:N | 4:R:104:GLY:O | 2.52 | 0.43 |
| 1:A:14:GLY:N | 1:A:34:MET:O | 2.47 | 0.43 |
| 1:A:147:THR:O | 1:A:371:LEU:N | 2.28 | 0.43 |
| 1:A:223:LEU:HD23 | 1:A:224:PRO:O | 2.18 | 0.43 |
| 1:A:274:TYR:CD1 | 4:R:102:LEU:HD12 | 2.54 | 0.43 |
| 1:E:214:HIS:CE1 | 2:F:12:LEU:HD23 | 2.53 | 0.43 |
| 4:N:143:LEU:HG | 4:N:215:ILE:HG21 | 2.00 | 0.43 |
| 3:Q:33:TYR:HE1 | 4:R:103:TYR:CE1 | 2.37 | 0.43 |
| 4:R:150:TYR:HE1 | 4:R:153:GLU:HA | 1.83 | 0.43 |
| 1:A:351:VAL:HG23 | 1:A:352:GLY:N | 2.33 | 0.42 |
| 1:A:379:GLY:N | 1:A:398:LYS:O | 2.49 | 0.42 |
| 1:C:456:MET:CB | 1:C:461:GLN:HB3 | 2.49 | 0.42 |
| 1:E:57:ARG:HD2 | 1:E:59:TYR:CE2 | 2.54 | 0.42 |
| 4:N:4:LEU:HD11 | 4:N:98:ARG:HB2 | 2.01 | 0.42 |
| 1:A:27:GLY:HA2 | 1:A:45:MET:O | 2.20 | 0.42 |
| 1:C:213:VAL:HA | 2:D:7:HIS:CE1 | 2.53 | 0.42 |
| 2:D:42:TYR:O | 2:D:45:LEU:HG | 2.19 | 0.42 |
| 1:E:25:LEU:HD11 | 1:E:285:LEU:HD23 | 1.99 | 0.42 |
| 1:E:201:PHE:HA | 1:E:215:ARG:H | 1.84 | 0.42 |
| 1:E:245:ALA:HA | 1:E:249:LYS:O | 2.19 | 0.42 |
| 1:E:370:VAL:HG12 | 1:E:372:VAL:HG23 | 2.00 | 0.42 |
| 1:E:416:ARG:O | 1:E:420:LEU:HD12 | 2.19 | 0.42 |
| 1:E:420:LEU:HB2 | 1:E:424:ALA:HB2 | 2.01 | 0.42 |
| 3:M:109:ARG:HH11 | 3:M:141:TYR:HB3 | 1.84 | 0.42 |
| 3:M:112:ALA:HB3 | 3:M:141:TYR:H | 1.83 | 0.42 |
| 4:R:155:VAL:HG12 | 4:R:204:HIS:CB | 2.48 | 0.42 |
| 4:R:167:GLY:O | 4:R:187:THR:N | 2.52 | 0.42 |
| 1:A:408:LEU:O | 1:A:412:LYS:N | 2.39 | 0.42 |
| 1:C:12:ILE:HD11 | 1:C:31:LEU:HD22 | 2.00 | 0.42 |
| 1:C:144:HIS:CE1 | 1:C:152:HIS:CE1 | 3.07 | 0.42 |
| 1:E:308:PHE:CG | 1:E:385:VAL:HG12 | 2.54 | 0.42 |
| 1:E:385:VAL:HB | 1:E:392:ILE:HG13 | 2.01 | 0.42 |
| 1:E:489:GLY:C | 1:E:491:LEU:N | 2.71 | 0.42 |
| 3:M:115:THR:N | 3:M:138:ASN:O | 2.35 | 0.42 |
| 3:M:121:PRO:HD2 | 3:M:187:TYR:OH | 2.19 | 0.42 |
| 4:R:3:GLN:O | 4:R:25:SER:OG | 2.31 | 0.42 |
| 1:A:179:LYS:HA | 1:A:185:GLU:HA | 2.02 | 0.42 |
| 1:A:214:HIS:NE2 | 2:B:10:SER:O | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:314:PRO:HB2 | 1:A:396:TRP:CE3 | 2.54 | 0.42 |
| 1:A:347:ASP:OD1 | 1:A:348:MET:N | 2.53 | 0.42 |
| 1:C:9:ARG:H | 1:C:319:HIS:CE1 | 2.36 | 0.42 |
| 1:C:16:SER:C | 1:C:18:ALA:H | 2.22 | 0.42 |
| 1:C:59:TYR:HB3 | 1:C:223:LEU:CD2 | 2.49 | 0.42 |
| 1:C:167:PHE:CZ | 1:C:188:LEU:HD22 | 2.53 | 0.42 |
| 1:C:201:PHE:HA | 1:C:215:ARG:N | 2.34 | 0.42 |
| 1:E:204:MET:O | 1:E:211:PHE:N | 2.52 | 0.42 |
| 1:E:308:PHE:HZ | 1:E:338:PRO:HD2 | 1.83 | 0.42 |
| 2:F:36:ILE:HG12 | 2:F:43:ALA:HB2 | 2.00 | 0.42 |
| 3:M:76:ILE:HG21 | 3:M:83:ASP:OD2 | 2.19 | 0.42 |
| 3:Q:6:GLN:NE2 | 3:Q:36:TRP:HZ3 | 2.18 | 0.42 |
| 3:Q:136:PHE:CG | 4:R:185:SER:HB3 | 2.54 | 0.42 |
| 4:R:136:THR:OG1 | 4:R:141:VAL:HG12 | 2.18 | 0.42 |
| 1:A:11:PHE:HD1 | 1:A:32:THR:HB | 1.84 | 0.42 |
| 1:A:19:THR:HB | 1:A:292:ASP:N | 2.34 | 0.42 |
| 1:A:202:TYR:CE1 | 1:A:215:ARG:CZ | 3.02 | 0.42 |
| 2:B:8:GLY:HA2 | 2:B:9:GLU:HA | 1.58 | 0.42 |
| 1:C:456:MET:HE1 | 1:C:460:THR:HB | 2.01 | 0.42 |
| 1:C:461:GLN:HB2 | 1:C:491:LEU:HD11 | 2.01 | 0.42 |
| 1:E:60:CYS:N | 1:E:224:PRO:O | 2.36 | 0.42 |
| 1:E:304:CYS:HB2 | 1:E:338:PRO:HD3 | 2.01 | 0.42 |
| 3:M:35:HIS:CE1 | 4:N:103:TYR:HA | 2.55 | 0.42 |
| 3:M:91:HIS:HE1 | 3:M:96:THR:O | 2.03 | 0.42 |
| 4:N:158:THR:HB | 4:N:162:GLY:N | 2.35 | 0.42 |
| 3:Q:81:ALA:HA | 3:Q:84:GLU:HG2 | 2.00 | 0.42 |
| 3:Q:187:TYR:O | 3:Q:193:TYR:OH | 2.35 | 0.42 |
| 4:R:156:THR:HB | 4:R:203:ALA:HB3 | 2.02 | 0.42 |
| 1:A:53:LEU:HD22 | 1:A:130:ILE:HA | 2.02 | 0.42 |
| 1:A:91:VAL:HG11 | 1:A:237:GLU:HG3 | 2.01 | 0.42 |
| 1:C:2:ASN:ND2 | 1:C:153:GLY:HA2 | 2.34 | 0.42 |
| 1:C:137:TYR:CD1 | 1:C:285:LEU:HD22 | 2.55 | 0.42 |
| 2:D:48:VAL:O | 2:D:52:MET:HG2 | 2.19 | 0.42 |
| 1:E:11:PHE:CD1 | 1:E:32:THR:HB | 2.53 | 0.42 |
| 1:E:292:ASP:OD1 | 1:E:293:LYS:N | 2.51 | 0.42 |
| 2:F:40:PRO:HA | 2:F:43:ALA:HB3 | 2.02 | 0.42 |
| 4:N:199:THR:HA | 4:N:214:LYS:HA | 2.01 | 0.42 |
| 3:Q:95:LEU:HD13 | 4:R:50:TRP:HE1 | 1.85 | 0.42 |
| 4:R:41:PRO:HD3 | 4:R:92:ALA:HA | 2.00 | 0.42 |
| 1:A:340:VAL:HG23 | 1:A:342:VAL:HG13 | 2.02 | 0.42 |
| 1:C:42:ASP:OD1 | 1:C:144:HIS:NE2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:58:SER:OG | 1:C:126:ILE:HG12 | 2.19 | 0.42 |
| 1:C:187:THR:O | 1:C:290:LYS:N | 2.49 | 0.42 |
| 1:C:355:VAL:N | 1:C:374:MET:HA | 2.21 | 0.42 |
| 1:C:422:ASP:CG | 1:C:443:GLN:HA | 2.40 | 0.42 |
| 1:E:21:VAL:O | 1:E:288:ARG:HA | 2.19 | 0.42 |
| 1:E:138:GLU:HG2 | 1:E:168:THR:OG1 | 2.19 | 0.42 |
| 1:E:217:TRP:HE1 | 2:F:5:GLN:C | 2.15 | 0.42 |
| 3:M:95:LEU:HD22 | 4:N:47:TRP:CH2 | 2.54 | 0.42 |
| 4:N:46:LYS:HE3 | 4:N:64:PHE:CZ | 2.55 | 0.42 |
| 3:Q:37:TYR:HB2 | 3:Q:88:TYR:HB2 | 2.01 | 0.42 |
| 3:Q:175:SER:C | 4:R:171:PHE:HE1 | 2.23 | 0.42 |
| 1:A:344:SER:HA | 1:A:382:TYR:HD2 | 1.85 | 0.42 |
| 1:C:489:GLY:O | 1:C:491:LEU:N | 2.53 | 0.42 |
| 1:E:183:TYR:HB3 | 1:E:294:LEU:HD12 | 2.01 | 0.42 |
| 1:E:413:GLY:HA2 | 1:E:416:ARG:NE | 2.35 | 0.42 |
| 3:M:116:VAL:HG13 | 3:M:137:LEU:HG | 2.01 | 0.42 |
| 4:N:4:LEU:HD21 | 4:N:98:ARG:N | 2.35 | 0.42 |
| 4:N:159:TRP:CH2 | 4:N:200:CYS:HB3 | 2.54 | 0.42 |
| 3:Q:91:HIS:CD2 | 3:Q:98:SER:HG | 2.33 | 0.42 |
| 1:A:143:VAL:O | 1:A:163:GLN:HB3 | 2.20 | 0.42 |
| 1:A:185:GLU:O | 1:A:293:LYS:HB2 | 2.20 | 0.42 |
| 1:A:392:ILE:O | 1:A:392:ILE:HG13 | 2.20 | 0.42 |
| 1:C:313:ASN:HB3 | 1:C:314:PRO:HD2 | 2.01 | 0.42 |
| 2:D:8:GLY:HA2 | 2:D:9:GLU:HA | 1.43 | 0.42 |
| 1:E:225:TRP:O | 1:E:234:ARG:N | 2.28 | 0.42 |
| 1:E:261:GLY:HA2 | 1:E:264:GLN:HB2 | 2.02 | 0.42 |
| 1:E:468:LEU:CB | 1:E:487:THR:HG22 | 2.50 | 0.42 |
| 3:M:39:GLN:NE2 | 3:M:43:GLN:O | 2.53 | 0.42 |
| 4:R:122:THR:N | 4:R:151:PHE:O | 2.35 | 0.42 |
| 1:A:59:TYR:HB3 | 1:A:223:LEU:HD22 | 2.01 | 0.42 |
| 1:A:110:LYS:HD2 | 1:A:110:LYS:HA | 1.85 | 0.42 |
| 1:C:84:LYS:HB3 | 1:C:90:TYR:CG | 2.55 | 0.42 |
| 1:E:489:GLY:O | 1:E:491:LEU:N | 2.53 | 0.42 |
| 3:M:44:PRO:HB3 | 4:N:109:GLY:O | 2.20 | 0.42 |
| 4:N:35:HIS:O | 4:N:97:ALA:N | 2.49 | 0.42 |
| 3:Q:109:ARG:HG3 | 3:Q:110:ALA:O | 2.20 | 0.42 |
| 3:Q:122:SER:HB2 | 3:Q:124:GLU:OE1 | 2.19 | 0.42 |
| 4:R:110:GLN:OE1 | 4:R:110:GLN:N | 2.51 | 0.42 |
| 4:R:147:VAL:O | 4:R:181:THR:HA | 2.20 | 0.42 |
| 4:R:173:ALA:HB2 | 4:R:182:LEU:HD23 | 2.00 | 0.42 |
| 1:A:73:ARG:NH2 | 1:A:77:THR:HB | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:151:ASN:O | 1:A:158:GLN:HG2 | 2.19 | 0.41 |
| 1:A:204:MET:O | 1:A:211:PHE:N | 2.52 | 0.41 |
| 1:A:459:ILE:HG22 | 2:B:28:TYR:CD2 | 2.54 | 0.41 |
| 1:C:85:ARG:NH2 | 1:C:94:GLN:HG2 | 2.35 | 0.41 |
| 1:E:131:GLN:HB2 | 1:E:134:ASN:ND2 | 2.35 | 0.41 |
| 2:F:34:ASN:O | 2:F:38:ARG:N | 2.49 | 0.41 |
| 3:M:36:TRP:CZ3 | 3:M:89:CYS:HB3 | 2.55 | 0.41 |
| 3:M:119:PHE:HE1 | 4:N:135:ASP:HB3 | 1.85 | 0.41 |
| 3:M:159:GLY:HA3 | 3:M:181:THR:O | 2.19 | 0.41 |
| 3:M:187:TYR:O | 3:M:212:ARG:NE | 2.52 | 0.41 |
| 4:R:129:LEU:HD11 | 4:R:146:LEU:HB2 | 2.01 | 0.41 |
| 4:R:158:THR:HB | 4:R:162:GLY:N | 2.35 | 0.41 |
| 1:A:288:ARG:HH11 | 1:E:346:ASN:ND2 | 2.17 | 0.41 |
| 1:A:480:ILE:O | 1:A:484:PHE:N | 2.53 | 0.41 |
| 2:B:66:LEU:O | 2:B:70:VAL:HG23 | 2.20 | 0.41 |
| 1:C:91:VAL:HG11 | 1:C:237:GLU:HG3 | 2.01 | 0.41 |
| 1:C:493:PHE:O | 1:C:497:ASN:N | 2.46 | 0.41 |
| 1:E:48:ILE:CD1 | 1:E:283:GLY:HA2 | 2.46 | 0.41 |
| 1:E:90:TYR:CD1 | 1:E:118:LYS:HB2 | 2.54 | 0.41 |
| 1:E:121:CYS:SG | 1:E:124:LYS:HB3 | 2.60 | 0.41 |
| 1:E:142:PHE:HE2 | 1:E:144:HIS:ND1 | 2.17 | 0.41 |
| 1:E:218:PHE:HD2 | 1:E:219:HIS:CD2 | 2.38 | 0.41 |
| 1:E:308:PHE:CZ | 1:E:338:PRO:HD2 | 2.55 | 0.41 |
| 1:E:428:GLY:O | 1:E:435:ASN:HB3 | 2.20 | 0.41 |
| 3:Q:171:ASP:N | 3:Q:171:ASP:OD1 | 2.49 | 0.41 |
| 4:R:147:VAL:O | 4:R:182:LEU:N | 2.51 | 0.41 |
| 1:A:146:THR:HG21 | 1:A:362:ALA:HB2 | 2.02 | 0.41 |
| 1:A:155:TYR:O | 1:A:159:VAL:HG23 | 2.20 | 0.41 |
| 1:A:327:SER:HA | 1:A:369:LYS:HA | 2.01 | 0.41 |
| 1:C:65:VAL:HG11 | 1:C:252:VAL:O | 2.20 | 0.41 |
| 1:C:202:TYR:N | 1:C:213:VAL:O | 2.42 | 0.41 |
| 1:E:8:ASN:HD22 | 1:E:29:SER:HB3 | 1.85 | 0.41 |
| 1:E:321:THR:HA | 1:E:376:PRO:HD2 | 2.02 | 0.41 |
| 3:M:6:GLN:NE2 | 3:M:36:TRP:HZ3 | 2.18 | 0.41 |
| 3:M:48:LEU:O | 3:M:56:GLU:HG2 | 2.19 | 0.41 |
| 2:D:39:ASN:ND2 | 1:E:454:GLY:O | 2.53 | 0.41 |
| 1:E:311:ALA:N | 1:E:325:GLU:O | 2.53 | 0.41 |
| 3:Q:13:VAL:HG22 | 3:Q:17:GLN:HB3 | 2.02 | 0.41 |
| 3:Q:116:VAL:O | 3:Q:208:LYS:HG3 | 2.20 | 0.41 |
| 1:A:321:THR:OG1 | 1:A:373:GLU:OE2 | 2.22 | 0.41 |
| 1:E:12:ILE:HD11 | 1:E:31:LEU:HD13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:38:LYS:HD2 | 1:E:294:LEU:HG | 2.03 | 0.41 |
| 1:E:75:PRO:CD | 1:E:111:GLY:HA2 | 2.47 | 0.41 |
| 2:F:40:PRO:O | 2:F:44:PHE:N | 2.47 | 0.41 |
| 4:N:6:GLU:OE2 | 4:N:96:CYS:N | 2.39 | 0.41 |
| 4:N:41:PRO:HD3 | 4:N:92:ALA:HB2 | 2.02 | 0.41 |
| 4:N:128:PRO:HB2 | 4:N:215:ILE:HA | 2.02 | 0.41 |
| 3:Q:35:HIS:NE2 | 3:Q:92:ILE:HG13 | 2.35 | 0.41 |
| 4:R:36:TRP:O | 4:R:48:MET:N | 2.52 | 0.41 |
| 4:R:87:LYS:O | 4:R:90:ASP:N | 2.54 | 0.41 |
| 1:A:34:MET:SD | 1:A:355:VAL:HA | 2.60 | 0.41 |
| 1:A:38:LYS:HE3 | 1:A:291:MET:HB3 | 2.01 | 0.41 |
| 1:A:50:ALA:HB3 | 1:A:278:VAL:CG1 | 2.51 | 0.41 |
| 1:A:97:THR:O | 1:A:99:ARG:HG2 | 2.21 | 0.41 |
| 1:A:139:VAL:HB | 1:A:167:PHE:CZ | 2.56 | 0.41 |
| 1:A:268:GLY:H | 2:B:8:GLY:HA2 | 1.85 | 0.41 |
| 2:B:30:MET:O | 2:B:34:ASN:N | 2.37 | 0.41 |
| 1:C:3:CYS:O | 1:C:9:ARG:HD2 | 2.21 | 0.41 |
| 1:C:156:SER:O | 1:C:159:VAL:HB | 2.21 | 0.41 |
| 1:C:201:PHE:O | 1:C:215:ARG:NE | 2.51 | 0.41 |
| 1:C:360:PHE:CE2 | 1:C:362:ALA:HA | 2.56 | 0.41 |
| 1:E:307:LYS:N | 1:E:390:LYS:HD2 | 2.35 | 0.41 |
| 1:E:384:VAL:HG13 | 1:E:391:GLN:HB2 | 2.02 | 0.41 |
| 3:M:46:ARG:HH12 | 4:N:107:TYR:HD1 | 1.65 | 0.41 |
| 3:Q:31:THR:OG1 | 3:Q:32:SER:N | 2.53 | 0.41 |
| 3:Q:109:ARG:HH11 | 3:Q:141:TYR:HB3 | 1.85 | 0.41 |
| 1:A:141:ILE:O | 1:A:165:ALA:N | 2.41 | 0.41 |
| 1:A:148:THR:HG23 | 1:A:151:ASN:HD21 | 1.86 | 0.41 |
| 1:A:224:PRO:HG3 | 1:A:236:ARG:HA | 2.01 | 0.41 |
| 1:C:48:ILE:CD1 | 1:C:283:GLY:HA2 | 2.51 | 0.41 |
| 1:C:308:PHE:CD1 | 1:C:385:VAL:HG12 | 2.55 | 0.41 |
| 1:E:56:VAL:HG11 | 1:E:202:TYR:CZ | 2.56 | 0.41 |
| 3:M:95:LEU:HD23 | 3:M:97:ARG:HG3 | 2.03 | 0.41 |
| 3:M:182:LEU:HB2 | 3:M:187:TYR:HB2 | 2.03 | 0.41 |
| 4:N:29:PHE:HZ | 4:N:72:LEU:HD22 | 1.86 | 0.41 |
| 4:R:12:LYS:HB2 | 4:R:116:VAL:HG22 | 2.03 | 0.41 |
| 4:R:147:VAL:HB | 4:R:182:LEU:HG | 2.03 | 0.41 |
| 1:A:72:ALA:HB1 | 1:A:99:ARG:HH21 | 1.85 | 0.41 |
| 1:A:99:ARG:HG3 | 1:A:105:CYS:SG | 2.60 | 0.41 |
| 1:A:119:PHE:CZ | 1:A:236:ARG:HB2 | 2.55 | 0.41 |
| 1:A:261:GLY:O | 1:A:265:ALA:N | 2.46 | 0.41 |
| 1:C:27:GLY:CA | 1:C:45:MET:HB3 | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:456:MET:CE | 1:C:460:THR:HB | 2.51 | 0.41 |
| 4:N:52:ASN:OD1 | 4:N:53:THR:N | 2.54 | 0.41 |
| 3:Q:2:ILE:HG13 | 3:Q:27:GLN:HB3 | 2.02 | 0.41 |
| 3:Q:148:LYS:HB2 | 3:Q:196:GLU:CG | 2.51 | 0.41 |
| 4:R:2:VAL:HG21 | 4:R:98:ARG:HH12 | 1.85 | 0.41 |
| 4:R:152:PRO:HD2 | 4:R:206:ALA:HB1 | 2.02 | 0.41 |
| 1:A:31:LEU:O | 1:A:43:VAL:N | 2.45 | 0.41 |
| 1:A:48:ILE:CD1 | 1:A:283:GLY:HA2 | 2.51 | 0.41 |
| 1:A:88:SER:O | 1:A:236:ARG:NH2 | 2.54 | 0.41 |
| 1:A:155:TYR:CD1 | 1:A:166:LYS:HE3 | 2.55 | 0.41 |
| 1:A:229:SER:OG | 1:A:230:SER:N | 2.54 | 0.41 |
| 1:A:354:LEU:HD13 | 1:A:359:PRO:HD3 | 2.03 | 0.41 |
| 1:A:468:LEU:CB | 1:A:487:THR:HG22 | 2.51 | 0.41 |
| 1:C:40:THR:HG22 | 1:C:144:HIS:HD2 | 1.86 | 0.41 |
| 2:D:67:LEU:HA | 2:D:70:VAL:HG23 | 2.03 | 0.41 |
| 1:E:9:ARG:HG2 | 1:E:11:PHE:CE1 | 2.56 | 0.41 |
| 1:E:128:ARG:HH12 | 1:E:205:THR:HG1 | 1.67 | 0.41 |
| 1:E:137:TYR:HE2 | 1:E:192:PRO:HA | 1.86 | 0.41 |
| 1:E:274:TYR:HA | 1:E:277:SER:O | 2.21 | 0.41 |
| 3:M:13:VAL:HG22 | 3:M:17:GLN:HB3 | 2.03 | 0.41 |
| 3:M:140:PHE:HB2 | 3:M:199:HIS:NE2 | 2.35 | 0.41 |
| 4:N:2:VAL:HG21 | 4:N:98:ARG:NH1 | 2.36 | 0.41 |
| 4:N:39:GLN:HB3 | 4:N:95:PHE:HE2 | 1.85 | 0.41 |
| 4:N:64:PHE:HB3 | 4:N:68:PHE:HD2 | 1.86 | 0.41 |
| 3:Q:29:VAL:O | 3:Q:31:THR:HG23 | 2.21 | 0.41 |
| 3:Q:48:LEU:O | 3:Q:59:VAL:HG21 | 2.20 | 0.41 |
| 3:Q:55:LEU:HD11 | 3:Q:61:SER:CA | 2.47 | 0.41 |
| 3:Q:149:TRP:CD1 | 3:Q:160:VAL:HG22 | 2.56 | 0.41 |
| 4:R:4:LEU:HD13 | 4:R:107:TYR:HB2 | 2.03 | 0.41 |
| 4:R:46:LYS:HE3 | 4:R:64:PHE:CZ | 2.56 | 0.41 |
| 4:R:141:VAL:HG23 | 4:R:188:VAL:HG23 | 2.01 | 0.41 |
| 1:A:1:PHE:CG | 1:A:2:ASN:N | 2.89 | 0.41 |
| 1:A:53:LEU:CD2 | 1:A:130:ILE:HG12 | 2.50 | 0.41 |
| 1:A:55:GLU:HG2 | 1:A:128:ARG:NE | 2.36 | 0.41 |
| 1:A:65:VAL:HG11 | 1:A:252:VAL:O | 2.21 | 0.41 |
| 1:A:291:MET:O | 1:A:294:LEU:HB3 | 2.21 | 0.41 |
| 1:C:203:VAL:HG12 | 1:C:210:SER:HB3 | 2.03 | 0.41 |
| 1:C:410:THR:O | 1:C:413:GLY:N | 2.52 | 0.41 |
| 1:E:42:ASP:O | 1:E:141:ILE:HG13 | 2.21 | 0.41 |
| 1:E:67:ASP:HB3 | 1:E:118:LYS:HB2 | 2.03 | 0.41 |
| 1:E:316:ASP:HA | 1:E:322:VAL:HG22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:M:25:ALA:HB3 | 3:M:70:THR:HA | 2.03 | 0.41 |
| 3:M:47:LEU:CD2 | 4:N:106:ASP:HA | 2.51 | 0.41 |
| 3:M:47:LEU:HD23 | 4:N:106:ASP:HA | 2.01 | 0.41 |
| 4:R:37:VAL:N | 4:R:48:MET:HE2 | 2.36 | 0.41 |
| 4:R:70:PHE:CE1 | 4:R:81:LEU:HD13 | 2.55 | 0.41 |
| 4:R:86:LEU:HA | 4:R:90:ASP:OD2 | 2.21 | 0.41 |
| 1:A:46:ILE:HD11 | 1:A:166:LYS:HG2 | 2.02 | 0.40 |
| 1:C:51:SER:HB2 | 4:N:31:ASP:O | 2.21 | 0.40 |
| 1:E:63:ALA:HA | 1:E:122:THR:H | 1.86 | 0.40 |
| 1:E:69:SER:OG | 1:E:116:CYS:HB2 | 2.20 | 0.40 |
| 1:E:336:LYS:O | 1:E:338:PRO:HD3 | 2.21 | 0.40 |
| 3:M:109:ARG:HG3 | 3:M:110:ALA:O | 2.21 | 0.40 |
| 4:N:145:CYS:O | 4:N:183:SER:HA | 2.21 | 0.40 |
| 4:R:73:GLU:OE2 | 4:R:76:ALA:N | 2.32 | 0.40 |
| 1:A:26:GLU:C | 1:A:45:MET:HB3 | 2.41 | 0.40 |
| 1:A:93:LYS:HG3 | 1:A:94:GLN:O | 2.21 | 0.40 |
| 2:B:13:VAL:HG12 | 2:B:14:ASN:N | 2.36 | 0.40 |
| 1:C:461:GLN:HE21 | 1:C:494:LEU:CD1 | 2.34 | 0.40 |
| 1:E:37:ASP:O | 1:E:296:LEU:HG | 2.21 | 0.40 |
| 1:E:242:PHE:HB3 | 1:E:250:GLN:HE21 | 1.85 | 0.40 |
| 1:E:430:ILE:HG13 | 1:E:430:ILE:O | 2.21 | 0.40 |
| 1:E:431:GLY:HA2 | 1:E:435:ASN:HB2 | 2.02 | 0.40 |
| 1:E:459:ILE:HG12 | 1:E:463:LEU:HB2 | 2.04 | 0.40 |
| 3:M:44:PRO:HG3 | 4:N:110:GLN:HA | 2.03 | 0.40 |
| 4:N:8:GLY:O | 4:N:112:THR:HG23 | 2.21 | 0.40 |
| 4:N:47:TRP:CH2 | 4:N:49:GLY:HA2 | 2.57 | 0.40 |
| 3:Q:92:ILE:HG21 | 4:R:101:GLY:O | 2.21 | 0.40 |
| 1:A:123:SER:HA | 3:Q:28:SER:CA | 2.47 | 0.40 |
| 1:A:203:VAL:HG13 | 1:A:272:VAL:HG21 | 2.04 | 0.40 |
| 1:A:324:ILE:HD12 | 1:A:326:LEU:HD21 | 2.02 | 0.40 |
| 1:A:413:GLY:O | 1:A:417:LEU:HG | 2.22 | 0.40 |
| 1:C:93:LYS:HG3 | 1:C:94:GLN:O | 2.22 | 0.40 |
| 1:C:412:LYS:HG2 | 1:C:416:ARG:HG3 | 2.04 | 0.40 |
| 1:E:143:VAL:N | 1:E:163:GLN:O | 2.37 | 0.40 |
| 1:E:304:CYS:N | 1:E:338:PRO:HD3 | 2.34 | 0.40 |
| 1:E:328:TYR:HE2 | 1:E:332:ASP:OD1 | 2.04 | 0.40 |
| 1:E:389:ASP:OD1 | 1:E:390:LYS:HG2 | 2.21 | 0.40 |
| 4:N:35:HIS:CD2 | 4:N:105:VAL:HG12 | 2.56 | 0.40 |
| 4:N:52:ASN:OD1 | 4:N:54:GLY:N | 2.54 | 0.40 |
| 4:N:150:TYR:CE1 | 4:N:155:VAL:HG13 | 2.56 | 0.40 |
| 3:Q:12:ALA:HA | 3:Q:106:GLU:HB2 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:118:ILE:HG23 | 3:Q:118:ILE:O | 2.22 | 0.40 |
| 4:R:64:PHE:HD1 | 4:R:68:PHE:HE2 | 1.68 | 0.40 |
| 1:A:24:VAL:HG12 | 1:A:286:LYS:HG2 | 2.04 | 0.40 |
| 1:C:39:PRO:HD2 | 1:C:294:LEU:HD11 | 2.03 | 0.40 |
| 1:C:127:GLY:HA3 | 1:C:218:PHE:CZ | 2.56 | 0.40 |
| 1:C:396:TRP:CG | 1:C:397:HIS:N | 2.90 | 0.40 |
| 2:D:13:VAL:HG12 | 2:D:14:ASN:N | 2.35 | 0.40 |
| 1:E:54:ALA:O | 1:E:129:THR:HG22 | 2.21 | 0.40 |
| 3:M:149:TRP:CD1 | 3:M:160:VAL:HG22 | 2.56 | 0.40 |
| 4:N:151:PHE:HA | 4:N:152:PRO:HA | 1.85 | 0.40 |
| 3:Q:44:PRO:HA | 4:R:95:PHE:CE1 | 2.56 | 0.40 |
| 3:Q:89:CYS:SG | 3:Q:100:ALA:HB3 | 2.61 | 0.40 |
| 3:Q:112:ALA:N | 3:Q:141:TYR:O | 2.54 | 0.40 |
| 1:A:8:ASN:HD22 | 1:A:29:SER:HB3 | 1.86 | 0.40 |
| 1:C:19:THR:HB | 1:C:291:MET:HB2 | 2.03 | 0.40 |
| 1:C:99:ARG:HA | 1:C:103:ASN:HD21 | 1.87 | 0.40 |
| 1:E:196:LEU:HD23 | 2:F:13:VAL:HG21 | 2.04 | 0.40 |
| 1:E:314:PRO:HG3 | 1:E:394:HIS:CG | 2.57 | 0.40 |
| 3:M:44:PRO:HA | 3:M:45:PRO:HD3 | 1.98 | 0.40 |
| 4:R:170:THR:HG23 | 4:R:184:SER:HB2 | 2.03 | 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 | 498/500 (100%) | 455 (91%) | 40 (8%) | 3 (1%) | 25 65 |
| 1 | C | 498/500 (100%) | 450 (90%) | 46 (9%) | 2 (0%) | 34 72 |
| 1 | E | 498/500 (100%) | 458 (92%) | 37 (7%) | 3 (1%) | 25 65 |
| 2 | B | 72/74 (97%) | 62 (86%) | 9 (12%) | 1 (1%) | 11 47 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | D | 72/74 (97%) | 59 (82%) | 12 (17%) | 1 (1%) | 11 | 47 |
| 2 | F | 72/74 (97%) | 62 (86%) | 8 (11%) | 2 (3%) | 5 | 33 |
| 3 | M | 213/215 (99%) | 200 (94%) | 11 (5%) | 2 (1%) | 17 | 56 |
| 3 | Q | 213/215 (99%) | 201 (94%) | 10 (5%) | 2 (1%) | 17 | 56 |
| 4 | N | 216/218 (99%) | 209 (97%) | 7 (3%) | 0 | 100 | 100 |
| 4 | R | 216/218 (99%) | 208 (96%) | 8 (4%) | 0 | 100 | 100 |
| All | All | 2568/2588 (99%) | 2364 (92%) | 188 (7%) | 16 (1%) | 29 | 65 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 490 | VAL |
| 1 | C | 490 | VAL |
| 1 | E | 490 | VAL |
| 3 | M | 52 | VAL |
| 3 | Q | 52 | VAL |
| 1 | A | 433 | VAL |
| 2 | B | 13 | VAL |
| 1 | C | 433 | VAL |
| 2 | D | 13 | VAL |
| 1 | E | 433 | VAL |
| 2 | F | 13 | VAL |
| 2 | F | 64 | THR |
| 3 | Q | 78 | PRO |
| 3 | M | 78 | PRO |
| 1 | A | 430 | ILE |
| 1 | E | 430 | ILE |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 399/399 (100%) | 399 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | C | 399/399 (100%) | 399 (100%) | 0 | 100 | 100 |
| 1 | E | 399/399 (100%) | 399 (100%) | 0 | 100 | 100 |
| 2 | B | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 2 | D | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 2 | F | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 3 | M | 186/192 (97%) | 186 (100%) | 0 | 100 | 100 |
| 3 | Q | 186/192 (97%) | 186 (100%) | 0 | 100 | 100 |
| 4 | N | 183/185 (99%) | 183 (100%) | 0 | 100 | 100 |
| 4 | R | 183/185 (99%) | 183 (100%) | 0 | 100 | 100 |
| All | All | 2121/2140 (99%) | 2121 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 52 | GLN |
| 1 | A | 81 | HIS |
| 1 | A | 131 | GLN |
| 1 | A | 134 | ASN |
| 1 | A | 152 | HIS |
| 1 | A | 158 | GLN |
| 1 | A | 163 | GLN |
| 1 | A | 250 | GLN |
| 1 | A | 319 | HIS |
| 1 | A | 358 | ASN |
| 2 | B | 56 | ASN |
| 1 | C | 8 | ASN |
| 1 | C | 36 | ASN |
| 1 | C | 81 | HIS |
| 1 | C | 94 | GLN |
| 1 | C | 219 | HIS |
| 1 | C | 250 | GLN |
| 1 | C | 263 | HIS |
| 2 | D | 59 | GLN |
| 1 | E | 36 | ASN |
| 1 | E | 62 | HIS |
| 1 | E | 94 | GLN |
| 1 | E | 134 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 152 | HIS |
| 1 | E | 197 | ASN |
| 1 | E | 214 | HIS |
| 1 | E | 219 | HIS |
| 1 | E | 250 | GLN |
| 1 | E | 263 | HIS |
| 1 | E | 264 | GLN |
| 1 | E | 319 | HIS |
| 1 | E | 358 | ASN |
| 2 | F | 5 | GLN |
| 2 | F | 7 | HIS |
| 2 | F | 59 | GLN |
| 3 | M | 27 | GLN |
| 3 | M | 162 | ASN |
| 4 | N | 176 | GLN |
| 3 | Q | 27 | GLN |
| 3 | Q | 139 | ASN |
| 3 | Q | 162 | ASN |
| 4 | R | 52 | ASN |

### 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)

There are no chain breaks in this entry.

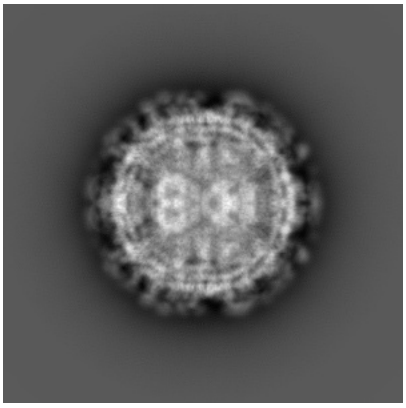
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6855. These allow visual inspection of the internal detail of the map and identification of artifacts.

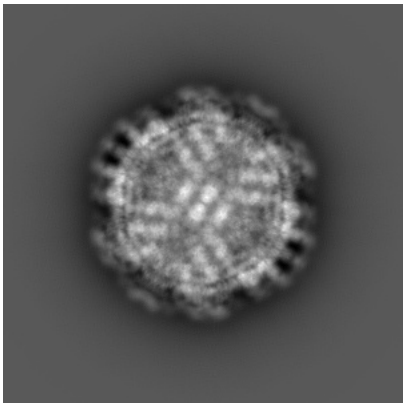
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

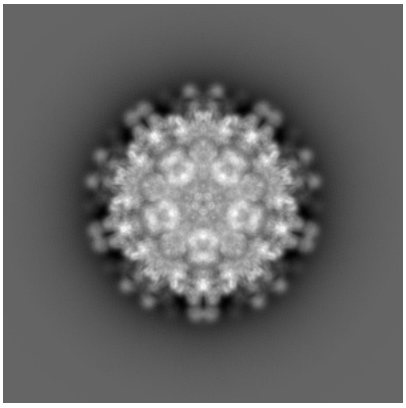
### 6.1.1 Primary map



X



Y

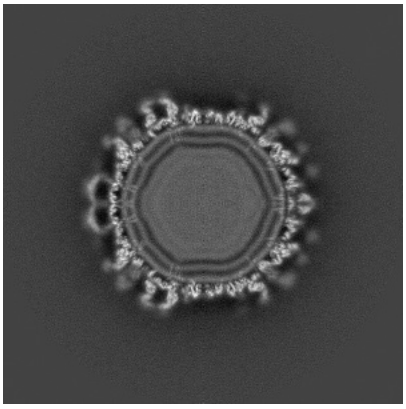


Z

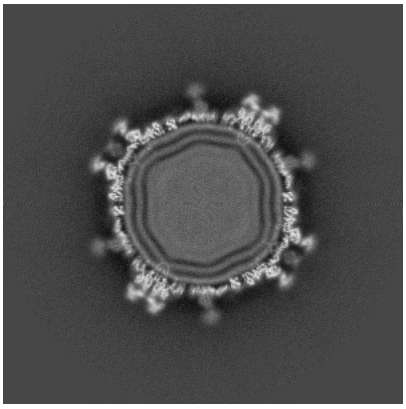
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

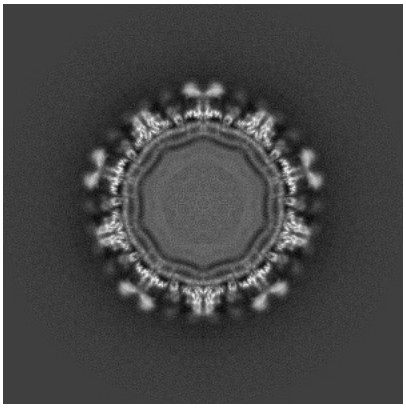
### 6.2.1 Primary map



X Index: 360



Y Index: 360

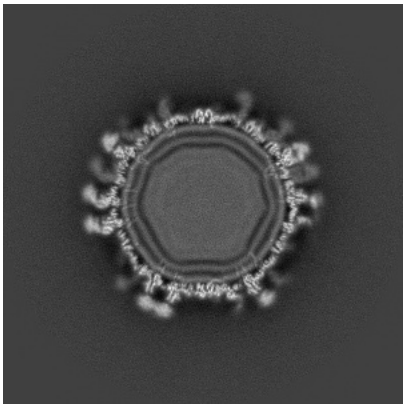


Z Index: 360

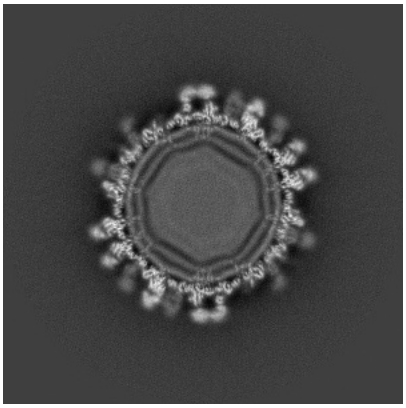
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

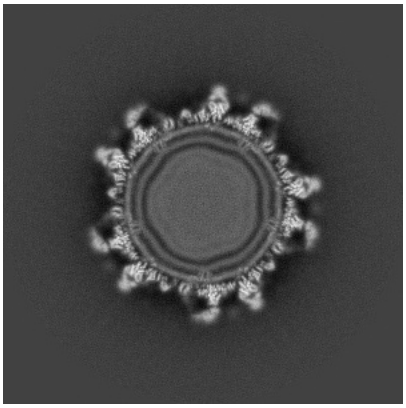
### 6.3.1 Primary map



X Index: 372



Y Index: 402

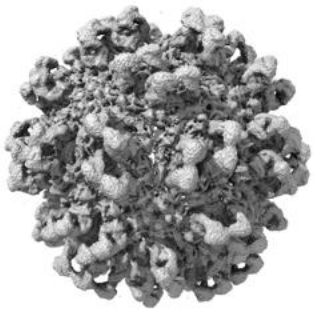


Z Index: 328

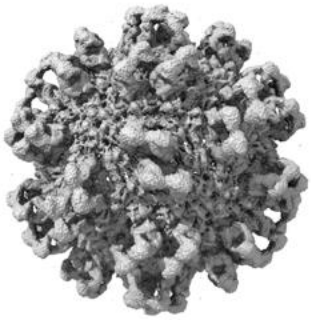
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

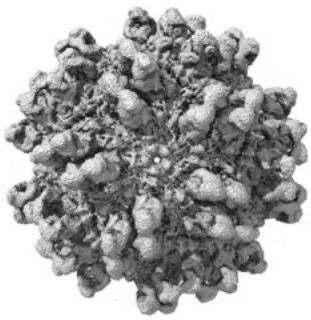
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

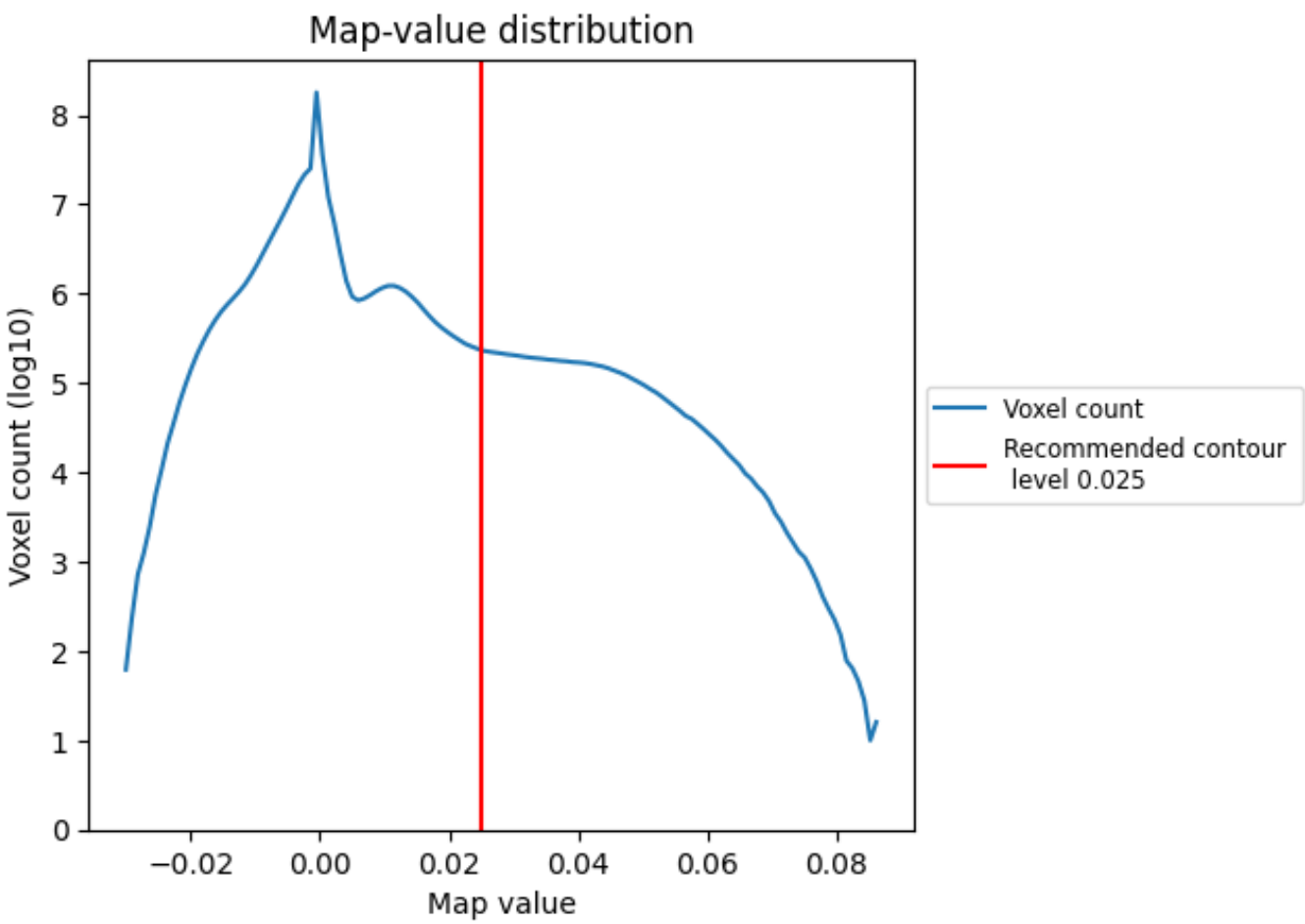
## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis (i)

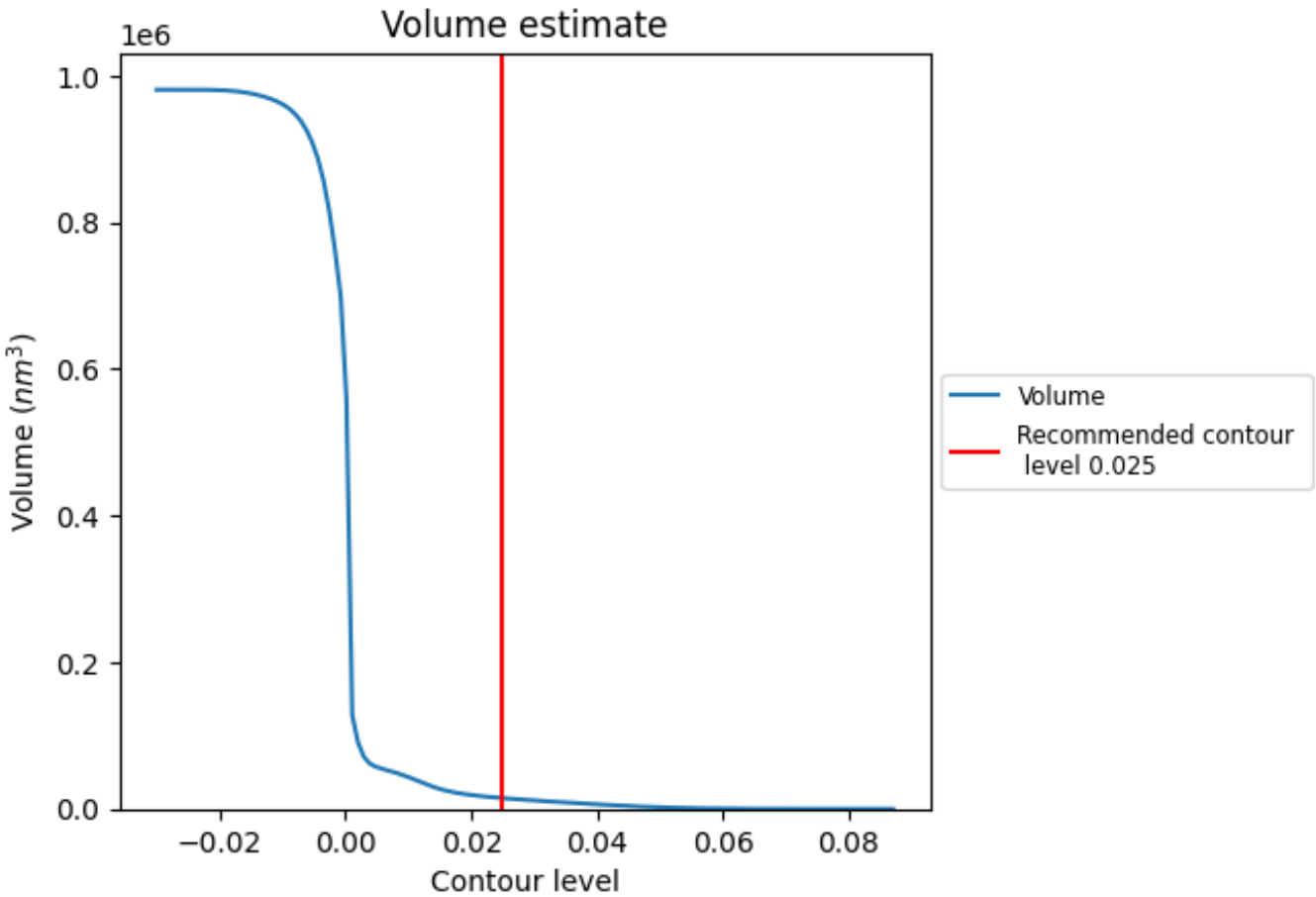
This section contains the results of statistical analysis of the map.

## 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.

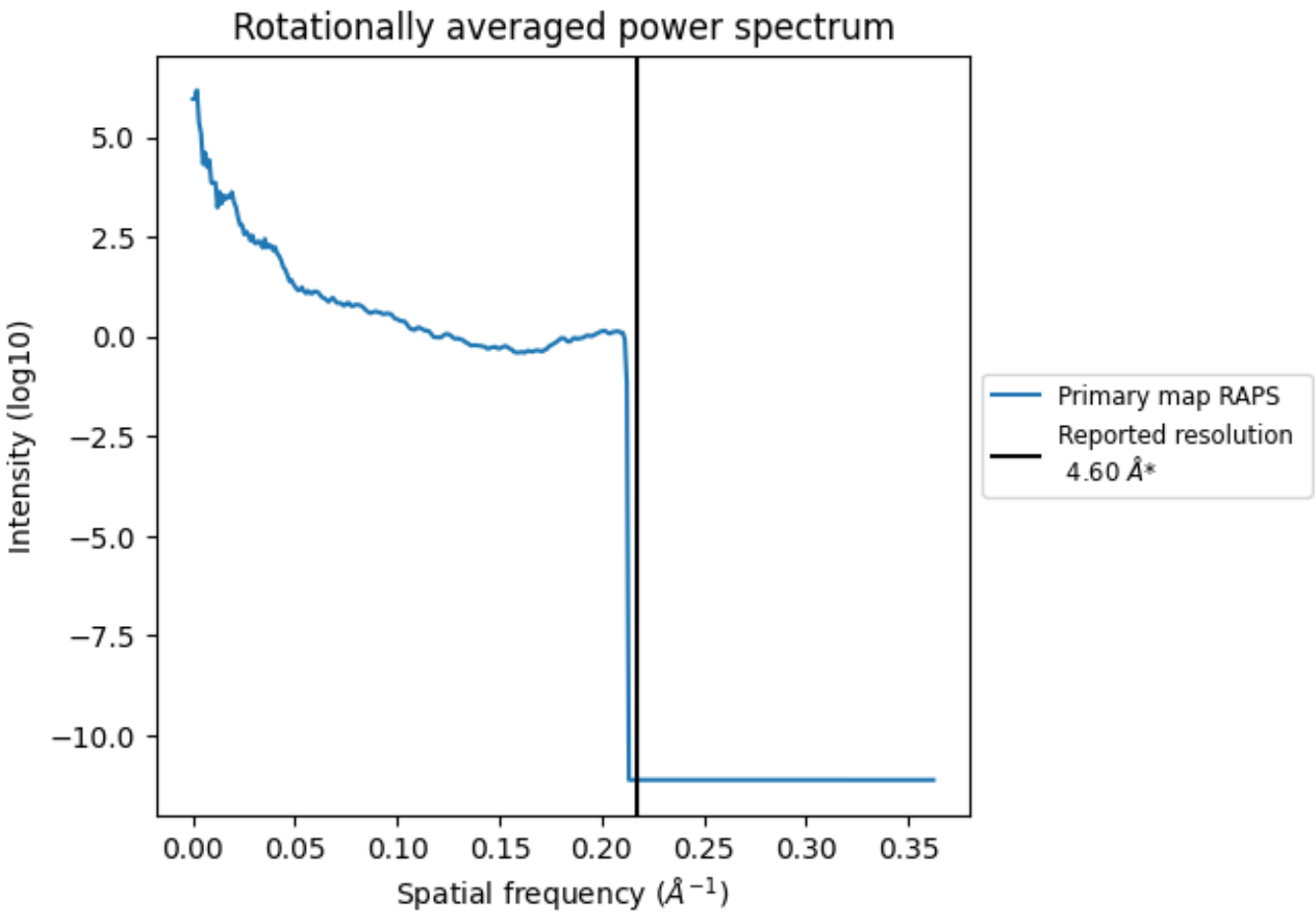
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 14735 $nm^3$; this corresponds to an approximate mass of 13310 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 0.217 Å$^{-1}$

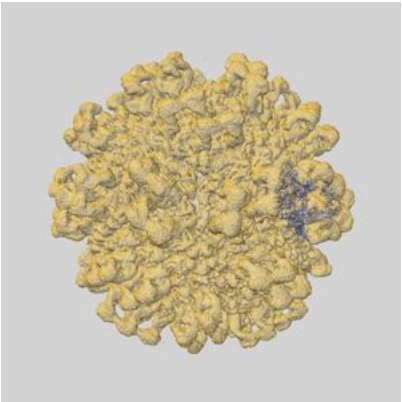
# 8 Fourier-Shell correlation (i)

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

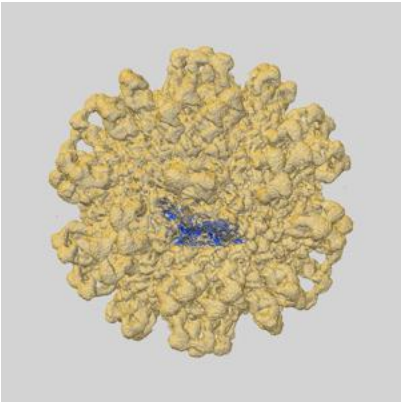
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6855 and PDB model 5YWP. Per-residue inclusion information can be found in section 3 on page 5.

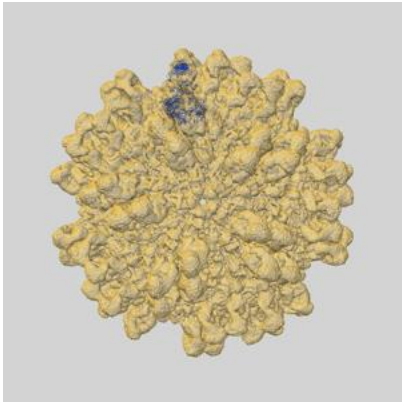
## 9.1 Map-model overlay (i)



X



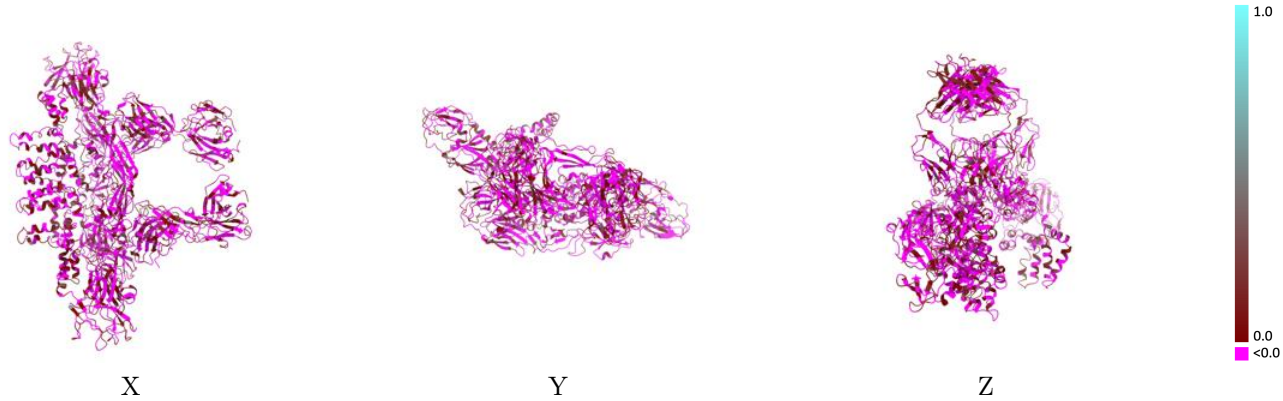
Y



Z

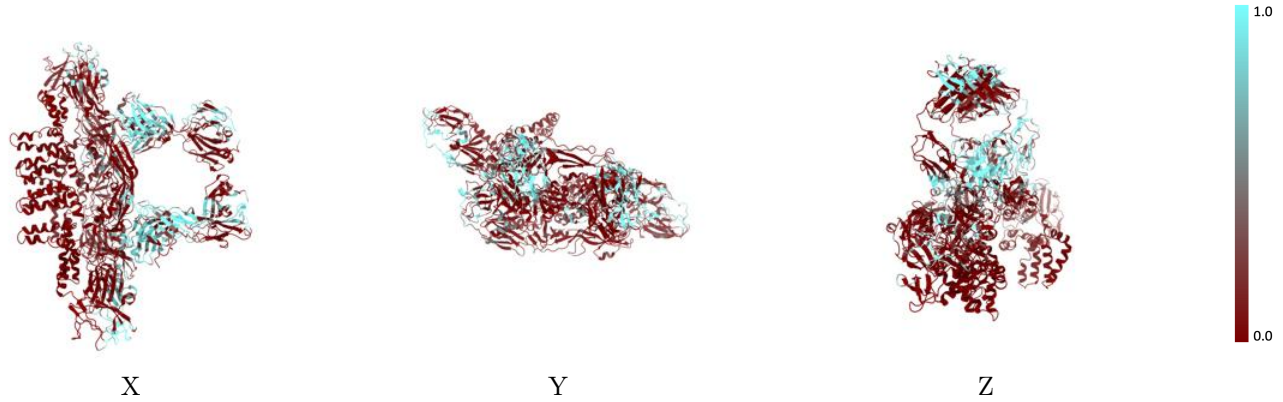
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



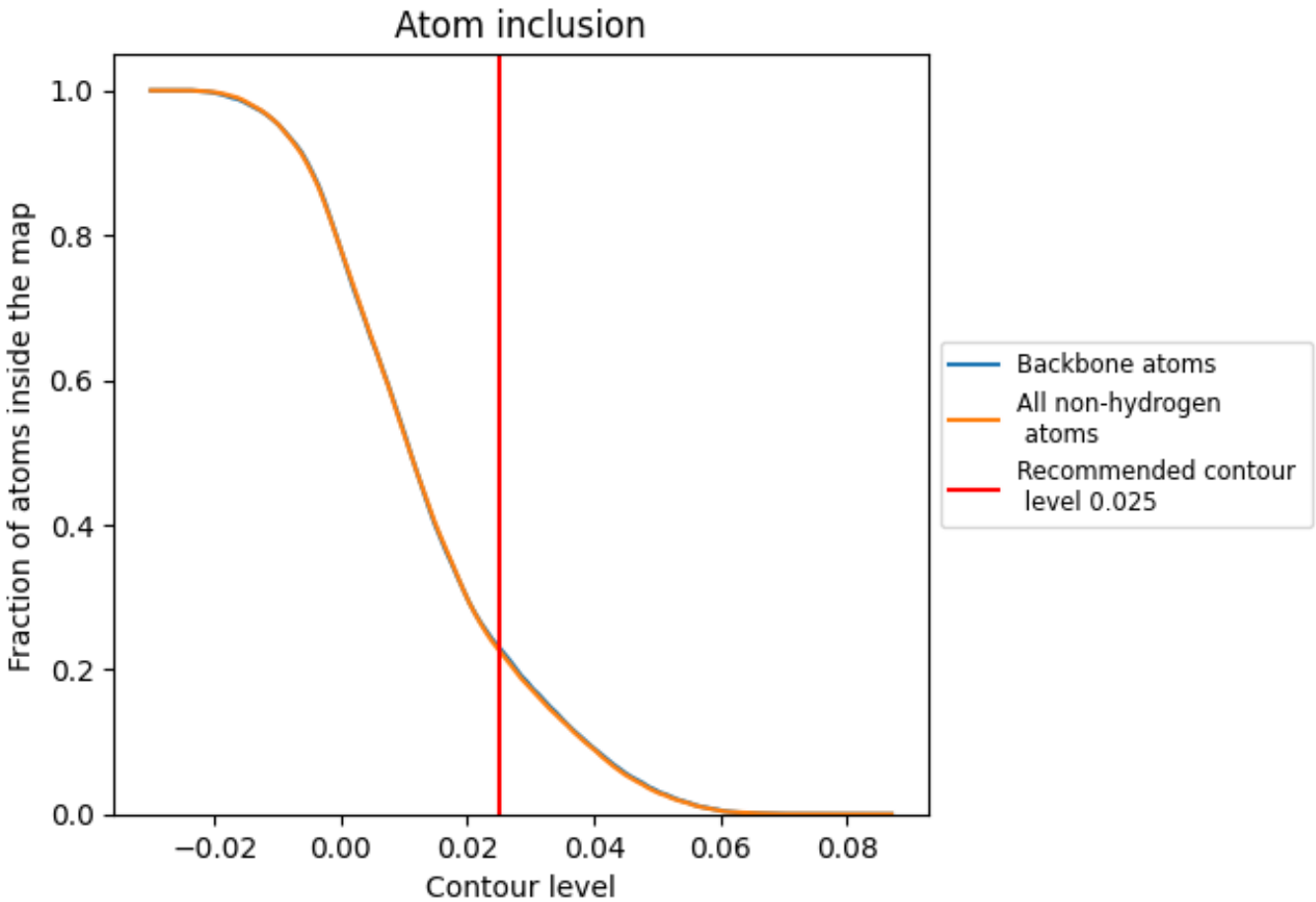

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)




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 (0.025).

## 9.4 Atom inclusion (i)




At the recommended contour level, 23% of all backbone atoms, 23% 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 (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.2267 | -0.0120 |
| A | 0.1639 | -0.0150 |
| B | 0.0728 | 0.0120 |
| C | 0.1615 | -0.0170 |
| D | 0.0409 | 0.0100 |
| E | 0.0976 | -0.0320 |
| F | 0.0337 | -0.0050 |
| M | 0.1872 | -0.0290 |
| N | 0.6086 | 0.0240 |
| Q | 0.5006 | 0.0030 |
| R | 0.3840 | -0.0010 |