# Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 08:54 am GMT

| | | |
|---|---|---|
| PDB ID | : | 7NFC |
| EMDB ID | : | EMD-12299 |
| Title | : | Cryo-EM structure of NHEJ super-complex (dimer) |
| Authors | : | Chaplin, A.K.; Hardwick, S.W.; Kefala Stavridi, A.; Chirgadze, D.Y.; Blundell, T.L. |
| Deposited on | : | 2021-02-05 |
| Resolution | : | 4.14 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 ⓘ symbol.

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

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

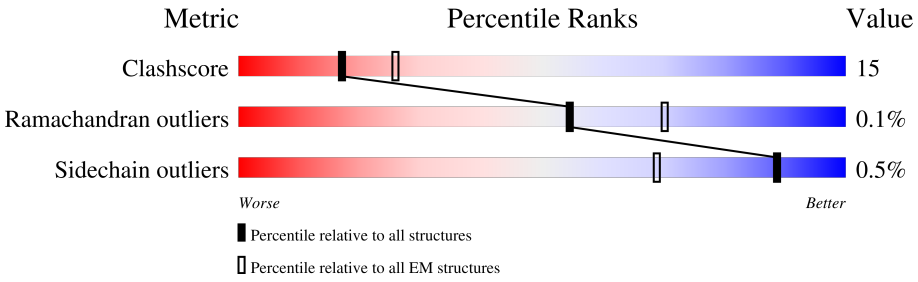
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 4.14 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 | 4148 | 55% 31% 14% |
| 1 | F | 4148 | 56% 30% 14% |
| 2 | B | 609 | 44% 34% 22% |
| 2 | G | 609 | 46% 34% 20% |
| 3 | C | 732 | 43% 22% 35% |
| 3 | H | 732 | 13% 60% 28% 12% |
| 4 | K | 336 | 19% 45% 14% 40% |
| 4 | L | 336 | 20% 43% 14% 42% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | N | 336 | 21% 47% 12% 40% |
| 4 | O | 336 | 27% 45% 13% 42% |
| 5 | M | 911 | 6% 22% 7% 72% |
| 5 | P | 911 | 16% 10% 73% |
| 6 | Q | 299 | 31% 51% 19% 29% |
| 6 | R | 299 | 30% 51% 22% 27% |
| 7 | D | 27 | 19% 81% |
| 8 | E | 28 | 21% 79% |
| 8 | I | 28 | 21% 79% |
| 9 | J | 27 | 33% 67% |

# 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 89069 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 3562 | Total | C | N | O | S | 0 | 0 |
| | | | 28076 | 18032 | 4728 | 5132 | 184 | | |
| 1 | F | 3557 | Total | C | N | O | S | 0 | 0 |
| | | | 28060 | 18026 | 4720 | 5131 | 183 | | |

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 476 | Total | C | N | O | S | 0 | 0 |
| | | | 3822 | 2452 | 648 | 705 | 17 | | |
| 2 | G | 489 | Total | C | N | O | S | 0 | 0 |
| | | | 3948 | 2529 | 669 | 732 | 18 | | |

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 477 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2466 | 646 | 714 | 23 | | |
| 3 | H | 642 | Total | C | N | O | S | 0 | 0 |
| | | | 5150 | 3298 | 864 | 963 | 25 | | |

- Molecule 4 is a protein called DNA repair protein XRCC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | K | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1625 | 1028 | 278 | 312 | 7 | | |
| 4 | L | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1592 | 1009 | 272 | 304 | 7 | | |
| 4 | N | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1625 | 1028 | 278 | 312 | 7 | | |
| 4 | O | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1579 | 1000 | 271 | 301 | 7 | | |

- Molecule 5 is a protein called DNA ligase 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | M | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 2095 | 1333 | 353 | 396 | 13 | | |
| 5 | P | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1965 | 1248 | 330 | 374 | 13 | | |

- Molecule 6 is a protein called Non-homologous end-joining factor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | Q | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1690 | 1084 | 282 | 310 | 14 | | |
| 6 | R | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1728 | 1105 | 288 | 320 | 15 | | |

- Molecule 7 is a DNA chain called DNA (27-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | D | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 556 | 268 | 95 | 166 | 27 | | |

- Molecule 8 is a DNA chain called DNA (28-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | E | 28 | Total | C | N | O | P | 0 | 0 |
| | | | 576 | 277 | 107 | 164 | 28 | | |
| 8 | I | 28 | Total | C | N | O | P | 0 | 0 |
| | | | 576 | 277 | 107 | 164 | 28 | | |

- Molecule 9 is a DNA chain called DNA (27-MER).

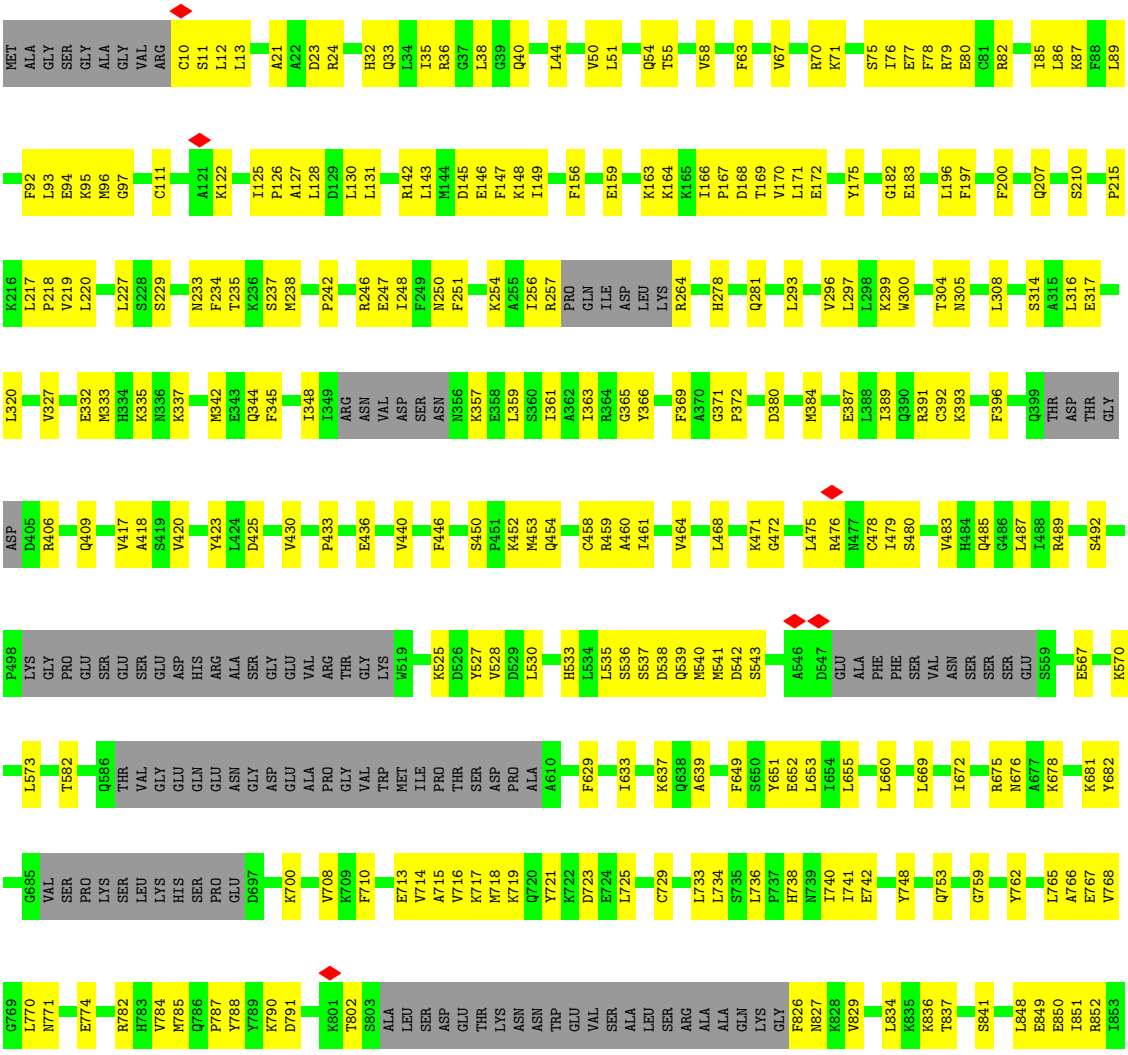
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 557 | 269 | 94 | 167 | 27 | | |

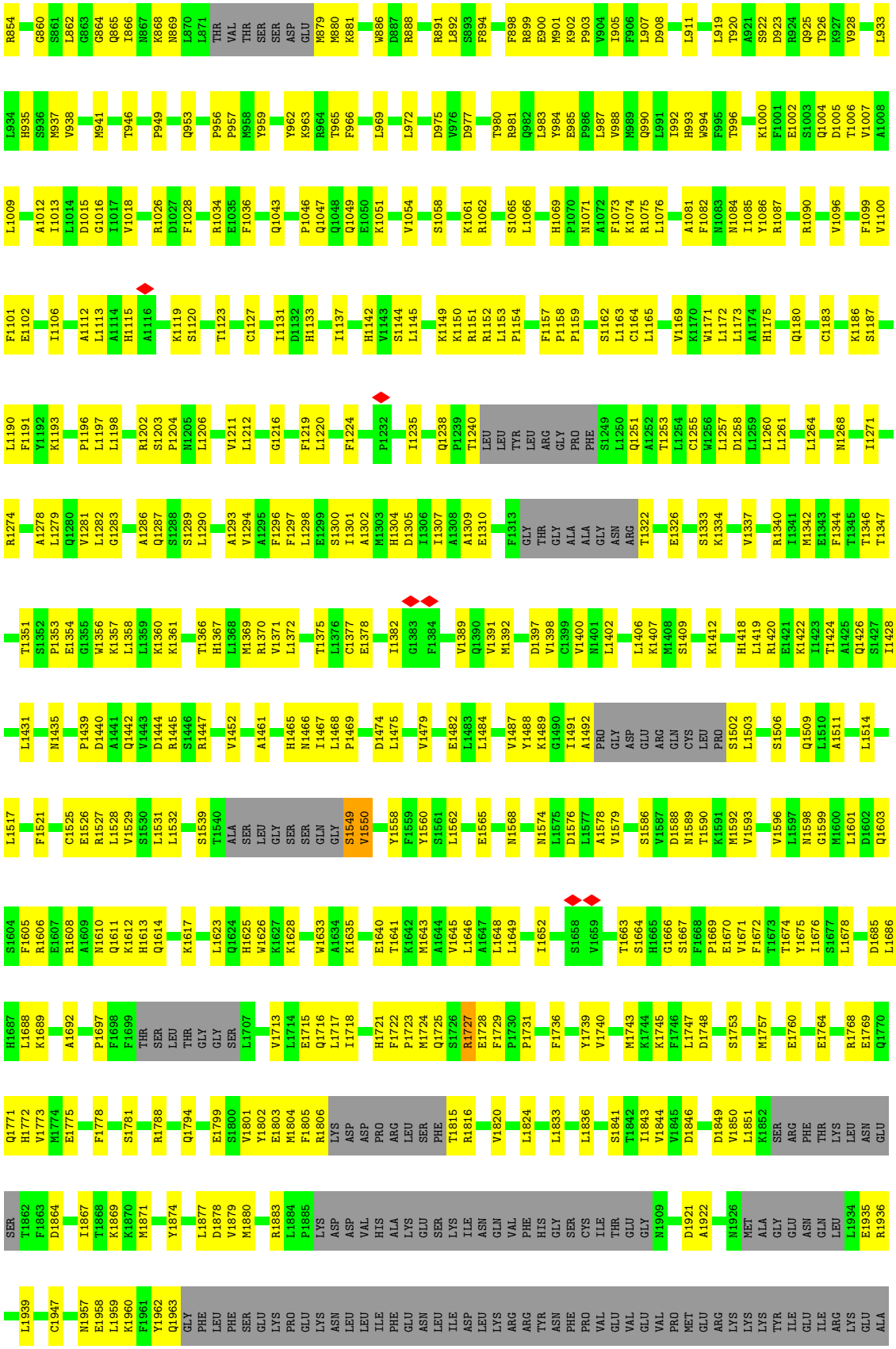
# 3 Residue-property plots (i)

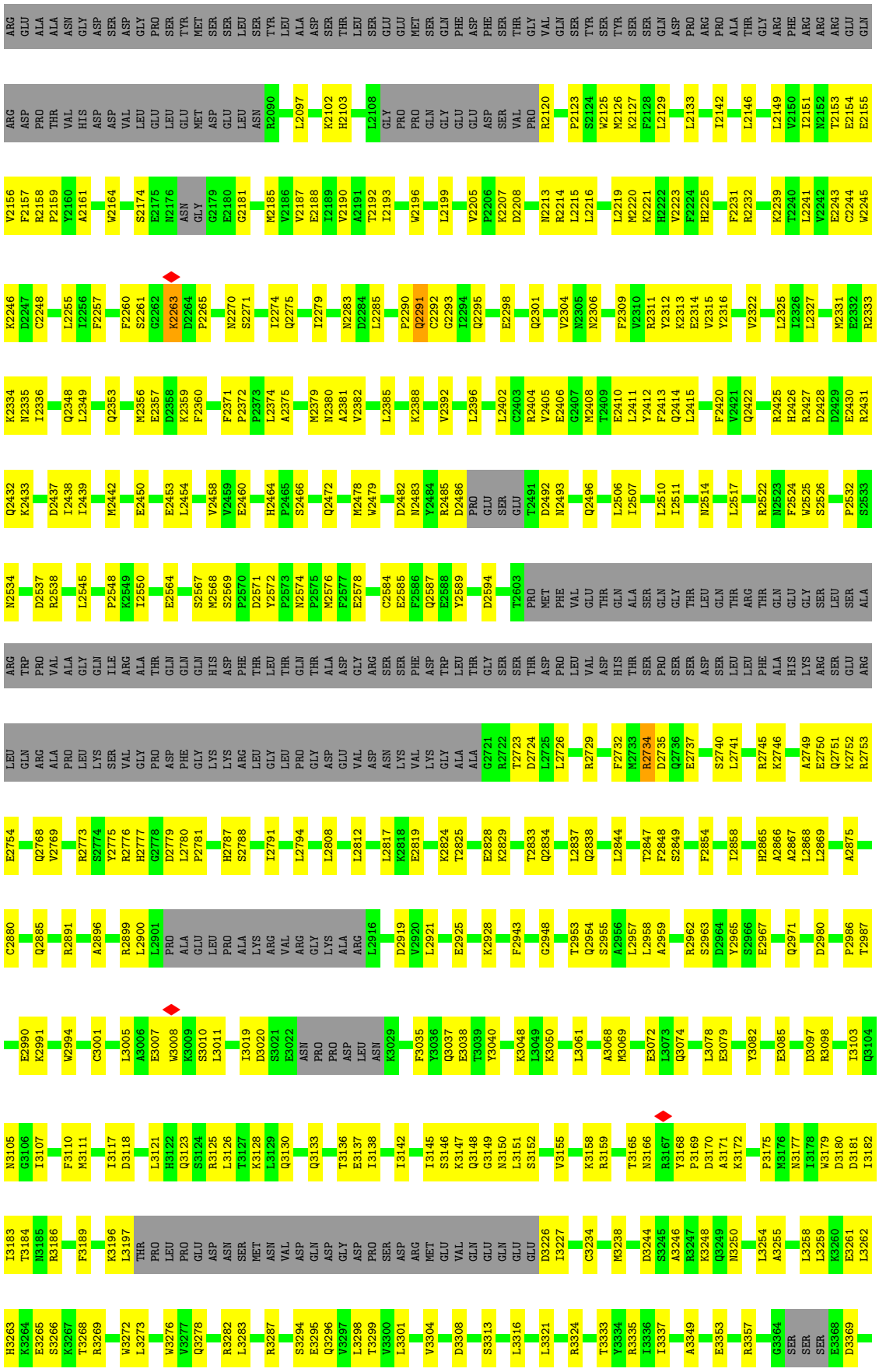
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

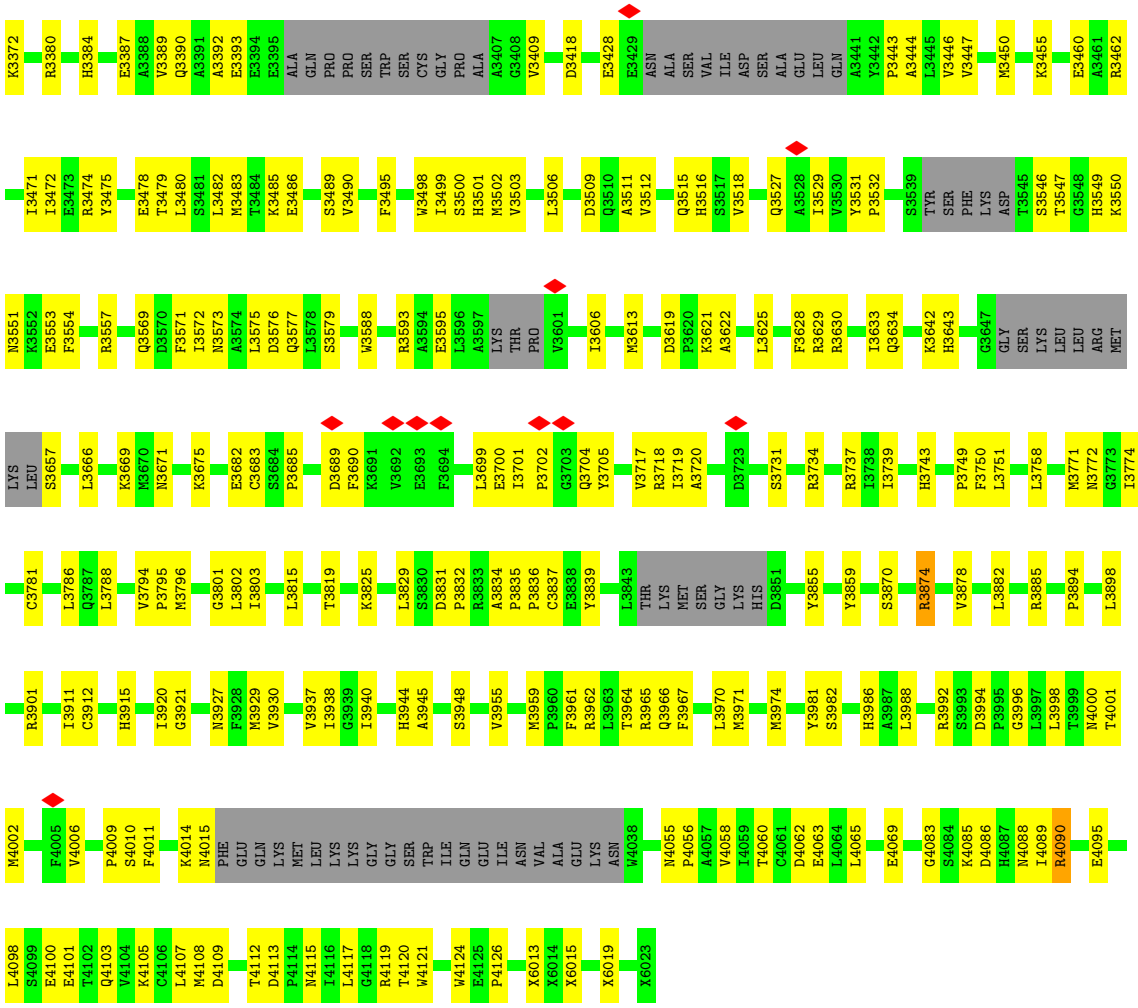
• Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs

Chain A:

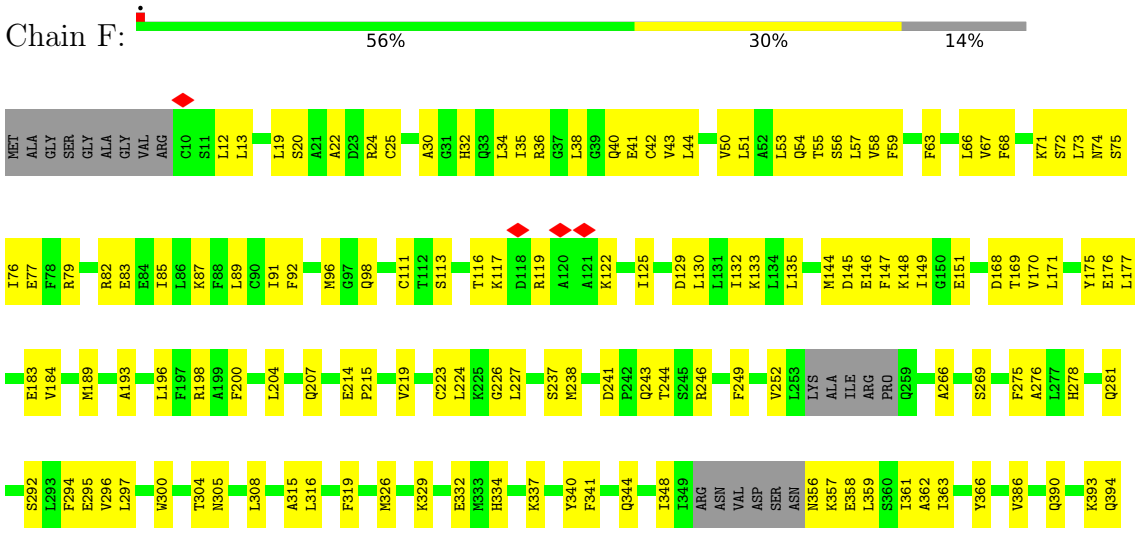


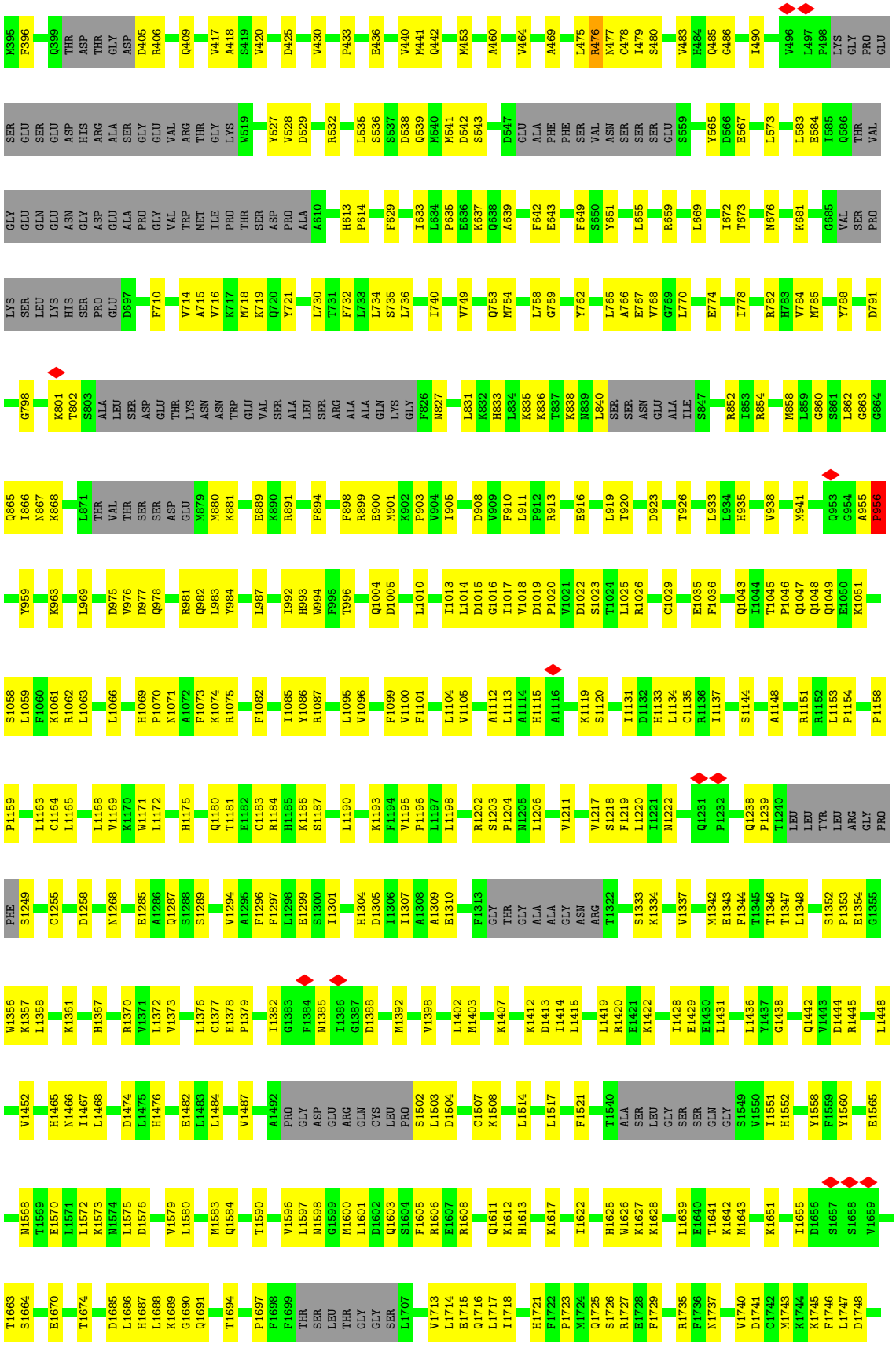


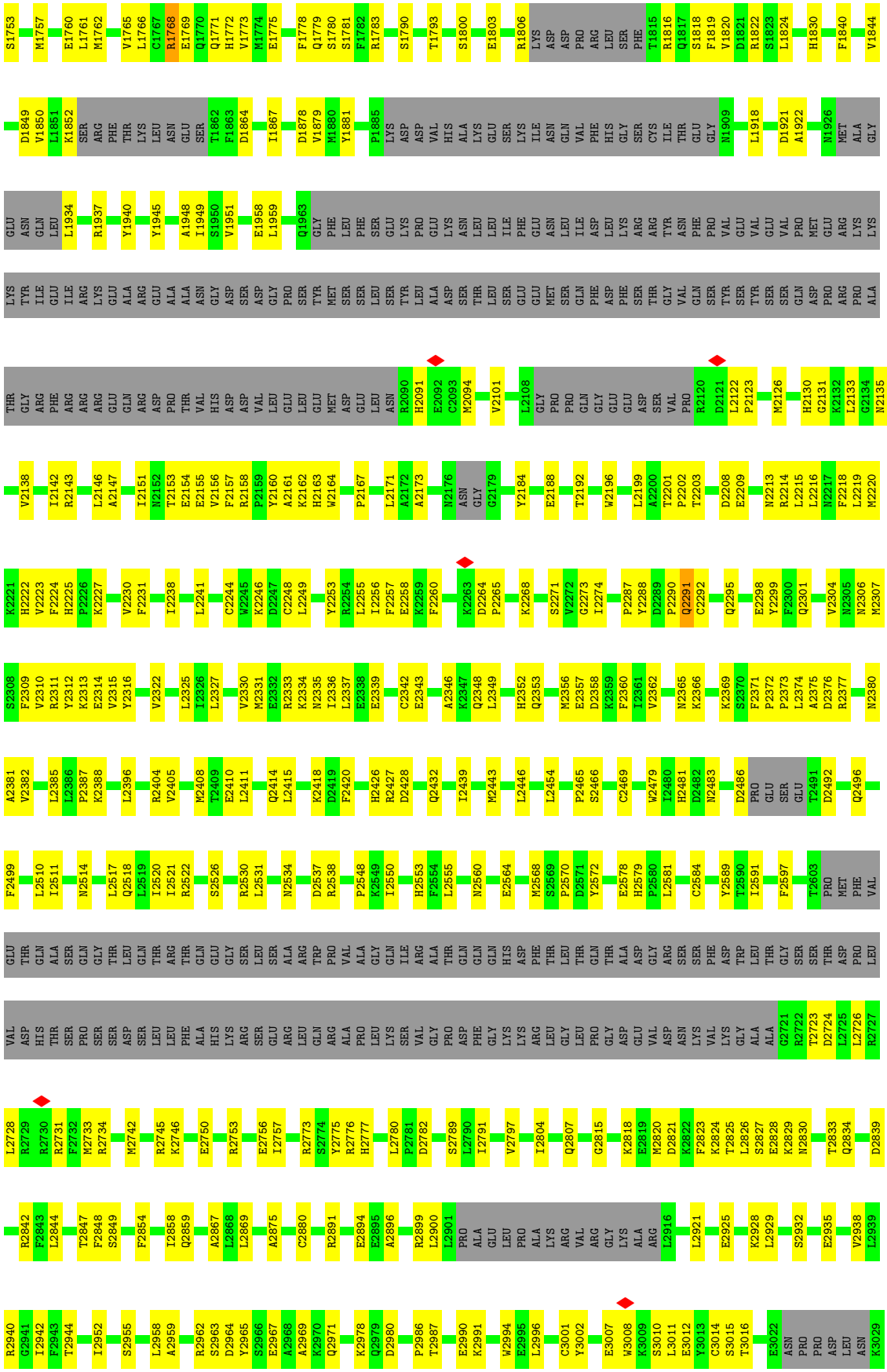


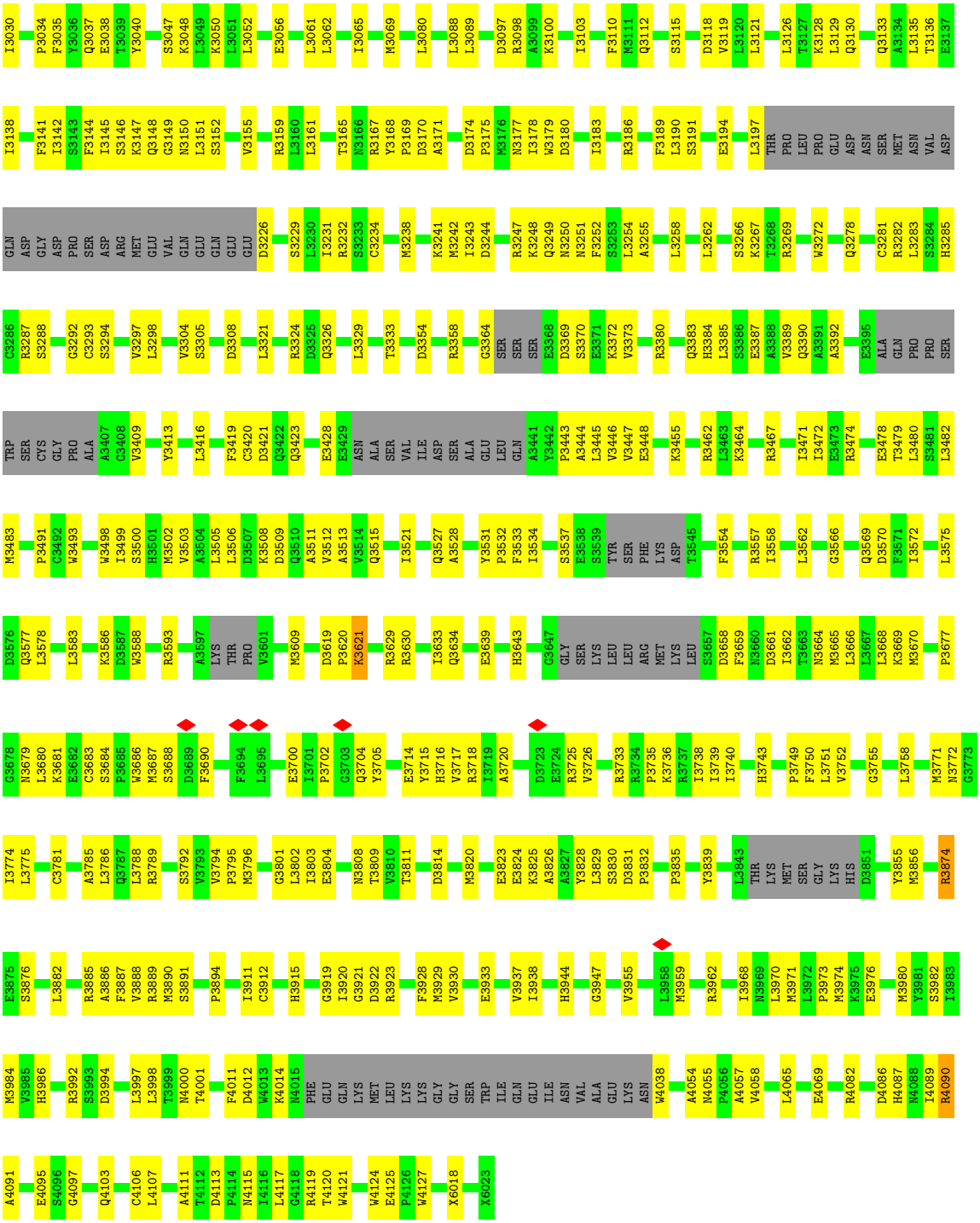
• Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs

Chain F:



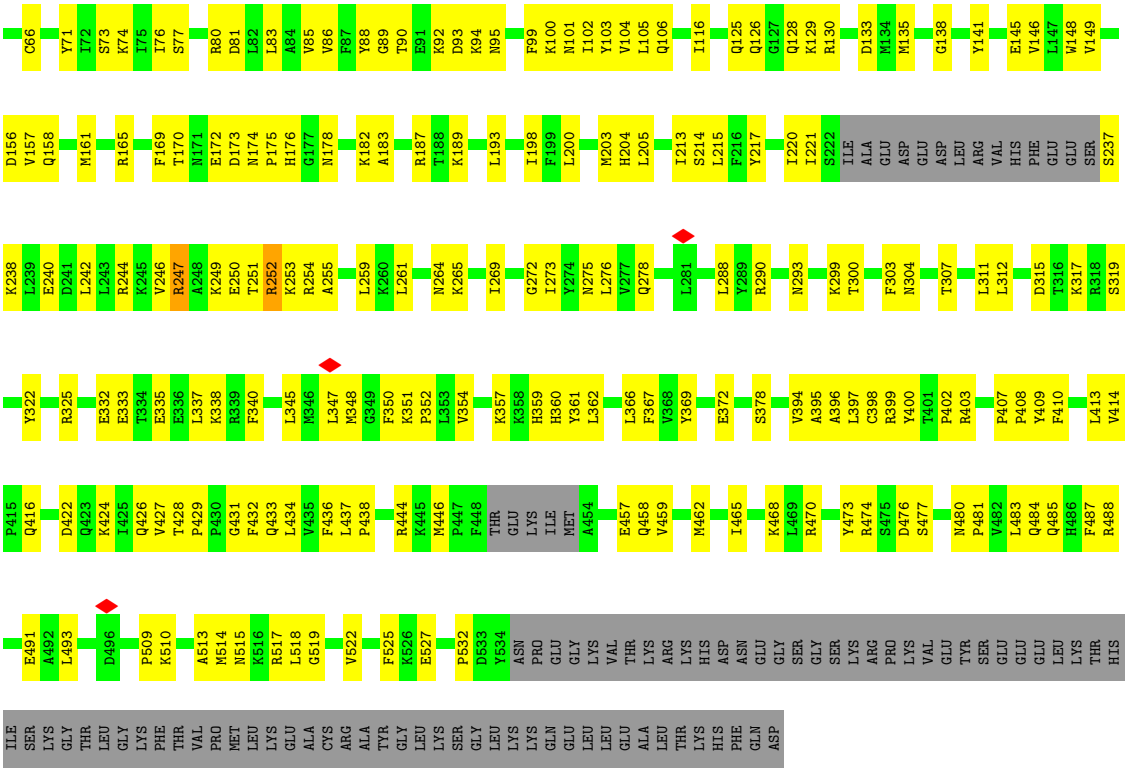






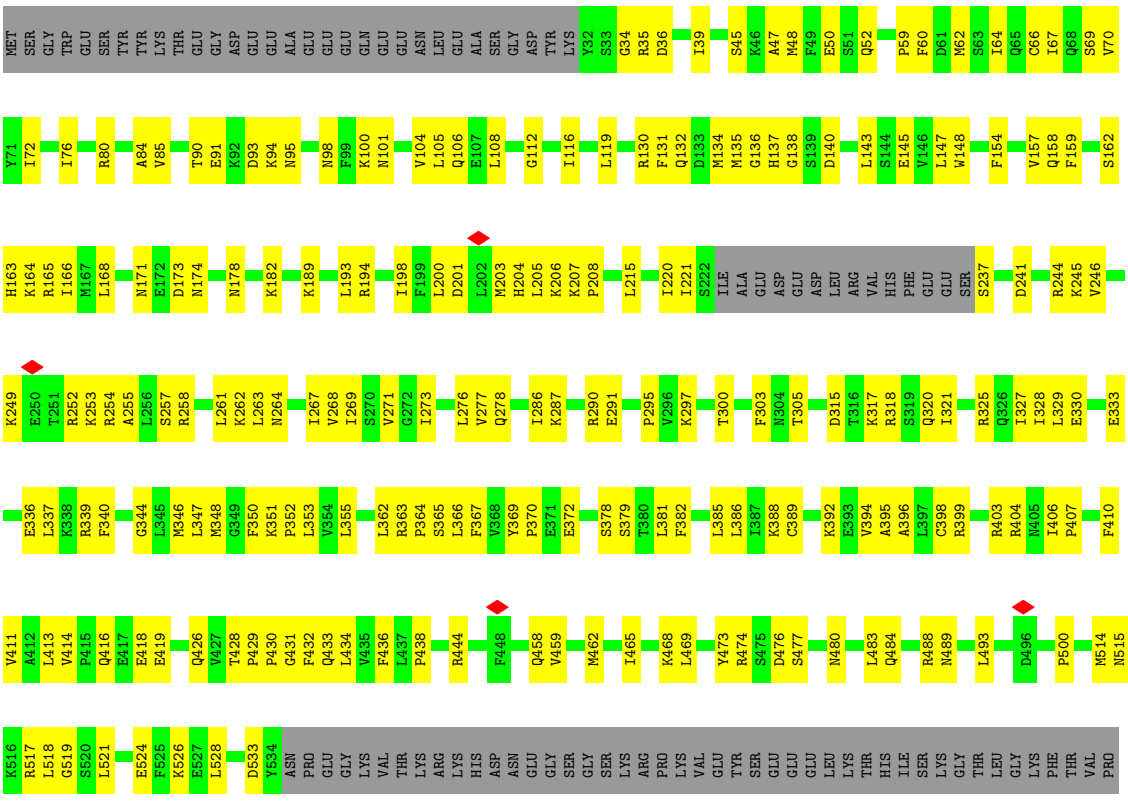
• Molecule 2: X-ray repair cross-complementing protein 6

Chain B:

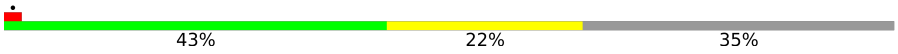
• Molecule 2: X-ray repair cross-complementing protein 6

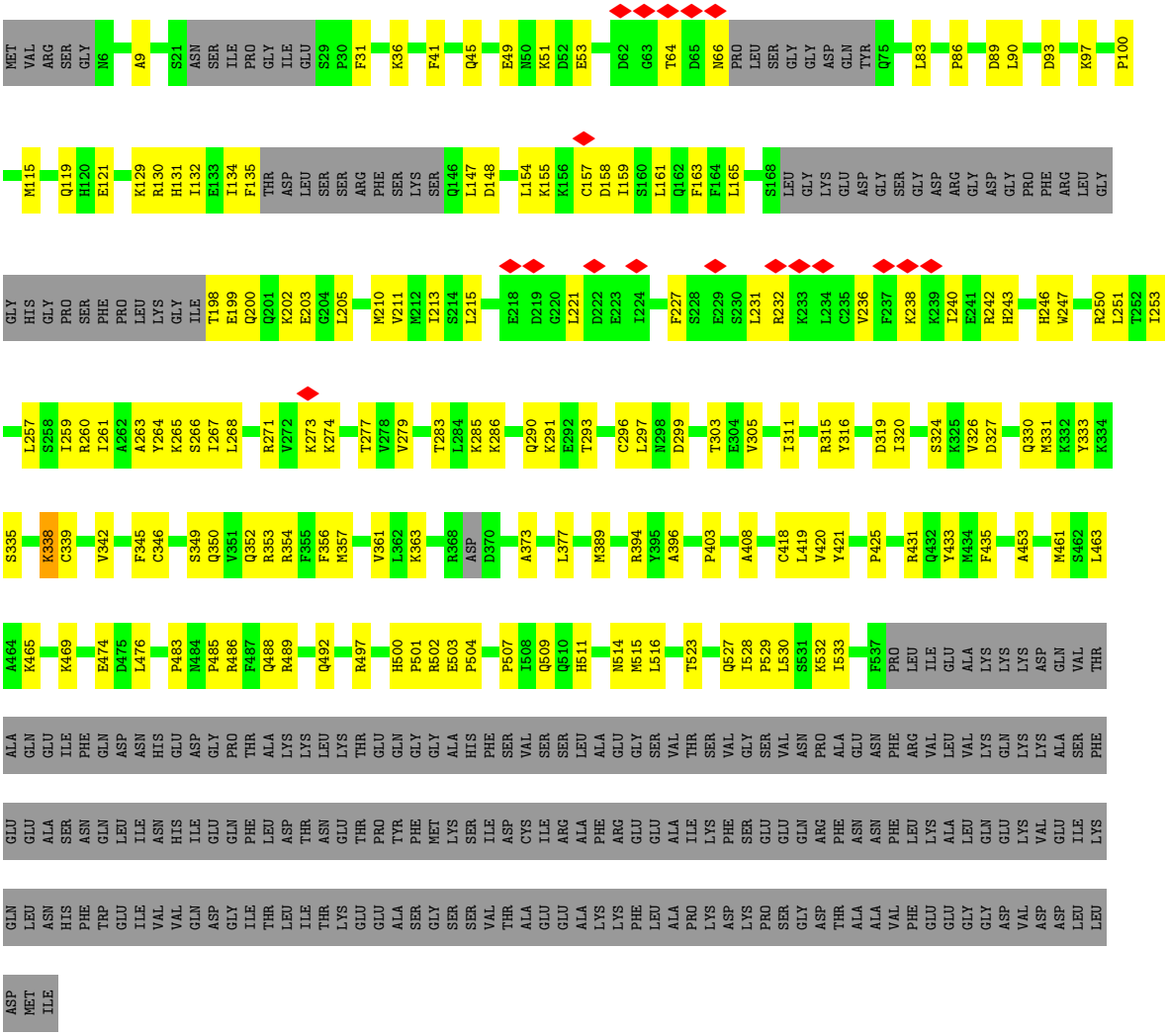
Chain G:

• Molecule 3: X-ray repair cross-complementing protein 5

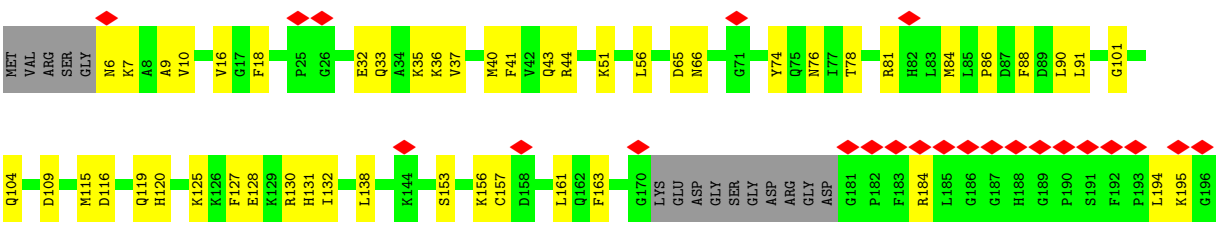
Chain C:

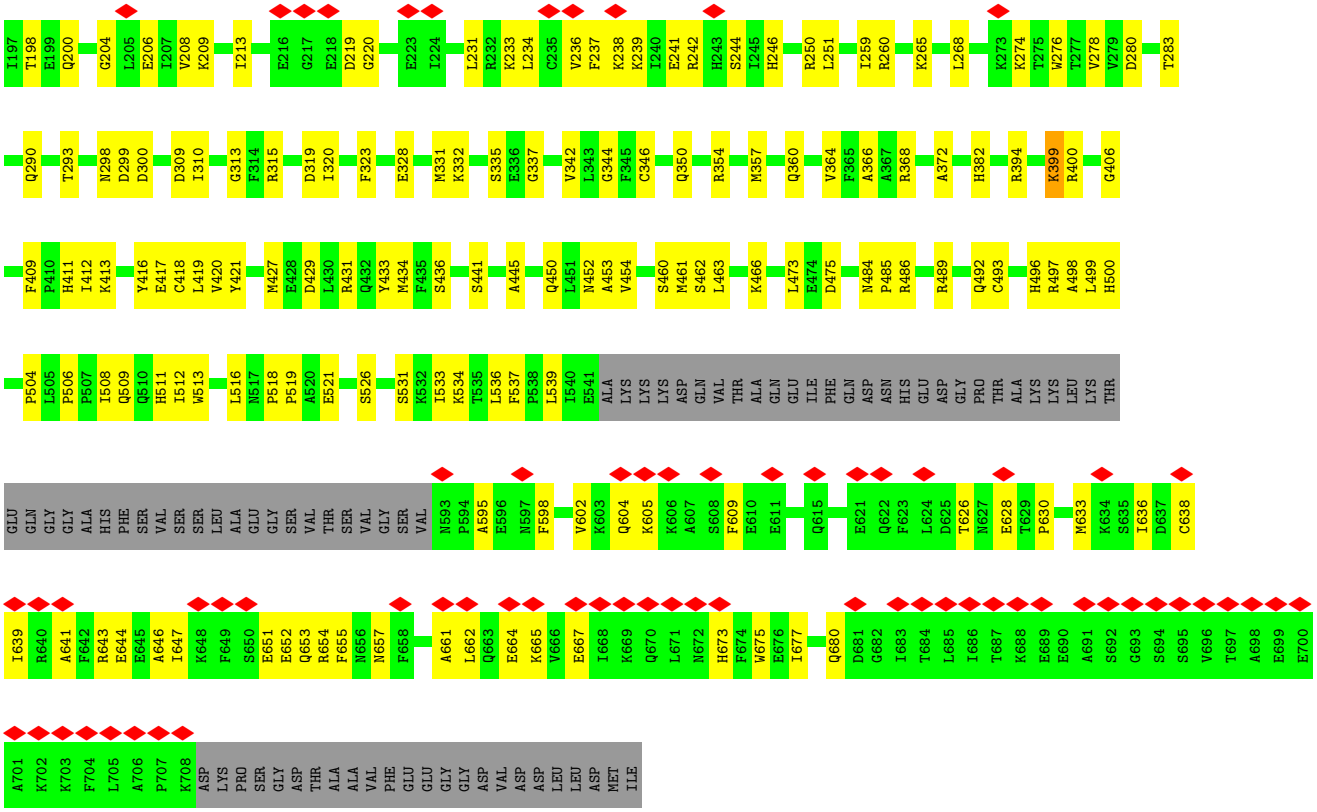


• Molecule 3: X-ray repair cross-complementing protein 5

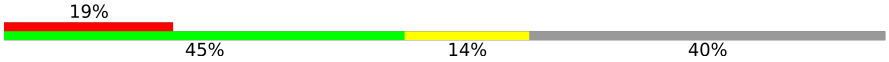
Chain H:

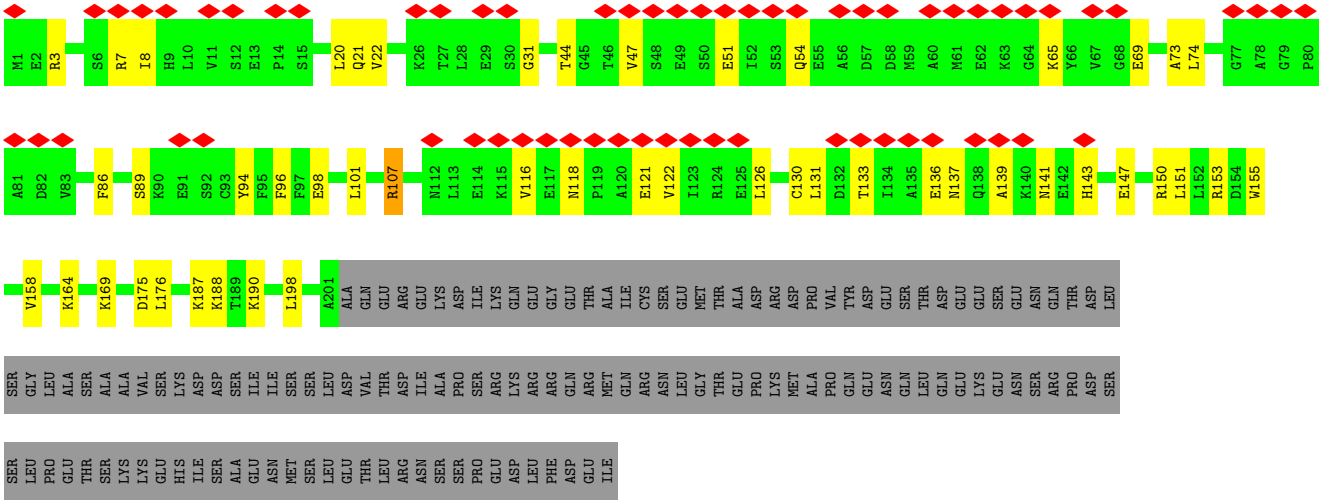





• Molecule 4: DNA repair protein XRCC4

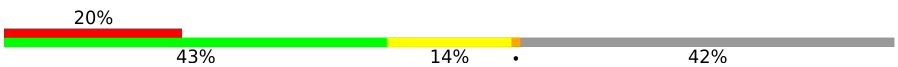
Chain K:

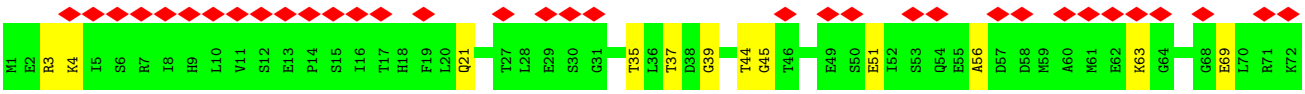


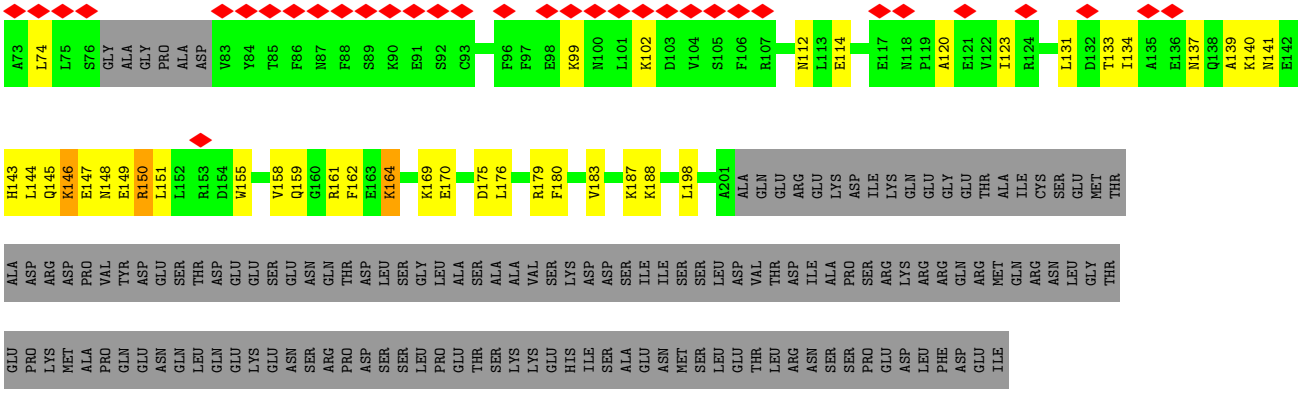



• Molecule 4: DNA repair protein XRCC4

Chain L:

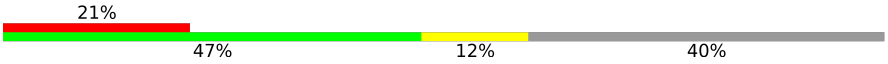


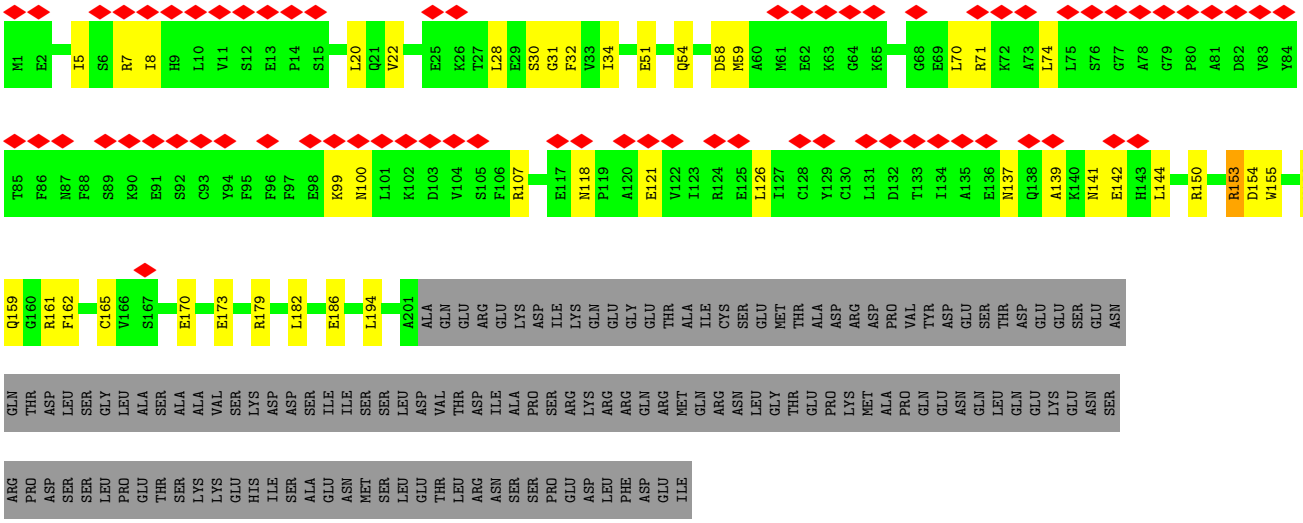






• Molecule 4: DNA repair protein XRCC4

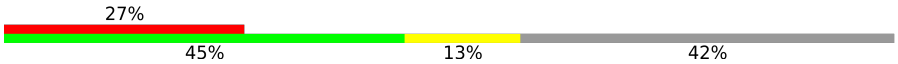
Chain N:

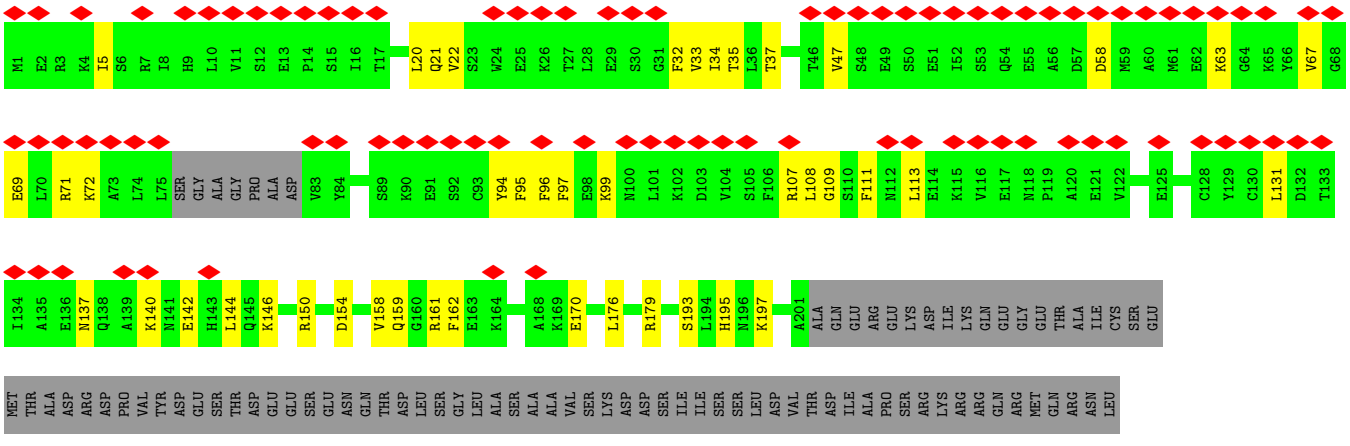


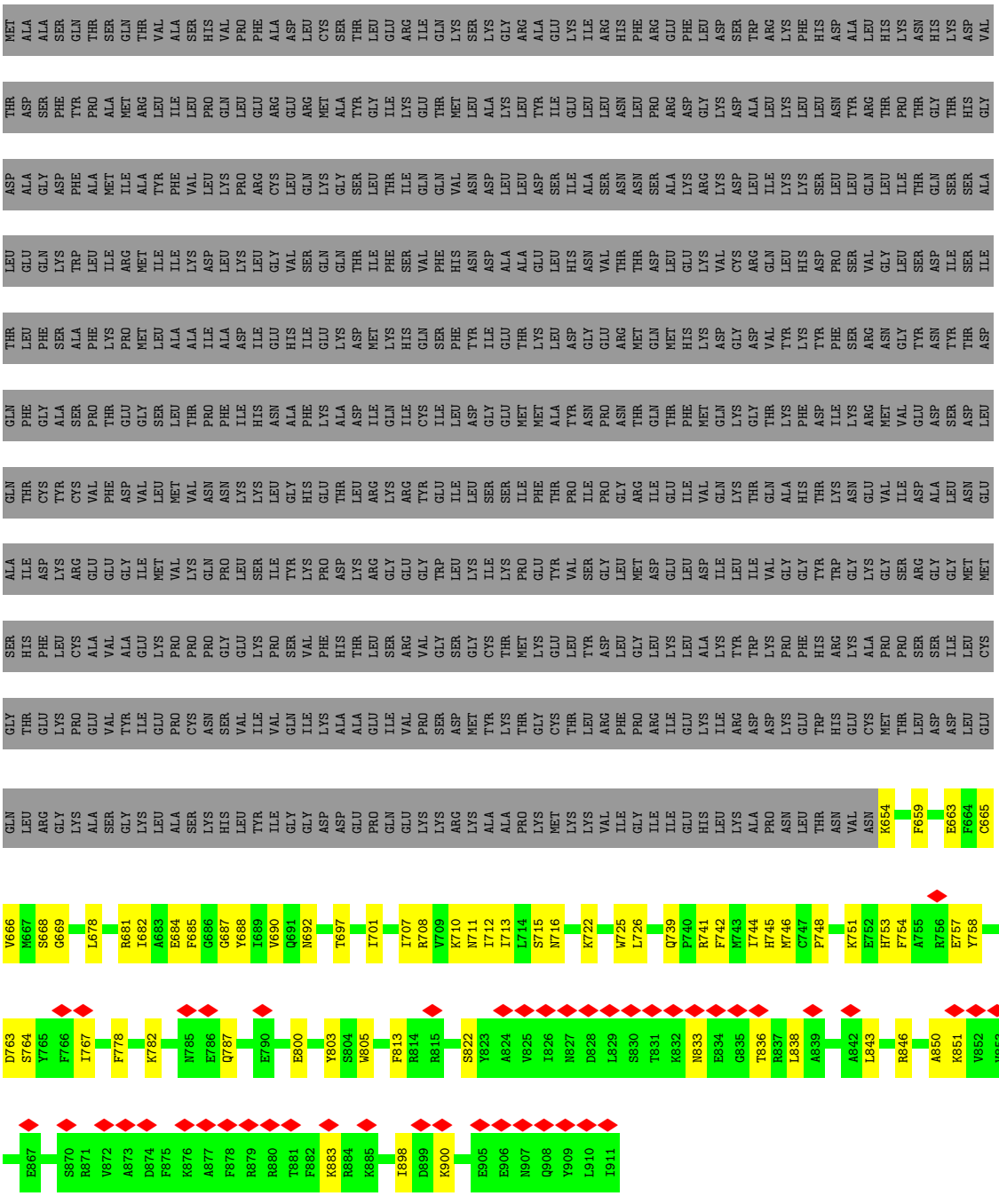

• Molecule 4: DNA repair protein XRCC4

Chain O:

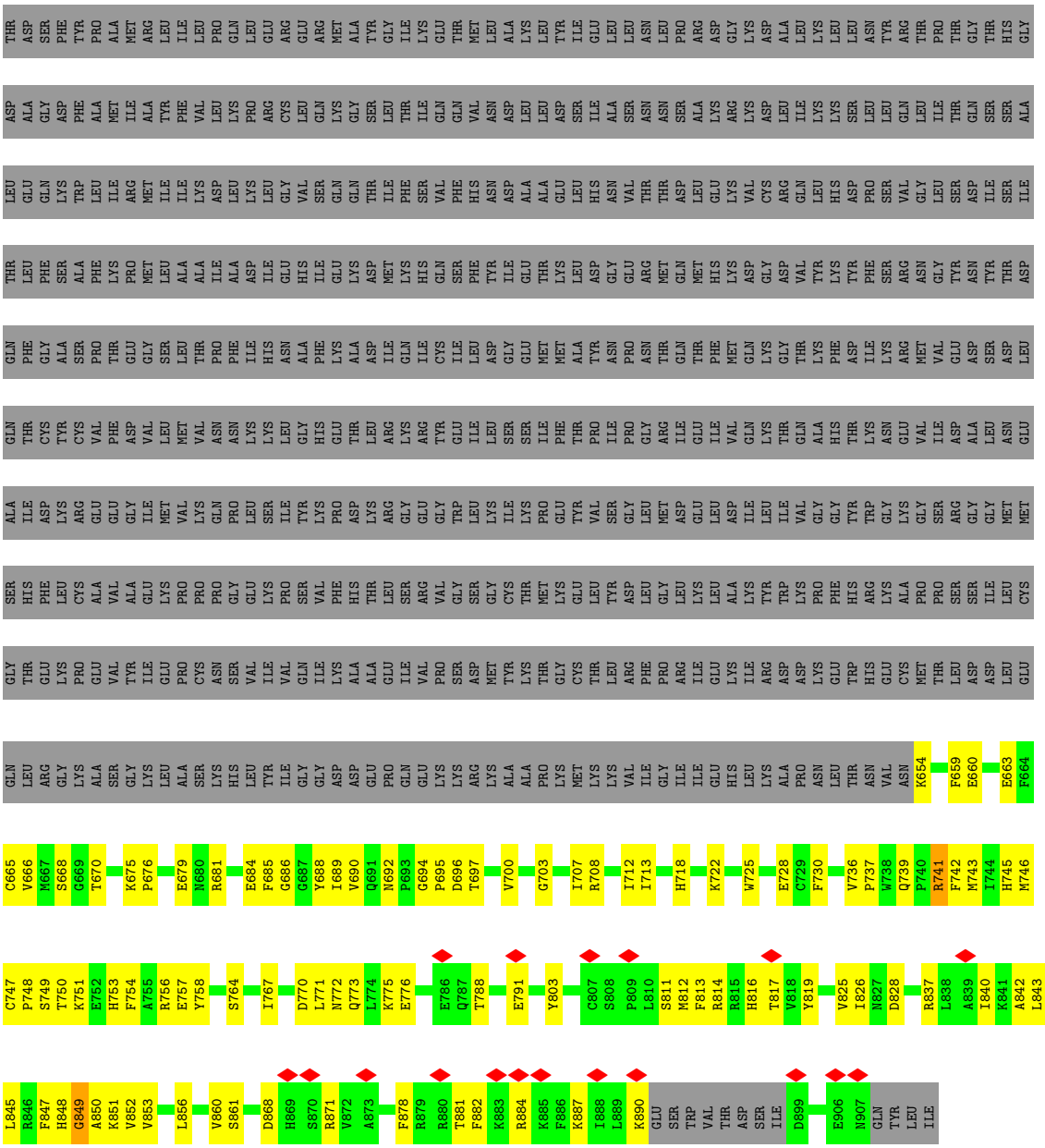



• Molecule 5: DNA ligase 4

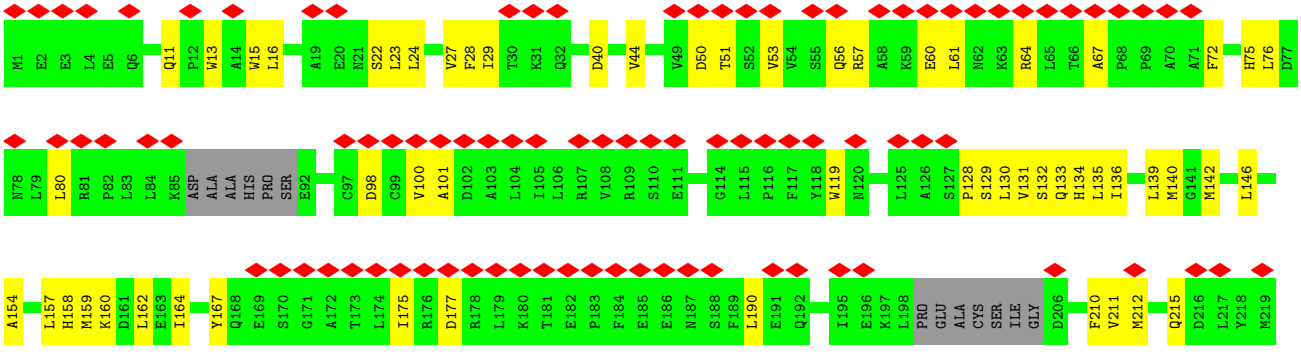



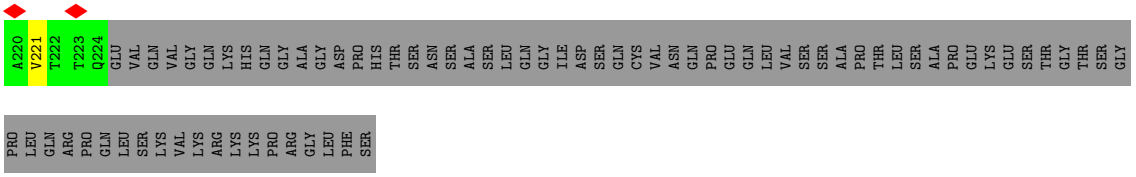

• Molecule 5: DNA ligase 4

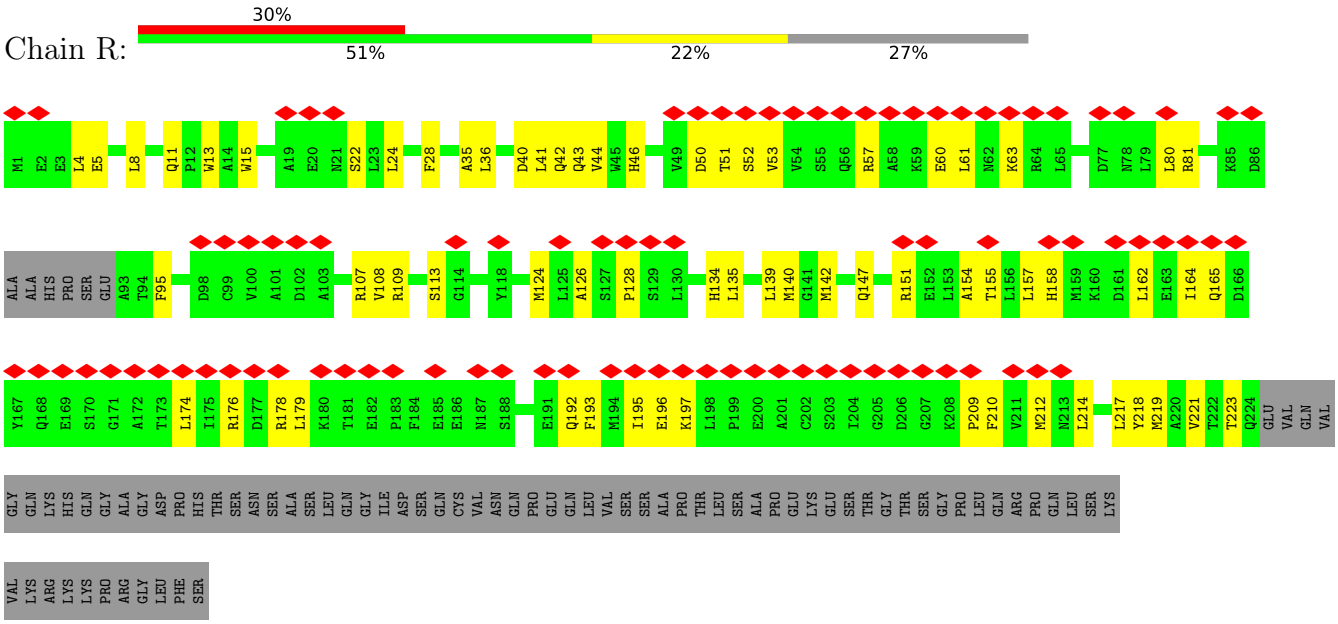
• Molecule 6: Non-homologous end-joining factor 1

Chain Q:

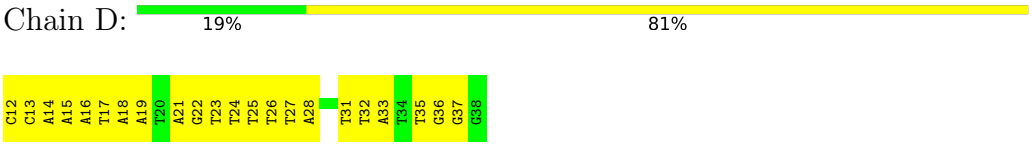





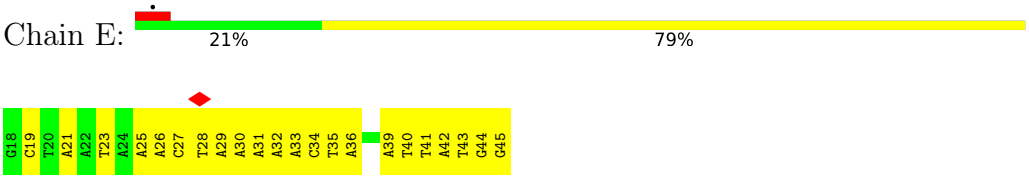

• Molecule 6: Non-homologous end-joining factor 1



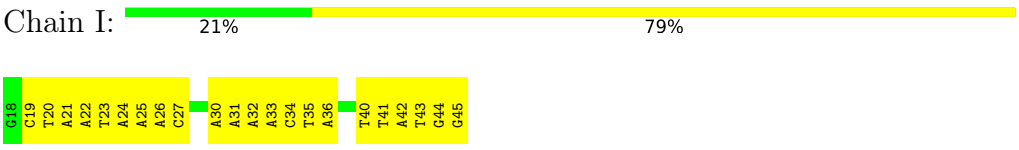

• Molecule 7: DNA (27-MER)




• Molecule 8: DNA (28-MER)

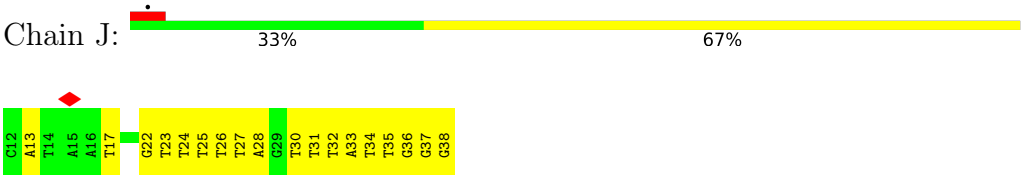



• Molecule 8: DNA (28-MER)




• Molecule 9: DNA (27-MER)

Chain J:


33%
67%
C12
A13
T14
A15
A16
T17
G22
T23
T24
T25
T26
T27
A28
G29
T30
T31
T32
A33
T34
T35
G36
G37
G38

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 23421 | 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 ($e^-/Å^2$) | 46.8 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.695 | Depositor |
| Minimum map value | -0.275 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.024 | Depositor |
| Recommended contour level | 0.175 | Depositor |
| Map size (Å) | 704.16003, 704.16003, 704.16003 | wwPDB |
| Map dimensions | 540, 540, 540 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.304, 1.304, 1.304 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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 | 0.27 | 0/28527 | 0.47 | 0/38582 |
| 1 | F | 0.27 | 0/28510 | 0.47 | 1/38552 (0.0%) |
| 2 | B | 0.26 | 0/3896 | 0.50 | 0/5248 |
| 2 | G | 0.27 | 0/4025 | 0.49 | 0/5421 |
| 3 | C | 0.25 | 0/3921 | 0.46 | 0/5282 |
| 3 | H | 0.26 | 0/5254 | 0.47 | 0/7085 |
| 4 | K | 0.24 | 0/1654 | 0.47 | 0/2224 |
| 4 | L | 0.24 | 0/1619 | 0.49 | 0/2174 |
| 4 | N | 0.24 | 0/1654 | 0.47 | 0/2224 |
| 4 | O | 0.24 | 0/1605 | 0.46 | 0/2155 |
| 5 | M | 0.25 | 0/2144 | 0.45 | 0/2895 |
| 5 | P | 0.28 | 0/2008 | 0.48 | 0/2712 |
| 6 | Q | 0.24 | 0/1722 | 0.53 | 0/2332 |
| 6 | R | 0.24 | 0/1762 | 0.51 | 0/2389 |
| 7 | D | 0.54 | 0/622 | 0.96 | 0/959 |
| 8 | E | 0.55 | 0/647 | 0.96 | 0/996 |
| 8 | I | 0.59 | 0/647 | 0.95 | 0/996 |
| 9 | J | 0.53 | 0/623 | 1.02 | 0/961 |
| All | All | 0.28 | 0/90840 | 0.50 | 1/123187 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 956 | PRO | N-CA-CB | 6.22 | 110.77 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 28076 | 0 | 28047 | 898 | 0 |
| 1 | F | 28060 | 0 | 28056 | 856 | 0 |
| 2 | B | 3822 | 0 | 3899 | 176 | 0 |
| 2 | G | 3948 | 0 | 4036 | 181 | 0 |
| 3 | C | 3849 | 0 | 3892 | 121 | 0 |
| 3 | H | 5150 | 0 | 5176 | 173 | 0 |
| 4 | K | 1625 | 0 | 1611 | 40 | 0 |
| 4 | L | 1592 | 0 | 1583 | 45 | 0 |
| 4 | N | 1625 | 0 | 1611 | 35 | 0 |
| 4 | O | 1579 | 0 | 1571 | 39 | 0 |
| 5 | M | 2095 | 0 | 2046 | 42 | 0 |
| 5 | P | 1965 | 0 | 1904 | 74 | 0 |
| 6 | Q | 1690 | 0 | 1699 | 51 | 0 |
| 6 | R | 1728 | 0 | 1728 | 62 | 0 |
| 7 | D | 556 | 0 | 310 | 35 | 0 |
| 8 | E | 576 | 0 | 318 | 28 | 0 |
| 8 | I | 576 | 0 | 318 | 34 | 0 |
| 9 | J | 557 | 0 | 311 | 29 | 0 |
| All | All | 89069 | 0 | 88116 | 2724 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2724) 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:1549:SER:O | 1:A:1550:VAL:HG22 | 1.17 | 1.29 |
| 1:A:1549:SER:O | 1:A:1550:VAL:CG2 | 2.04 | 1.05 |
| 3:H:56:LEU:H | 3:H:81:ARG:HB2 | 1.39 | 0.88 |
| 1:A:327:VAL:HG13 | 1:A:333:MET:HB2 | 1.58 | 0.85 |
| 5:P:811:SER:HB2 | 5:P:849:GLY:HA3 | 1.57 | 0.84 |
| 1:A:2965:TYR:HB3 | 1:A:3001:CYS:HB2 | 1.58 | 0.83 |
| 4:L:179:ARG:HD3 | 5:M:778:PHE:HB3 | 1.60 | 0.83 |
| 2:B:352:PRO:HA | 2:B:394:VAL:HA | 1.61 | 0.83 |
| 1:F:1115:HIS:HA | 1:F:1119:LYS:HD2 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Q:133:GLN:H | 6:R:42:GLN:H | 1.28 | 0.81 |
| 1:F:50:VAL:HG13 | 1:F:51:LEU:HG | 1.62 | 0.81 |
| 1:A:168:ASP:H | 1:A:171:LEU:HD12 | 1.45 | 0.81 |
| 1:F:1428:ILE:HA | 1:F:1431:LEU:HB2 | 1.63 | 0.80 |
| 1:F:901:MET:HG2 | 1:F:903:PRO:HD3 | 1.63 | 0.79 |
| 7:D:24:DT:H3 | 8:E:34:DC:H42 | 1.26 | 0.79 |
| 5:P:812:MET:H | 5:P:848:HIS:HB3 | 1.46 | 0.79 |
| 1:F:1104:LEU:HD22 | 1:F:1134:LEU:HD13 | 1.66 | 0.78 |
| 3:H:242:ARG:NH2 | 8:I:22:DA:N7 | 2.31 | 0.78 |
| 1:A:2433:LYS:HG3 | 1:A:2472:GLN:HE22 | 1.47 | 0.77 |
| 1:A:1611:GLN:HE21 | 1:A:1614:GLN:HE21 | 1.32 | 0.77 |
| 1:A:2594:ASP:HA | 1:A:2768:GLN:HE22 | 1.47 | 0.77 |
| 1:A:2357:GLU:HA | 1:A:2360:PHE:HB3 | 1.65 | 0.77 |
| 1:A:3255:ALA:HB1 | 1:A:3258:LEU:HB2 | 1.65 | 0.77 |
| 5:M:813:PHE:HB3 | 5:M:850:ALA:HB2 | 1.66 | 0.77 |
| 1:A:3750:PHE:HB3 | 1:A:3802:LEU:HD11 | 1.67 | 0.76 |
| 1:F:149:ILE:HD11 | 1:F:183:GLU:HB2 | 1.65 | 0.76 |
| 6:Q:132:SER:HB3 | 6:R:44:VAL:HA | 1.67 | 0.76 |
| 1:F:12:LEU:HD21 | 1:F:44:LEU:HD22 | 1.68 | 0.76 |
| 6:R:15:TRP:HE1 | 6:R:22:SER:HA | 1.50 | 0.76 |
| 1:A:1803:GLU:HA | 1:A:1806:ARG:HH21 | 1.51 | 0.75 |
| 4:N:28:LEU:HD22 | 4:N:71:ARG:HH12 | 1.50 | 0.75 |
| 6:Q:135:LEU:HB2 | 6:R:41:LEU:HB2 | 1.66 | 0.75 |
| 1:A:1307:ILE:HG23 | 1:A:1309:ALA:H | 1.50 | 0.75 |
| 2:B:322:TYR:HE1 | 3:C:274:LYS:HG3 | 1.52 | 0.74 |
| 1:F:2776:ARG:HH21 | 1:F:2782:ASP:HB2 | 1.50 | 0.74 |
| 4:L:45:GLY:HA3 | 4:L:114:GLU:H | 1.51 | 0.74 |
| 6:Q:132:SER:HA | 6:R:40:ASP:H | 1.50 | 0.74 |
| 1:A:3321:LEU:HD13 | 1:A:3324:ARG:HH12 | 1.52 | 0.74 |
| 6:R:57:ARG:HG2 | 6:R:61:LEU:HD22 | 1.70 | 0.74 |
| 2:G:403:ARG:H | 2:G:406:ILE:HD11 | 1.53 | 0.74 |
| 1:F:3142:ILE:O | 1:F:3147:LYS:NZ | 2.21 | 0.73 |
| 2:G:533:ASP:OD1 | 3:H:250:ARG:NH2 | 2.20 | 0.73 |
| 3:C:501:PRO:HB2 | 3:C:502:ARG:HH21 | 1.53 | 0.73 |
| 2:G:69:SER:HB3 | 2:G:245:LYS:HB3 | 1.69 | 0.73 |
| 1:F:3684:SER:HB3 | 1:F:3687:MET:HB2 | 1.70 | 0.73 |
| 1:A:3971:MET:SD | 1:A:3974:MET:HG3 | 2.29 | 0.73 |
| 2:G:255:ALA:HB3 | 2:G:258:ARG:HH22 | 1.53 | 0.73 |
| 7:D:21:DA:H2" | 8:E:33:DA:H62 | 1.54 | 0.72 |
| 1:F:2859:GLN:HE22 | 1:F:2880:CYS:HB3 | 1.54 | 0.72 |
| 2:B:173:ASP:HB2 | 2:B:214:SER:H | 1.55 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3593:ARG:NH2 | 1:A:3657:SER:O | 2.22 | 0.72 |
| 1:F:3982:SER:O | 1:F:3986:HIS:ND1 | 2.21 | 0.72 |
| 3:H:647:ILE:HA | 3:H:652:GLU:HG2 | 1.70 | 0.72 |
| 2:G:47:ALA:O | 2:G:171:ASN:ND2 | 2.23 | 0.72 |
| 3:H:605:LYS:HB2 | 3:H:609:PHE:HZ | 1.54 | 0.72 |
| 4:K:139:ALA:O | 4:K:143:HIS:ND1 | 2.22 | 0.72 |
| 1:F:1268:ASN:ND2 | 1:F:1347:THR:OG1 | 2.23 | 0.72 |
| 8:I:21:DA:H4' | 9:J:36:DG:H1' | 1.71 | 0.72 |
| 1:A:197:PHE:O | 1:A:246:ARG:NH2 | 2.23 | 0.72 |
| 2:B:303:PHE:HB3 | 3:C:290:GLN:HB3 | 1.72 | 0.72 |
| 1:F:1220:LEU:HD11 | 1:F:1287:GLN:HB2 | 1.70 | 0.72 |
| 1:F:1151:ARG:NH1 | 1:F:1163:LEU:O | 2.23 | 0.71 |
| 5:P:860:VAL:O | 5:P:884:ARG:NH2 | 2.23 | 0.71 |
| 1:A:901:MET:HG2 | 1:A:903:PRO:HD3 | 1.72 | 0.71 |
| 1:A:3137:GLU:OE2 | 1:A:3166:ASN:ND2 | 2.23 | 0.71 |
| 5:M:707:ILE:HA | 5:M:710:LYS:HD2 | 1.72 | 0.71 |
| 1:F:833:HIS:O | 1:F:838:LYS:NZ | 2.21 | 0.71 |
| 1:F:2290:PRO:O | 1:F:2292:CYS:N | 2.23 | 0.71 |
| 2:G:261:LEU:HB2 | 2:G:269:ILE:HB | 1.71 | 0.71 |
| 6:Q:134:HIS:H | 6:R:42:GLN:HB2 | 1.56 | 0.71 |
| 1:A:4055:ASN:HB2 | 1:A:4095:GLU:HA | 1.71 | 0.71 |
| 5:M:663:GLU:HB3 | 5:M:697:THR:HA | 1.71 | 0.71 |
| 5:M:682:ILE:HG12 | 5:M:687:GLY:HA3 | 1.72 | 0.71 |
| 1:A:3349:ALA:O | 1:A:3357:ARG:NH2 | 2.23 | 0.70 |
| 2:B:90:THR:HG21 | 2:B:103:TYR:HB2 | 1.73 | 0.70 |
| 3:H:662:LEU:HD23 | 3:H:665:LYS:HE2 | 1.74 | 0.70 |
| 1:A:3511:ALA:O | 1:A:3515:GLN:NE2 | 2.25 | 0.70 |
| 6:R:11:GLN:HB2 | 6:R:28:PHE:HB2 | 1.73 | 0.70 |
| 1:A:1172:LEU:HD11 | 1:A:1187:SER:HB2 | 1.73 | 0.70 |
| 1:A:2408:MET:HA | 1:A:2411:LEU:HD22 | 1.73 | 0.70 |
| 1:A:1151:ARG:NH1 | 1:A:1163:LEU:O | 2.22 | 0.70 |
| 1:A:865:GLN:HB2 | 1:A:3168:TYR:HB3 | 1.73 | 0.70 |
| 5:P:814:ARG:H | 5:P:850:ALA:N | 1.90 | 0.70 |
| 2:G:366:LEU:H | 2:G:434:LEU:HB2 | 1.57 | 0.69 |
| 4:K:22:VAL:HG21 | 4:K:74:LEU:HB3 | 1.74 | 0.69 |
| 3:H:65:ASP:H | 3:H:78:THR:HG22 | 1.57 | 0.69 |
| 1:A:2959:ALA:HA | 1:A:2962:ARG:HD3 | 1.74 | 0.69 |
| 1:A:3622:ALA:HB3 | 1:A:3630:ARG:HD2 | 1.74 | 0.69 |
| 4:N:153:ARG:NH1 | 4:N:154:ASP:OD1 | 2.25 | 0.69 |
| 1:A:2225:HIS:HB2 | 1:A:2231:PHE:HB2 | 1.72 | 0.69 |
| 2:B:366:LEU:HB2 | 2:B:434:LEU:HD12 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1171:TRP:O | 1:A:1175:HIS:ND1 | 2.25 | 0.69 |
| 1:A:2331:MET:O | 1:A:2334:LYS:NZ | 2.26 | 0.69 |
| 1:F:827:ASN:HB3 | 1:F:836:LYS:HE2 | 1.74 | 0.69 |
| 1:A:248:ILE:HA | 1:A:251:PHE:HD2 | 1.57 | 0.69 |
| 1:F:3593:ARG:NH2 | 1:F:3661:ASP:OD1 | 2.26 | 0.69 |
| 1:F:3679:ASN:HA | 1:F:3726:VAL:HG22 | 1.74 | 0.69 |
| 4:O:5:ILE:HA | 4:O:21:GLN:HA | 1.74 | 0.69 |
| 7:D:27:DT:H2" | 7:D:28:DA:C5 | 2.28 | 0.69 |
| 1:A:71:LYS:HB3 | 1:A:82:ARG:HH22 | 1.57 | 0.69 |
| 1:A:78:PHE:HB3 | 1:A:82:ARG:HH21 | 1.57 | 0.69 |
| 1:A:4086:ASP:HA | 1:A:4089:ILE:HG12 | 1.73 | 0.68 |
| 5:P:746:MET:O | 5:P:751:LYS:NZ | 2.25 | 0.68 |
| 6:Q:134:HIS:HB3 | 6:R:42:GLN:HG3 | 1.75 | 0.68 |
| 1:A:2353:GLN:HA | 1:A:2356:MET:HG3 | 1.75 | 0.68 |
| 1:F:2295:GLN:HG3 | 1:F:2298:GLU:HB3 | 1.75 | 0.68 |
| 1:F:3151:LEU:HA | 1:F:3197:LEU:HD22 | 1.74 | 0.68 |
| 3:H:337:GLY:H | 3:H:399:LYS:HB3 | 1.58 | 0.68 |
| 1:A:3266:SER:HB3 | 1:A:3273:LEU:HA | 1.73 | 0.68 |
| 5:P:861:SER:O | 5:P:887:LYS:NZ | 2.25 | 0.68 |
| 1:F:207:GLN:NE2 | 1:F:215:PRO:O | 2.26 | 0.68 |
| 1:F:1354:GLU:HA | 1:F:1357:LYS:HB3 | 1.76 | 0.68 |
| 1:F:4055:ASN:HD22 | 1:F:4058:VAL:HG23 | 1.58 | 0.68 |
| 1:A:3266:SER:HA | 1:A:3272:TRP:CD1 | 2.28 | 0.68 |
| 2:G:468:LYS:NZ | 2:G:517:ARG:O | 2.27 | 0.68 |
| 1:A:1238:GLN:HA | 1:A:1296:PHE:HZ | 1.59 | 0.68 |
| 1:A:2987:THR:HG23 | 1:A:2990:GLU:H | 1.59 | 0.68 |
| 1:F:867:ASN:HB3 | 1:F:3129:LEU:HD11 | 1.75 | 0.68 |
| 4:N:118:ASN:ND2 | 4:N:121:GLU:OE1 | 2.25 | 0.68 |
| 1:F:2572:TYR:HE1 | 1:F:2791:ILE:HD11 | 1.59 | 0.68 |
| 2:G:339:ARG:O | 3:H:489:ARG:NH1 | 2.26 | 0.68 |
| 5:P:663:GLU:HA | 5:P:688:TYR:HB2 | 1.75 | 0.68 |
| 5:P:868:ASP:HB3 | 5:P:871:ARG:HE | 1.58 | 0.68 |
| 1:A:304:THR:HG22 | 1:A:305:ASN:H | 1.58 | 0.68 |
| 1:A:3443:PRO:HB3 | 1:A:3471:ILE:HD11 | 1.76 | 0.68 |
| 1:F:3493:TRP:HD1 | 1:F:3521:ILE:HG12 | 1.58 | 0.68 |
| 1:F:3659:PHE:HA | 1:F:3662:ILE:HD12 | 1.76 | 0.68 |
| 1:A:919:LEU:HG | 1:A:920:THR:HG23 | 1.74 | 0.67 |
| 1:A:3998:LEU:HB3 | 1:A:4002:MET:HE1 | 1.74 | 0.67 |
| 3:H:138:LEU:HD12 | 3:H:204:GLY:HA2 | 1.77 | 0.67 |
| 2:B:348:MET:HB2 | 2:B:397:LEU:HB3 | 1.76 | 0.67 |
| 1:F:40:GLN:OE1 | 1:F:2427:ARG:NH1 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:H:489:ARG:HD2 | 3:H:508:ILE:HG13 | 1.76 | 0.67 |
| 1:A:1304:HIS:HE1 | 1:A:1307:ILE:HG22 | 1.59 | 0.67 |
| 1:A:1420:ARG:NH2 | 1:A:1466:ASN:O | 2.28 | 0.67 |
| 1:A:715:ALA:O | 1:A:719:LYS:NZ | 2.27 | 0.67 |
| 1:A:2791:ILE:HA | 1:A:2794:LEU:HD12 | 1.76 | 0.67 |
| 1:F:304:THR:HG22 | 1:F:305:ASN:H | 1.58 | 0.67 |
| 2:G:287:LYS:HB3 | 3:H:310:ILE:HD11 | 1.75 | 0.67 |
| 8:E:39:DA:N6 | 8:E:40:DT:O4 | 2.27 | 0.67 |
| 1:F:2959:ALA:HA | 1:F:2962:ARG:HD3 | 1.75 | 0.67 |
| 2:G:193:LEU:HB2 | 2:G:198:ILE:HB | 1.76 | 0.67 |
| 1:A:1442:GLN:OE1 | 1:A:1445:ARG:NH2 | 2.27 | 0.67 |
| 1:A:3837:CYS:SG | 1:A:3874:ARG:NH1 | 2.68 | 0.67 |
| 2:G:94:LYS:NZ | 2:G:104:VAL:O | 2.28 | 0.67 |
| 5:M:692:ASN:OD1 | 5:M:708:ARG:NH2 | 2.28 | 0.67 |
| 8:I:21:DA:N3 | 9:J:35:DT:N3 | 2.35 | 0.67 |
| 1:F:2965:TYR:HB3 | 1:F:3001:CYS:HB2 | 1.77 | 0.67 |
| 8:I:35:DT:H3 | 9:J:22:DG:H22 | 1.41 | 0.67 |
| 1:A:672:ILE:O | 1:A:676:ASN:ND2 | 2.29 | 0.66 |
| 2:B:95:ASN:HD21 | 2:B:99:PHE:H | 1.43 | 0.66 |
| 1:A:3911:ILE:HD12 | 1:A:3937:VAL:HG23 | 1.77 | 0.66 |
| 1:F:1015:ASP:OD1 | 1:F:1016:GLY:N | 2.28 | 0.66 |
| 1:F:2511:ILE:HD12 | 1:F:2550:ILE:HD12 | 1.76 | 0.66 |
| 1:F:767:GLU:OE2 | 1:F:854:ARG:NH1 | 2.29 | 0.66 |
| 5:P:665:CYS:HB2 | 5:P:697:THR:HG21 | 1.76 | 0.66 |
| 1:A:3944:HIS:ND1 | 1:A:3948:SER:O | 2.28 | 0.66 |
| 1:A:170:VAL:HA | 1:A:219:VAL:HG11 | 1.78 | 0.66 |
| 1:A:468:LEU:HD21 | 1:A:478:CYS:HB2 | 1.78 | 0.66 |
| 1:A:2181:GLY:H | 1:A:2185:MET:HE1 | 1.59 | 0.66 |
| 1:F:24:ARG:HG3 | 1:F:25:CYS:H | 1.60 | 0.66 |
| 1:F:3554:PHE:HD1 | 1:F:3557:ARG:HH21 | 1.42 | 0.66 |
| 1:A:111:CYS:HB2 | 1:A:130:LEU:HD22 | 1.76 | 0.66 |
| 6:Q:175:ILE:HG22 | 6:Q:177:ASP:H | 1.60 | 0.66 |
| 1:A:23:ASP:O | 1:A:70:ARG:NH2 | 2.29 | 0.66 |
| 1:A:996:THR:HG23 | 1:A:1043:GLN:HE21 | 1.61 | 0.66 |
| 5:P:654:LYS:N | 5:P:684:GLU:O | 2.29 | 0.66 |
| 7:D:37:DG:OP1 | 8:E:21:DA:N6 | 2.21 | 0.66 |
| 1:A:58:VAL:HG21 | 1:A:3098:ARG:HD2 | 1.79 | 0.65 |
| 1:A:1305:ASP:OD1 | 1:A:1334:LYS:NZ | 2.27 | 0.65 |
| 1:F:1171:TRP:O | 1:F:1175:HIS:ND1 | 2.27 | 0.65 |
| 1:F:3751:LEU:HD22 | 1:F:3803:ILE:HD11 | 1.79 | 0.65 |
| 2:G:90:THR:HB | 2:G:101:ASN:HA | 1.75 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:87:LYS:NZ | 1:A:829:VAL:O | 2.30 | 0.65 |
| 2:G:50:GLU:OE2 | 2:G:52:GLN:NE2 | 2.30 | 0.65 |
| 4:K:3:ARG:NH2 | 4:K:21:GLN:OE1 | 2.27 | 0.65 |
| 1:A:2869:LEU:HD13 | 1:A:2896:ALA:HA | 1.78 | 0.65 |
| 1:F:672:ILE:O | 1:F:676:ASN:ND2 | 2.30 | 0.65 |
| 9:J:26:DT:H2" | 9:J:27:DT:H3 | 1.60 | 0.65 |
| 1:A:125:ILE:HG13 | 1:A:126:PRO:HD3 | 1.77 | 0.65 |
| 3:H:496:HIS:CD2 | 3:H:500:HIS:HE1 | 2.15 | 0.65 |
| 1:F:2213:ASN:ND2 | 1:F:2248:CYS:O | 2.29 | 0.65 |
| 1:F:2415:LEU:HB2 | 1:F:2420:PHE:HB2 | 1.78 | 0.65 |
| 1:F:2986:PRO:O | 1:F:2991:LYS:NZ | 2.30 | 0.65 |
| 1:F:2987:THR:HG23 | 1:F:2990:GLU:H | 1.61 | 0.65 |
| 2:G:414:VAL:HB | 2:G:433:GLN:HB2 | 1.79 | 0.65 |
| 6:Q:129:SER:HA | 6:R:44:VAL:HB | 1.78 | 0.65 |
| 1:A:2322:VAL:HA | 1:A:2325:LEU:HD12 | 1.79 | 0.65 |
| 1:F:1663:THR:HG22 | 1:F:1664:SER:H | 1.62 | 0.65 |
| 1:F:3062:LEU:HD13 | 1:F:3089:LEU:HD21 | 1.77 | 0.65 |
| 2:G:200:LEU:HD21 | 2:G:221:ILE:HG12 | 1.79 | 0.65 |
| 1:A:418:ALA:HB2 | 1:A:464:VAL:HG12 | 1.77 | 0.65 |
| 1:A:1397:ASP:OD1 | 1:A:1398:VAL:N | 2.30 | 0.65 |
| 1:A:2263:LYS:HE3 | 1:A:2265:PRO:HB3 | 1.77 | 0.65 |
| 1:A:3428:GLU:OE1 | 1:A:3474:ARG:NH1 | 2.30 | 0.65 |
| 1:F:3700:GLU:HG3 | 1:F:3718:ARG:HA | 1.79 | 0.65 |
| 2:G:157:VAL:HG22 | 2:G:159:PHE:H | 1.61 | 0.65 |
| 3:H:43:GLN:HB3 | 3:H:91:LEU:HD21 | 1.78 | 0.65 |
| 4:K:65:LYS:NZ | 4:K:69:GLU:OE2 | 2.29 | 0.65 |
| 5:M:663:GLU:HA | 5:M:688:TYR:HB2 | 1.79 | 0.65 |
| 1:A:3126:LEU:O | 1:A:3130:GLN:NE2 | 2.29 | 0.65 |
| 1:A:1264:LEU:HD23 | 1:A:1340:ARG:HG3 | 1.78 | 0.65 |
| 2:B:357:LYS:HE2 | 2:B:359:HIS:HE1 | 1.61 | 0.65 |
| 1:F:2196:TRP:HB2 | 1:F:2199:LEU:HB2 | 1.77 | 0.65 |
| 1:F:2894:GLU:HG3 | 1:F:3973:PRO:HG2 | 1.77 | 0.65 |
| 1:F:3444:ALA:HB2 | 1:F:3478:GLU:HG3 | 1.79 | 0.65 |
| 1:F:3511:ALA:O | 1:F:3515:GLN:NE2 | 2.30 | 0.64 |
| 1:A:2295:GLN:HG3 | 1:A:2298:GLU:HB3 | 1.79 | 0.64 |
| 2:B:156:ASP:O | 2:B:158:GLN:NE2 | 2.30 | 0.64 |
| 2:B:458:GLN:HE22 | 2:B:527:GLU:HG3 | 1.62 | 0.64 |
| 1:A:2312:TYR:HD2 | 1:A:2315:VAL:HG23 | 1.62 | 0.64 |
| 1:F:3796:MET:H | 1:F:3801:GLY:HA2 | 1.62 | 0.64 |
| 1:F:3882:LEU:HA | 1:F:3885:ARG:HE | 1.63 | 0.64 |
| 1:F:3998:LEU:HA | 1:F:4001:THR:HG22 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:453:ALA:HB1 | 3:C:533:ILE:HG12 | 1.79 | 0.64 |
| 1:F:2356:MET:HE1 | 1:F:2358:ASP:HB3 | 1.79 | 0.64 |
| 2:B:261:LEU:HB3 | 2:B:269:ILE:HB | 1.78 | 0.64 |
| 2:B:428:THR:OG1 | 3:C:354:ARG:NH1 | 2.31 | 0.64 |
| 1:F:3444:ALA:HA | 1:F:3482:LEU:HD11 | 1.80 | 0.64 |
| 1:F:1442:GLN:OE1 | 1:F:1445:ARG:NH2 | 2.31 | 0.64 |
| 1:F:2830:ASN:O | 1:F:2834:GLN:NE2 | 2.30 | 0.64 |
| 1:A:2943:PHE:HB3 | 1:A:2954:GLN:HG2 | 1.80 | 0.64 |
| 2:B:300:THR:OG1 | 3:C:291:LYS:NZ | 2.29 | 0.64 |
| 1:F:418:ALA:HB2 | 1:F:464:VAL:HG12 | 1.80 | 0.64 |
| 1:F:3138:ILE:HG22 | 1:F:3189:PHE:HZ | 1.62 | 0.64 |
| 1:F:3258:LEU:O | 1:F:3262:LEU:HG | 1.97 | 0.64 |
| 1:F:3467:ARG:NH1 | 1:F:4000:ASN:OD1 | 2.31 | 0.64 |
| 3:H:44:ARG:HB2 | 3:H:237:PHE:HB2 | 1.80 | 0.64 |
| 1:A:1788:ARG:O | 1:A:1794:GLN:NE2 | 2.31 | 0.64 |
| 1:A:3142:ILE:O | 1:A:3147:LYS:NZ | 2.28 | 0.64 |
| 1:A:256:ILE:HG23 | 1:A:257:ARG:HG2 | 1.78 | 0.63 |
| 1:A:3758:LEU:HB2 | 1:A:3795:PRO:HB3 | 1.81 | 0.63 |
| 1:F:2891:ARG:HG2 | 1:F:3894:PRO:HB3 | 1.81 | 0.63 |
| 1:F:3739:ILE:HA | 1:F:3749:PRO:HA | 1.78 | 0.63 |
| 4:L:139:ALA:O | 4:L:143:HIS:ND1 | 2.25 | 0.63 |
| 4:N:51:GLU:HB3 | 4:N:54:GLN:HE22 | 1.63 | 0.63 |
| 1:A:278:HIS:HB3 | 1:A:281:GLN:HB2 | 1.79 | 0.63 |
| 1:A:865:GLN:NE2 | 1:A:3171:ALA:O | 2.30 | 0.63 |
| 1:A:1625:HIS:HA | 1:A:1628:LYS:HD3 | 1.80 | 0.63 |
| 1:A:2507:ILE:HA | 1:A:2510:LEU:HD23 | 1.80 | 0.63 |
| 1:F:3512:VAL:HA | 1:F:3515:GLN:HE21 | 1.62 | 0.63 |
| 1:F:3874:ARG:NH2 | 1:F:4117:LEU:O | 2.32 | 0.63 |
| 4:K:198:LEU:HD13 | 4:L:198:LEU:HA | 1.80 | 0.63 |
| 1:A:953:GLN:H | 1:A:956:PRO:HG3 | 1.63 | 0.63 |
| 1:A:3483:MET:HA | 1:A:3486:GLU:HB2 | 1.80 | 0.63 |
| 1:A:3718:ARG:H | 1:A:3743:HIS:CE1 | 2.16 | 0.63 |
| 1:A:975:ASP:O | 1:A:981:ARG:NH2 | 2.27 | 0.63 |
| 1:A:1283:GLY:H | 1:A:1286:ALA:HB2 | 1.63 | 0.63 |
| 1:F:340:TYR:O | 1:F:344:GLN:NE2 | 2.31 | 0.63 |
| 1:A:864:GLY:N | 1:A:3168:TYR:O | 2.32 | 0.63 |
| 5:M:746:MET:O | 5:M:751:LYS:NZ | 2.24 | 0.63 |
| 6:Q:136:ILE:HB | 6:R:40:ASP:HA | 1.81 | 0.63 |
| 1:A:1112:ALA:HA | 1:A:1180:GLN:HG2 | 1.79 | 0.63 |
| 1:F:3369:ASP:HB3 | 1:F:3372:LYS:HG2 | 1.80 | 0.63 |
| 1:F:3835:PRO:HA | 1:F:3839:TYR:HB2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:303:PHE:HB3 | 3:H:290:GLN:HB2 | 1.78 | 0.63 |
| 6:Q:142:MET:HG2 | 6:Q:221:VAL:HB | 1.80 | 0.63 |
| 1:A:1009:LEU:O | 1:A:1013:ILE:HD12 | 1.98 | 0.63 |
| 2:G:404:ARG:NH2 | 8:I:32:DA:OP1 | 2.32 | 0.63 |
| 6:Q:131:VAL:HG13 | 6:R:135:LEU:HD23 | 1.81 | 0.63 |
| 1:A:82:ARG:HA | 1:A:85:ILE:HD12 | 1.80 | 0.62 |
| 1:A:2380:ASN:OD1 | 1:A:2381:ALA:N | 2.32 | 0.62 |
| 1:F:396:PHE:HE1 | 1:F:441:MET:HG3 | 1.64 | 0.62 |
| 1:F:4086:ASP:HA | 1:F:4089:ILE:HG12 | 1.80 | 0.62 |
| 2:G:194:ARG:HH22 | 2:G:221:ILE:HA | 1.63 | 0.62 |
| 2:G:352:PRO:HA | 2:G:394:VAL:HA | 1.81 | 0.62 |
| 5:M:711:ASN:O | 5:M:715:SER:N | 2.29 | 0.62 |
| 1:A:2891:ARG:HG2 | 1:A:3894:PRO:HB3 | 1.81 | 0.62 |
| 1:A:3982:SER:O | 1:A:3986:HIS:ND1 | 2.21 | 0.62 |
| 2:B:304:ASN:HB3 | 2:B:311:LEU:HD21 | 1.79 | 0.62 |
| 2:G:291:GLU:HA | 5:P:690:VAL:HG23 | 1.81 | 0.62 |
| 2:G:521:LEU:HA | 2:G:524:GLU:HB2 | 1.81 | 0.62 |
| 6:R:60:GLU:HG2 | 6:R:61:LEU:HD12 | 1.82 | 0.62 |
| 1:A:1502:SER:OG | 1:A:1503:LEU:N | 2.31 | 0.62 |
| 1:A:3278:GLN:HB3 | 1:A:3282:ARG:HH12 | 1.64 | 0.62 |
| 2:B:347:LEU:HD11 | 2:B:396:ALA:HB1 | 1.80 | 0.62 |
| 1:A:1589:ASN:HD21 | 1:A:1592:MET:HG2 | 1.64 | 0.62 |
| 2:B:141:TYR:O | 2:B:182:LYS:NZ | 2.33 | 0.62 |
| 1:F:2375:ALA:HB3 | 1:F:2404:ARG:HD3 | 1.80 | 0.62 |
| 1:F:3929:MET:O | 1:F:3938:ILE:N | 2.27 | 0.62 |
| 3:H:499:LEU:HD22 | 3:H:500:HIS:HD2 | 1.63 | 0.62 |
| 2:G:277:VAL:HG23 | 3:H:429:ASP:HB3 | 1.81 | 0.62 |
| 2:G:528:LEU:HD21 | 3:H:372:ALA:HB1 | 1.81 | 0.62 |
| 3:H:66:ASN:ND2 | 3:H:74:TYR:O | 2.33 | 0.62 |
| 1:F:736:LEU:HD12 | 1:F:740:ILE:HG21 | 1.82 | 0.62 |
| 1:A:1568:ASN:HD22 | 1:A:1603:GLN:HB2 | 1.63 | 0.62 |
| 1:A:2196:TRP:HB2 | 1:A:2199:LEU:HB2 | 1.82 | 0.62 |
| 1:A:3720:ALA:HB3 | 1:A:3743:HIS:HB3 | 1.80 | 0.62 |
| 1:F:835:LYS:HD3 | 1:F:838:LYS:HD2 | 1.81 | 0.62 |
| 8:I:35:DT:H3 | 9:J:22:DG:N2 | 1.98 | 0.62 |
| 1:F:759:GLY:HA3 | 1:F:766:ALA:HB2 | 1.81 | 0.62 |
| 1:F:3809:THR:OG1 | 1:F:3929:MET:SD | 2.51 | 0.62 |
| 1:F:785:MET:HA | 1:F:788:TYR:CZ | 2.35 | 0.62 |
| 1:F:1685:ASP:HB3 | 1:F:1688:LEU:HG | 1.81 | 0.62 |
| 2:G:95:ASN:OD1 | 2:G:98:ASN:N | 2.33 | 0.62 |
| 2:G:348:MET:HG3 | 2:G:410:PHE:HE1 | 1.65 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3681:LYS:HB2 | 1:F:3687:MET:HG2 | 1.82 | 0.62 |
| 8:E:41:DT:H2" | 8:E:42:DA:H5' | 1.81 | 0.62 |
| 1:F:1367:HIS:HB2 | 1:F:1370:ARG:HH12 | 1.63 | 0.61 |
| 2:G:132:GLN:OE1 | 2:G:137:HIS:ND1 | 2.33 | 0.61 |
| 5:M:739:GLN:OE1 | 5:M:741:ARG:NH1 | 2.33 | 0.61 |
| 2:B:410:PHE:HB3 | 2:B:437:LEU:HD12 | 1.80 | 0.61 |
| 1:F:3443:PRO:HB3 | 1:F:3471:ILE:HD11 | 1.82 | 0.61 |
| 1:A:166:ILE:HG13 | 1:A:167:PRO:HD3 | 1.82 | 0.61 |
| 3:H:653:GLN:O | 3:H:657:ASN:ND2 | 2.33 | 0.61 |
| 1:F:866:ILE:HG13 | 1:F:3168:TYR:HD2 | 1.64 | 0.61 |
| 1:F:2218:PHE:O | 1:F:2222:HIS:ND1 | 2.33 | 0.61 |
| 2:G:67:ILE:HG13 | 2:G:119:LEU:HD21 | 1.82 | 0.61 |
| 5:M:822:SER:HB3 | 5:M:838:LEU:HD13 | 1.82 | 0.61 |
| 4:N:58:ASP:O | 6:Q:75:HIS:NE2 | 2.34 | 0.61 |
| 5:P:666:VAL:HG11 | 5:P:679:GLU:HG2 | 1.81 | 0.61 |
| 1:A:1302:ALA:H | 1:A:1334:LYS:HZ1 | 1.47 | 0.61 |
| 1:F:3620:PRO:O | 1:F:3630:ARG:NH1 | 2.31 | 0.61 |
| 1:F:2742:MET:HE1 | 8:I:44:DG:H1 | 1.65 | 0.61 |
| 1:F:3035:PHE:HA | 1:F:3038:GLU:HB2 | 1.82 | 0.61 |
| 4:L:69:GLU:OE1 | 4:L:99:LYS:NZ | 2.33 | 0.61 |
| 4:L:158:VAL:HA | 4:L:161:ARG:HG2 | 1.82 | 0.61 |
| 1:F:2514:ASN:HD22 | 1:F:2517:LEU:HG | 1.64 | 0.61 |
| 6:Q:139:LEU:HA | 6:Q:142:MET:HE3 | 1.82 | 0.61 |
| 1:F:1016:GLY:HA3 | 1:F:1029:CYS:SG | 2.41 | 0.61 |
| 1:F:2151:ILE:HG12 | 1:F:2192:THR:HG21 | 1.83 | 0.61 |
| 1:F:2268:LYS:HE3 | 1:F:2312:TYR:HB2 | 1.81 | 0.61 |
| 3:H:598:PHE:HZ | 3:H:638:CYS:HB2 | 1.65 | 0.61 |
| 1:F:996:THR:HG23 | 1:F:1043:GLN:HE21 | 1.66 | 0.61 |
| 1:A:149:ILE:HD11 | 1:A:183:GLU:HB2 | 1.81 | 0.61 |
| 1:A:1082:PHE:HA | 1:A:1085:ILE:HG12 | 1.83 | 0.61 |
| 1:A:3700:GLU:HA | 1:A:3719:ILE:H | 1.65 | 0.61 |
| 1:F:2967:GLU:O | 1:F:2971:GLN:HG2 | 2.01 | 0.61 |
| 3:H:508:ILE:HG23 | 3:H:509:GLN:H | 1.64 | 0.61 |
| 1:A:2213:ASN:ND2 | 1:A:2248:CYS:O | 2.33 | 0.60 |
| 3:C:238:LYS:HE2 | 3:C:483:PRO:HB3 | 1.82 | 0.60 |
| 1:F:1626:TRP:HZ2 | 1:F:1674:THR:HG21 | 1.65 | 0.60 |
| 1:F:2723:THR:HA | 1:F:2726:LEU:HD13 | 1.81 | 0.60 |
| 2:G:493:LEU:HD11 | 5:P:708:ARG:HE | 1.66 | 0.60 |
| 1:A:320:LEU:HD21 | 1:A:365:GLY:HA2 | 1.83 | 0.60 |
| 1:A:1375:THR:HG22 | 1:A:1382:ILE:HG21 | 1.82 | 0.60 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:CZ | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:20:SER:HB2 | 1:F:66:LEU:HD23 | 1.83 | 0.60 |
| 7:D:18:DA:H2" | 7:D:19:DA:C8 | 2.36 | 0.60 |
| 1:F:326:MET:HA | 1:F:329:LYS:HE3 | 1.83 | 0.60 |
| 1:F:1172:LEU:HD11 | 1:F:1187:SER:HB2 | 1.83 | 0.60 |
| 1:F:3666:LEU:HA | 1:F:3669:LYS:HZ2 | 1.66 | 0.60 |
| 4:N:155:TRP:HE1 | 4:O:158:VAL:HG21 | 1.66 | 0.60 |
| 1:A:3512:VAL:HA | 1:A:3515:GLN:HE21 | 1.66 | 0.60 |
| 3:C:93:ASP:HB3 | 3:C:97:LYS:HE2 | 1.83 | 0.60 |
| 1:F:3789:ARG:HD3 | 1:F:3938:ILE:HD11 | 1.83 | 0.60 |
| 2:G:329:LEU:HA | 3:H:497:ARG:HH21 | 1.66 | 0.60 |
| 4:L:170:GLU:OE2 | 5:M:851:LYS:NZ | 2.35 | 0.60 |
| 1:A:40:GLN:HB3 | 1:A:2427:ARG:HH21 | 1.66 | 0.60 |
| 1:A:771:ASN:OD1 | 1:A:854:ARG:NH2 | 2.34 | 0.60 |
| 1:A:1491:ILE:HG21 | 1:A:1558:TYR:HE2 | 1.67 | 0.60 |
| 1:A:3335:ARG:NH2 | 1:A:3418:ASP:OD2 | 2.33 | 0.60 |
| 1:F:919:LEU:HG | 1:F:920:THR:HG23 | 1.82 | 0.60 |
| 1:A:264:ARG:N | 8:E:40:DT:OP1 | 2.35 | 0.60 |
| 1:A:1145:LEU:HB3 | 1:A:1165:LEU:HB2 | 1.82 | 0.60 |
| 1:A:3628:PHE:HB2 | 1:A:3675:LYS:HB3 | 1.83 | 0.60 |
| 1:F:935:HIS:HB2 | 1:F:984:TYR:HE1 | 1.67 | 0.60 |
| 2:G:48:MET:HE3 | 2:G:60:PHE:HA | 1.84 | 0.60 |
| 1:A:2425:ARG:NH1 | 1:A:2460:GLU:OE1 | 2.34 | 0.60 |
| 1:A:2808:LEU:HD23 | 1:A:2812:LEU:HD23 | 1.82 | 0.60 |
| 1:A:3506:LEU:O | 1:A:3551:ASN:ND2 | 2.35 | 0.60 |
| 1:F:716:VAL:HG11 | 1:F:1120:SER:HB2 | 1.84 | 0.60 |
| 1:F:3380:ARG:O | 1:F:3384:HIS:ND1 | 2.35 | 0.60 |
| 6:R:193:PHE:HA | 6:R:197:LYS:HG2 | 1.84 | 0.60 |
| 1:A:3079:GLU:OE2 | 1:A:3105:ASN:ND2 | 2.35 | 0.60 |
| 3:C:339:CYS:H | 3:C:396:ALA:HB3 | 1.66 | 0.60 |
| 1:F:477:ASN:OD1 | 1:F:478:CYS:N | 2.35 | 0.60 |
| 1:F:1112:ALA:HA | 1:F:1180:GLN:HG2 | 1.83 | 0.60 |
| 1:F:2742:MET:SD | 9:J:13:DA:N6 | 2.65 | 0.60 |
| 1:F:3771:MET:HA | 1:F:3774:ILE:HD12 | 1.83 | 0.60 |
| 1:A:1532:LEU:HD11 | 1:A:1560:TYR:HB2 | 1.83 | 0.60 |
| 3:C:497:ARG:NH1 | 3:C:503:GLU:O | 2.35 | 0.60 |
| 1:F:1576:ASP:HA | 1:F:1579:VAL:HB | 1.84 | 0.60 |
| 1:F:3921:GLY:H | 1:F:3944:HIS:HB2 | 1.66 | 0.60 |
| 4:N:159:GLN:OE1 | 4:O:161:ARG:NH2 | 2.34 | 0.60 |
| 1:A:785:MET:HA | 1:A:788:TYR:CZ | 2.37 | 0.59 |
| 1:F:1204:PRO:HB2 | 1:F:1206:LEU:H | 1.67 | 0.59 |
| 1:F:2825:THR:HG22 | 1:F:2828:GLU:HG2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3103:ILE:HD13 | 1:F:3138:ILE:HD11 | 1.83 | 0.59 |
| 1:F:3392:ALA:HB1 | 1:F:3409:VAL:HG22 | 1.84 | 0.59 |
| 2:G:264:ASN:OD1 | 2:G:267:ILE:N | 2.31 | 0.59 |
| 1:A:54:GLN:OE1 | 1:A:54:GLN:N | 2.35 | 0.59 |
| 1:A:1211:VAL:HG13 | 1:A:1219:PHE:HZ | 1.67 | 0.59 |
| 1:A:2291:GLN:CD | 1:A:2292:CYS:H | 2.05 | 0.59 |
| 1:F:71:LYS:HB2 | 1:F:82:ARG:CZ | 2.32 | 0.59 |
| 6:Q:131:VAL:H | 6:R:44:VAL:HG23 | 1.68 | 0.59 |
| 1:A:1645:VAL:HA | 1:A:1648:LEU:HD12 | 1.84 | 0.59 |
| 1:A:2569:SER:OG | 1:A:2571:ASP:OD1 | 2.20 | 0.59 |
| 1:A:2825:THR:HG22 | 1:A:2828:GLU:HG2 | 1.84 | 0.59 |
| 1:A:3007:GLU:O | 1:A:3011:LEU:N | 2.35 | 0.59 |
| 1:F:1820:VAL:HA | 1:F:1824:LEU:HD23 | 1.83 | 0.59 |
| 1:F:2372:PRO:O | 1:F:2404:ARG:NH1 | 2.36 | 0.59 |
| 5:P:743:MET:SD | 5:P:746:MET:HB3 | 2.42 | 0.59 |
| 1:A:2514:ASN:HD22 | 1:A:2517:LEU:HG | 1.66 | 0.59 |
| 2:B:94:LYS:HE2 | 2:B:103:TYR:HE1 | 1.67 | 0.59 |
| 2:B:372:GLU:HG2 | 2:B:378:SER:HB2 | 1.83 | 0.59 |
| 3:C:210:MET:HA | 3:C:213:ILE:HG12 | 1.85 | 0.59 |
| 4:O:159:GLN:HG3 | 5:P:843:LEU:HD11 | 1.84 | 0.59 |
| 1:A:1015:ASP:OD1 | 1:A:1016:GLY:N | 2.36 | 0.59 |
| 1:A:1389:VAL:N | 1:A:1392:MET:SD | 2.70 | 0.59 |
| 1:A:2298:GLU:HG2 | 1:A:2301:GLN:HB3 | 1.84 | 0.59 |
| 1:A:3666:LEU:HA | 1:A:3669:LYS:HZ3 | 1.67 | 0.59 |
| 1:F:1765:VAL:O | 1:F:1768:ARG:NE | 2.36 | 0.59 |
| 1:F:3758:LEU:HB2 | 1:F:3795:PRO:HB3 | 1.85 | 0.59 |
| 3:H:431:ARG:HB3 | 3:H:433:TYR:CE1 | 2.38 | 0.59 |
| 3:H:509:GLN:HG3 | 3:H:511:HIS:H | 1.67 | 0.59 |
| 1:A:483:VAL:HG21 | 1:A:567:GLU:HG3 | 1.84 | 0.59 |
| 1:A:675:ARG:HA | 1:A:678:LYS:HE2 | 1.84 | 0.59 |
| 1:A:1465:HIS:HA | 1:A:1468:LEU:HB3 | 1.84 | 0.59 |
| 1:A:3103:ILE:HD13 | 1:A:3138:ILE:HD11 | 1.85 | 0.59 |
| 2:B:217:TYR:HB3 | 2:B:221:ILE:HD12 | 1.85 | 0.59 |
| 2:G:399:ARG:HA | 2:G:410:PHE:HA | 1.82 | 0.59 |
| 1:A:1144:SER:O | 1:A:1151:ARG:NH2 | 2.34 | 0.59 |
| 4:K:133:THR:O | 4:K:137:ASN:ND2 | 2.33 | 0.59 |
| 1:A:1002:GLU:O | 1:A:1004:GLN:NE2 | 2.36 | 0.59 |
| 1:A:2388:LYS:NZ | 2:B:157:VAL:O | 2.36 | 0.59 |
| 1:A:3392:ALA:HB1 | 1:A:3409:VAL:HG22 | 1.84 | 0.59 |
| 1:A:3625:LEU:H | 1:A:3683:CYS:HA | 1.68 | 0.59 |
| 3:C:349:SER:O | 3:C:352:GLN:NE2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:715:ALA:O | 1:F:719:LYS:NZ | 2.35 | 0.59 |
| 3:H:636:ILE:HA | 3:H:639:ILE:HG12 | 1.85 | 0.59 |
| 6:R:210:PHE:HA | 6:R:214:LEU:HB2 | 1.85 | 0.59 |
| 1:A:229:SER:O | 1:A:233:ASN:ND2 | 2.35 | 0.59 |
| 1:A:3855:TYR:OH | 1:A:4120:THR:O | 2.21 | 0.59 |
| 1:A:12:LEU:HD21 | 1:A:44:LEU:HD22 | 1.85 | 0.59 |
| 1:A:2824:LYS:O | 1:A:2829:LYS:NZ | 2.36 | 0.59 |
| 1:F:1115:HIS:CE1 | 1:F:1183:CYS:H | 2.20 | 0.59 |
| 1:F:2313:LYS:HA | 1:F:2316:TYR:CZ | 2.37 | 0.59 |
| 8:I:45:DG:H5' | 8:I:45:DG:H8 | 1.68 | 0.59 |
| 1:A:210:SER:OG | 1:A:257:ARG:NH1 | 2.35 | 0.58 |
| 1:A:1640:GLU:HA | 1:A:1643:MET:SD | 2.43 | 0.58 |
| 1:A:2243:GLU:HG2 | 1:A:2283:ASN:HD21 | 1.67 | 0.58 |
| 1:A:2414:GLN:OE1 | 1:A:2414:GLN:N | 2.34 | 0.58 |
| 1:A:2534:ASN:HB3 | 1:A:2537:ASP:HB2 | 1.84 | 0.58 |
| 1:F:305:ASN:ND2 | 8:I:41:DT:OP2 | 2.36 | 0.58 |
| 1:F:1717:LEU:O | 1:F:1721:HIS:ND1 | 2.35 | 0.58 |
| 1:F:2327:LEU:O | 1:F:2333:ARG:NH2 | 2.36 | 0.58 |
| 1:F:2388:LYS:NZ | 2:G:154:PHE:O | 2.33 | 0.58 |
| 2:G:39:ILE:HD12 | 2:G:84:ALA:HB3 | 1.85 | 0.58 |
| 2:B:362:LEU:HD23 | 2:B:436:PHE:HB3 | 1.84 | 0.58 |
| 1:F:933:LEU:HD22 | 1:F:2797:VAL:HG11 | 1.83 | 0.58 |
| 6:R:36:LEU:O | 6:R:46:HIS:ND1 | 2.36 | 0.58 |
| 1:A:207:GLN:NE2 | 1:A:215:PRO:O | 2.36 | 0.58 |
| 1:A:908:ASP:HA | 1:A:911:LEU:HD23 | 1.84 | 0.58 |
| 1:A:2925:GLU:HA | 1:A:2928:LYS:HD2 | 1.84 | 0.58 |
| 1:F:1190:LEU:HD12 | 1:F:1193:LYS:HD3 | 1.86 | 0.58 |
| 1:F:1297:PHE:HA | 1:F:1301:ILE:HG12 | 1.85 | 0.58 |
| 1:F:3750:PHE:HB3 | 1:F:3802:LEU:HD11 | 1.86 | 0.58 |
| 2:G:254:ARG:NH1 | 8:I:33:DA:O3' | 2.36 | 0.58 |
| 1:A:38:LEU:HD21 | 1:A:85:ILE:HG13 | 1.84 | 0.58 |
| 1:A:3380:ARG:O | 1:A:3384:HIS:ND1 | 2.36 | 0.58 |
| 1:F:1304:HIS:HE1 | 1:F:1307:ILE:HG22 | 1.69 | 0.58 |
| 3:H:44:ARG:NH2 | 3:H:233:LYS:O | 2.36 | 0.58 |
| 2:B:352:PRO:HB2 | 2:B:354:VAL:HG22 | 1.85 | 0.58 |
| 1:F:1502:SER:OG | 1:F:1503:LEU:N | 2.34 | 0.58 |
| 1:A:1487:VAL:HG23 | 1:A:1488:TYR:HD1 | 1.68 | 0.58 |
| 1:A:2372:PRO:O | 1:A:2404:ARG:NH1 | 2.36 | 0.58 |
| 1:A:2404:ARG:NH2 | 1:A:2406:GLU:OE2 | 2.36 | 0.58 |
| 1:A:2464:HIS:CE1 | 1:A:2466:SER:HG | 2.22 | 0.58 |
| 1:F:3455:LYS:O | 1:F:3455:LYS:NZ | 2.29 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1685:ASP:HB3 | 1:A:1688:LEU:HG | 1.84 | 0.58 |
| 1:F:3288:SER:HA | 1:F:3292:GLY:HA3 | 1.84 | 0.58 |
| 3:H:496:HIS:CD2 | 3:H:506:PRO:HD3 | 2.38 | 0.58 |
| 9:J:26:DT:H2" | 9:J:27:DT:N3 | 2.19 | 0.58 |
| 2:B:480:ASN:OD1 | 2:B:483:LEU:N | 2.30 | 0.58 |
| 2:B:522:VAL:HA | 2:B:525:PHE:HB2 | 1.85 | 0.58 |
| 2:G:300:THR:HA | 3:H:293:THR:HA | 1.86 | 0.58 |
| 4:L:150:ARG:NH1 | 4:L:151:LEU:HG | 2.18 | 0.58 |
| 1:A:2479:TRP:O | 1:A:2483:ASN:ND2 | 2.29 | 0.58 |
| 1:A:3474:ARG:NH2 | 1:A:3475:TYR:OH | 2.37 | 0.58 |
| 2:B:399:ARG:HA | 2:B:410:PHE:HA | 1.85 | 0.58 |
| 1:F:3048:LYS:HD2 | 1:F:3061:LEU:HB2 | 1.85 | 0.58 |
| 2:G:34:GLY:HA3 | 2:G:162:SER:HB3 | 1.83 | 0.58 |
| 5:P:660:GLU:HG2 | 5:P:686:GLY:HA3 | 1.84 | 0.58 |
| 1:A:1549:SER:C | 1:A:1550:VAL:HG22 | 2.16 | 0.58 |
| 1:F:3733:ARG:NH2 | 1:F:3755:GLY:O | 2.37 | 0.58 |
| 3:H:460:SER:OG | 3:H:461:MET:SD | 2.62 | 0.58 |
| 8:E:43:DT:H2" | 8:E:44:DG:H5' | 1.86 | 0.58 |
| 1:A:3546:SER:O | 1:A:3550:LYS:NZ | 2.37 | 0.57 |
| 1:A:4115:ASN:O | 1:A:4119:ARG:N | 2.36 | 0.57 |
| 1:F:802:THR:O | 1:F:852:ARG:NH1 | 2.36 | 0.57 |
| 1:F:3389:VAL:HG13 | 1:F:3413:TYR:HE1 | 1.69 | 0.57 |
| 3:H:519:PRO:HB2 | 3:H:521:GLU:HG2 | 1.85 | 0.57 |
| 1:A:1304:HIS:ND1 | 1:A:1307:ILE:O | 2.37 | 0.57 |
| 1:A:3148:GLN:NE2 | 1:A:3150:ASN:OD1 | 2.38 | 0.57 |
| 1:A:3151:LEU:HD21 | 1:A:3196:LYS:HE3 | 1.86 | 0.57 |
| 1:A:3313:SER:HB2 | 1:A:3316:LEU:HD22 | 1.87 | 0.57 |
| 2:B:247:ARG:NH2 | 2:B:491:GLU:OE2 | 2.36 | 0.57 |
| 1:F:469:ALA:HA | 1:F:475:LEU:HD13 | 1.85 | 0.57 |
| 1:F:2348:GLN:OE1 | 1:F:2353:GLN:NE2 | 2.36 | 0.57 |
| 1:F:2380:ASN:OD1 | 1:F:2381:ALA:N | 2.37 | 0.57 |
| 2:G:253:LYS:HD2 | 2:G:254:ARG:HB2 | 1.86 | 0.57 |
| 1:A:471:LYS:O | 1:A:475:LEU:N | 2.28 | 0.57 |
| 3:C:250:ARG:HA | 3:C:260:ARG:HA | 1.86 | 0.57 |
| 1:F:297:LEU:HD23 | 1:F:316:LEU:HA | 1.86 | 0.57 |
| 1:A:3117:ILE:O | 1:A:3125:ARG:NH2 | 2.37 | 0.57 |
| 2:B:252:ARG:NH1 | 2:B:254:ARG:O | 2.31 | 0.57 |
| 2:B:413:LEU:HB2 | 2:B:432:PHE:HB3 | 1.86 | 0.57 |
| 1:F:113:SER:O | 1:F:117:LYS:HB2 | 2.04 | 0.57 |
| 1:F:1151:ARG:HB2 | 1:F:1163:LEU:HD12 | 1.86 | 0.57 |
| 1:F:1195:VAL:HA | 1:F:1198:LEU:HD12 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1685:ASP:H | 1:F:1688:LEU:HD12 | 1.69 | 0.57 |
| 1:F:2388:LYS:NZ | 2:G:157:VAL:O | 2.38 | 0.57 |
| 1:F:3464:LYS:HD3 | 1:F:3997:LEU:HD21 | 1.85 | 0.57 |
| 1:A:3142:ILE:HA | 1:A:3145:ILE:HG12 | 1.86 | 0.57 |
| 3:C:335:SER:OG | 3:C:339:CYS:SG | 2.58 | 0.57 |
| 1:F:2257:PHE:HB2 | 1:F:2299:TYR:HE1 | 1.69 | 0.57 |
| 1:F:2271:SER:HA | 1:F:2274:ILE:HD12 | 1.87 | 0.57 |
| 1:F:2291:GLN:NE2 | 1:F:2292:CYS:SG | 2.78 | 0.57 |
| 1:A:984:TYR:HA | 1:A:987:LEU:HB3 | 1.86 | 0.57 |
| 1:A:2123:PRO:HA | 1:A:2127:LYS:HG2 | 1.86 | 0.57 |
| 1:F:639:ALA:O | 1:F:643:GLU:N | 2.37 | 0.57 |
| 1:F:1305:ASP:OD1 | 1:F:1334:LYS:NZ | 2.37 | 0.57 |
| 2:G:305:THR:HG23 | 3:H:290:GLN:HG3 | 1.85 | 0.57 |
| 1:A:89:LEU:O | 1:A:93:LEU:N | 2.36 | 0.57 |
| 1:A:2120:ARG:HE | 1:A:2159:PRO:HG2 | 1.70 | 0.57 |
| 1:A:3553:GLU:HG3 | 1:A:3557:ARG:HH22 | 1.69 | 0.57 |
| 3:H:9:ALA:HB3 | 3:H:130:ARG:HG3 | 1.85 | 0.57 |
| 6:Q:27:VAL:HG11 | 6:Q:80:LEU:HD12 | 1.85 | 0.57 |
| 1:A:753:GLN:NE2 | 1:A:791:ASP:O | 2.32 | 0.57 |
| 1:A:993:HIS:ND1 | 1:A:2779:ASP:OD1 | 2.32 | 0.57 |
| 1:A:1096:VAL:O | 1:A:1100:VAL:HG13 | 2.04 | 0.57 |
| 2:B:485:GLN:NE2 | 3:C:333:TYR:O | 2.38 | 0.57 |
| 1:F:3155:VAL:H | 1:F:3159:ARG:HH22 | 1.51 | 0.57 |
| 7:D:25:DT:H3' | 7:D:26:DT:H72 | 1.86 | 0.57 |
| 1:A:128:LEU:HD21 | 1:A:170:VAL:HB | 1.86 | 0.57 |
| 2:B:468:LYS:NZ | 2:B:517:ARG:O | 2.32 | 0.57 |
| 1:F:2342:CYS:HB3 | 1:F:2377:ARG:HH22 | 1.70 | 0.57 |
| 1:F:2815:GLY:HA2 | 1:F:2818:LYS:HZ2 | 1.70 | 0.57 |
| 1:F:2824:LYS:O | 1:F:2829:LYS:NZ | 2.38 | 0.57 |
| 2:G:131:PHE:CZ | 2:G:135:MET:HG2 | 2.39 | 0.57 |
| 1:A:1717:LEU:O | 1:A:1721:HIS:ND1 | 2.38 | 0.57 |
| 1:A:1843:ILE:HA | 1:A:1846:ASP:HB3 | 1.85 | 0.57 |
| 2:B:350:PHE:HD2 | 3:C:461:MET:HB2 | 1.70 | 0.57 |
| 5:P:746:MET:HE3 | 5:P:751:LYS:HG2 | 1.86 | 0.57 |
| 1:F:476:ARG:HH22 | 1:F:1558:TYR:HE1 | 1.52 | 0.56 |
| 1:F:1023:SER:OG | 1:F:1026:ARG:NH2 | 2.38 | 0.56 |
| 2:G:246:VAL:HB | 2:G:249:LYS:HZ1 | 1.70 | 0.56 |
| 1:A:1849:ASP:OD1 | 1:A:1850:VAL:N | 2.38 | 0.56 |
| 2:B:362:LEU:HB3 | 2:B:436:PHE:HB2 | 1.86 | 0.56 |
| 1:F:538:ASP:HA | 1:F:541:MET:HG3 | 1.87 | 0.56 |
| 1:F:2365:ASN:HD22 | 1:F:2396:LEU:HG | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:K:31:GLY:HA3 | 4:K:47:VAL:HG21 | 1.87 | 0.56 |
| 1:A:40:GLN:HG3 | 1:A:2427:ARG:HE | 1.70 | 0.56 |
| 1:A:1576:ASP:HA | 1:A:1579:VAL:HB | 1.86 | 0.56 |
| 1:A:2732:PHE:HA | 1:A:2734:ARG:HH11 | 1.70 | 0.56 |
| 1:A:3554:PHE:HD1 | 1:A:3557:ARG:HH21 | 1.54 | 0.56 |
| 2:B:276:LEU:HA | 3:C:433:TYR:HE2 | 1.69 | 0.56 |
| 1:F:68:PHE:O | 1:F:82:ARG:NH2 | 2.38 | 0.56 |
| 1:F:117:LYS:NZ | 3:H:298:ASN:O | 2.29 | 0.56 |
| 1:F:1048:GLN:HA | 1:F:1051:LYS:HG2 | 1.86 | 0.56 |
| 1:F:1377:CYS:SG | 1:F:1378:GLU:N | 2.78 | 0.56 |
| 1:F:1608:ARG:HE | 1:F:1612:LYS:HZ2 | 1.51 | 0.56 |
| 1:F:2534:ASN:HB3 | 1:F:2537:ASP:HB2 | 1.87 | 0.56 |
| 1:F:3639:GLU:O | 1:F:3643:HIS:ND1 | 2.34 | 0.56 |
| 1:F:3702:PRO:HB2 | 1:F:3794:VAL:HG21 | 1.87 | 0.56 |
| 2:G:271:VAL:HG12 | 2:G:370:PRO:HA | 1.85 | 0.56 |
| 2:G:318:ARG:HH21 | 3:H:278:VAL:HG13 | 1.70 | 0.56 |
| 3:H:409:PHE:HB3 | 3:H:420:VAL:HG23 | 1.87 | 0.56 |
| 5:P:813:PHE:HA | 5:P:850:ALA:O | 2.05 | 0.56 |
| 5:P:845:LEU:HD22 | 5:P:852:VAL:HG13 | 1.87 | 0.56 |
| 1:A:1820:VAL:HA | 1:A:1824:LEU:HD13 | 1.85 | 0.56 |
| 2:B:470:ARG:HH21 | 3:C:346:CYS:HA | 1.70 | 0.56 |
| 1:F:938:VAL:HA | 1:F:941:MET:HG3 | 1.86 | 0.56 |
| 2:G:476:ASP:HB2 | 3:H:427:MET:HG3 | 1.87 | 0.56 |
| 1:A:2232:ARG:NH1 | 1:A:2275:GLN:OE1 | 2.39 | 0.56 |
| 1:A:2522:ARG:HH21 | 1:A:2564:GLU:HG3 | 1.70 | 0.56 |
| 1:F:2330:VAL:HG22 | 1:F:2331:MET:SD | 2.46 | 0.56 |
| 5:P:694:GLY:O | 5:P:718:HIS:NE2 | 2.33 | 0.56 |
| 1:A:1354:GLU:HA | 1:A:1357:LYS:HB3 | 1.88 | 0.56 |
| 1:A:3151:LEU:HD22 | 1:A:3197:LEU:HA | 1.87 | 0.56 |
| 1:A:3737:ARG:HA | 1:A:3751:LEU:HA | 1.88 | 0.56 |
| 1:F:672:ILE:HG13 | 1:F:676:ASN:HD21 | 1.70 | 0.56 |
| 1:F:865:GLN:HE22 | 1:F:3171:ALA:N | 2.04 | 0.56 |
| 1:F:2131:GLY:O | 1:F:2135:ASN:ND2 | 2.38 | 0.56 |
| 1:A:852:ARG:NH2 | 1:A:922:SER:OG | 2.38 | 0.56 |
| 1:A:1354:GLU:HB3 | 1:A:1357:LYS:HD3 | 1.87 | 0.56 |
| 1:A:3110:PHE:CE1 | 1:A:3128:LYS:HG3 | 2.40 | 0.56 |
| 2:B:275:ASN:O | 2:B:278:GLN:NE2 | 2.38 | 0.56 |
| 1:F:529:ASP:HA | 1:F:532:ARG:HH11 | 1.70 | 0.56 |
| 1:F:1307:ILE:HG23 | 1:F:1309:ALA:H | 1.70 | 0.56 |
| 1:F:1605:PHE:O | 1:F:1608:ARG:NH2 | 2.39 | 0.56 |
| 1:F:2555:LEU:HD11 | 1:F:2854:PHE:HA | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Q:44:VAL:HG12 | 6:Q:130:LEU:HD21 | 1.87 | 0.56 |
| 1:F:116:THR:O | 2:G:297:LYS:NZ | 2.38 | 0.56 |
| 1:F:1238:GLN:HB2 | 1:F:1239:PRO:HD3 | 1.88 | 0.56 |
| 3:H:153:SER:HA | 3:H:156:LYS:HE2 | 1.87 | 0.56 |
| 3:H:315:ARG:HH11 | 3:H:320:ILE:HG13 | 1.70 | 0.56 |
| 1:A:2511:ILE:HD12 | 1:A:2550:ILE:HD12 | 1.87 | 0.56 |
| 3:C:514:ASN:OD1 | 3:C:515:MET:N | 2.39 | 0.56 |
| 1:F:584:GLU:O | 1:F:613:HIS:N | 2.38 | 0.56 |
| 1:F:3736:LYS:HB2 | 1:F:3752:VAL:HB | 1.87 | 0.56 |
| 1:F:3828:TYR:OH | 1:F:3876:SER:O | 2.24 | 0.56 |
| 4:K:169:LYS:HB2 | 4:L:169:LYS:HG3 | 1.87 | 0.56 |
| 5:M:710:LYS:HA | 5:M:713:ILE:HD12 | 1.86 | 0.56 |
| 1:A:168:ASP:OD1 | 1:A:169:THR:N | 2.35 | 0.55 |
| 1:A:1261:LEU:HG | 1:A:1340:ARG:HG2 | 1.89 | 0.55 |
| 1:A:2221:LYS:HZ2 | 1:A:2255:LEU:HD22 | 1.70 | 0.55 |
| 2:B:71:TYR:HB2 | 2:B:116:ILE:HD11 | 1.87 | 0.55 |
| 1:F:3826:ALA:O | 1:F:3830:SER:HB3 | 2.06 | 0.55 |
| 3:H:412:ILE:HA | 3:H:417:GLU:HG3 | 1.87 | 0.55 |
| 8:E:23:DT:H2" | 8:E:25:DA:N1 | 2.21 | 0.55 |
| 1:A:996:THR:HG23 | 1:A:1043:GLN:NE2 | 2.20 | 0.55 |
| 1:A:3447:VAL:HA | 1:A:3450:MET:HG3 | 1.88 | 0.55 |
| 1:F:1070:PRO:HA | 1:F:1113:LEU:HD21 | 1.88 | 0.55 |
| 1:F:1134:LEU:HD23 | 1:F:1137:ILE:HD11 | 1.89 | 0.55 |
| 5:M:666:VAL:HA | 5:M:701:ILE:HB | 1.88 | 0.55 |
| 1:A:3050:LYS:NZ | 1:A:3180:ASP:OD1 | 2.31 | 0.55 |
| 1:A:3294:SER:O | 1:A:3298:LEU:HG | 2.07 | 0.55 |
| 3:C:242:ARG:HD2 | 3:C:273:LYS:HE3 | 1.88 | 0.55 |
| 3:H:453:ALA:HB2 | 3:H:536:LEU:HD23 | 1.87 | 0.55 |
| 4:O:142:GLU:HB3 | 4:O:146:LYS:NZ | 2.22 | 0.55 |
| 7:D:18:DA:H2' | 7:D:18:DA:N3 | 2.20 | 0.55 |
| 1:A:200:PHE:CE2 | 1:A:227:LEU:HD21 | 2.41 | 0.55 |
| 1:A:2290:PRO:O | 1:A:2292:CYS:N | 2.39 | 0.55 |
| 1:A:3569:GLN:HA | 1:A:3572:ILE:HD12 | 1.88 | 0.55 |
| 1:A:3576:ASP:O | 1:A:3629:ARG:NH1 | 2.40 | 0.55 |
| 1:A:3717:VAL:HA | 1:A:3743:HIS:HE1 | 1.72 | 0.55 |
| 1:F:782:ARG:NH1 | 1:F:3168:TYR:OH | 2.40 | 0.55 |
| 4:K:187:LYS:HZ1 | 4:L:188:LYS:HG3 | 1.72 | 0.55 |
| 5:M:725:TRP:HE3 | 5:M:726:LEU:HD22 | 1.71 | 0.55 |
| 5:P:764:SER:OG | 5:P:767:ILE:O | 2.24 | 0.55 |
| 1:A:63:PHE:HE2 | 1:A:85:ILE:HG12 | 1.70 | 0.55 |
| 1:A:2205:VAL:HG22 | 1:A:2207:LYS:H | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:457:GLU:OE2 | 2:B:458:GLN:NE2 | 2.30 | 0.55 |
| 2:B:481:PRO:HA | 2:B:484:GLN:HE21 | 1.70 | 0.55 |
| 5:P:813:PHE:H | 5:P:848:HIS:HB2 | 1.70 | 0.55 |
| 1:A:71:LYS:CB | 1:A:82:ARG:HH22 | 2.20 | 0.55 |
| 1:A:1610:ASN:OD1 | 1:A:1611:GLN:N | 2.38 | 0.55 |
| 1:A:1614:GLN:HA | 1:A:1617:LYS:HE2 | 1.89 | 0.55 |
| 1:A:2737:GLU:HG2 | 1:A:2740:SER:HB2 | 1.88 | 0.55 |
| 3:H:86:PRO:HA | 3:H:90:LEU:HD12 | 1.88 | 0.55 |
| 8:I:34:DC:H42 | 9:J:23:DT:H3 | 1.53 | 0.55 |
| 1:A:983:LEU:HD22 | 1:A:2775:TYR:HE2 | 1.71 | 0.55 |
| 1:A:1841:SER:HA | 1:A:1844:VAL:HG23 | 1.89 | 0.55 |
| 1:F:538:ASP:OD1 | 1:F:539:GLN:N | 2.40 | 0.55 |
| 1:F:2331:MET:O | 1:F:2334:LYS:NZ | 2.32 | 0.55 |
| 1:F:2439:ILE:HD12 | 1:F:2454:LEU:HD21 | 1.89 | 0.55 |
| 1:F:3527:GLN:HB2 | 1:F:3705:TYR:HE2 | 1.72 | 0.55 |
| 1:F:4113:ASP:O | 1:F:4117:LEU:HG | 2.06 | 0.55 |
| 2:G:381:LEU:O | 2:G:385:LEU:HG | 2.05 | 0.55 |
| 1:A:3263:HIS:HB2 | 1:A:3276:TRP:CZ2 | 2.42 | 0.55 |
| 2:B:264:ASN:HD22 | 3:C:530:LEU:HD13 | 1.72 | 0.55 |
| 1:F:87:LYS:HE2 | 1:F:831:LEU:HD13 | 1.87 | 0.55 |
| 2:G:336:GLU:O | 3:H:489:ARG:NH2 | 2.40 | 0.55 |
| 7:D:37:DG:C8 | 8:E:19:DC:H2" | 2.42 | 0.55 |
| 1:A:1151:ARG:HB2 | 1:A:1163:LEU:HD12 | 1.89 | 0.55 |
| 1:F:2479:TRP:O | 1:F:2483:ASN:ND2 | 2.26 | 0.55 |
| 1:F:3255:ALA:HB1 | 1:F:3258:LEU:HB2 | 1.89 | 0.55 |
| 3:H:453:ALA:HB1 | 3:H:533:ILE:HG12 | 1.88 | 0.55 |
| 4:K:101:LEU:HD21 | 6:R:113:SER:HB3 | 1.89 | 0.55 |
| 5:P:665:CYS:HB3 | 5:P:700:VAL:HA | 1.88 | 0.55 |
| 1:A:3576:ASP:O | 1:A:3579:SER:OG | 2.21 | 0.55 |
| 3:C:253:ILE:HB | 3:C:257:LEU:HB3 | 1.88 | 0.55 |
| 1:F:3118:ASP:HB3 | 1:F:3121:LEU:HD13 | 1.88 | 0.55 |
| 1:F:3226:ASP:N | 1:F:3229:SER:HG | 2.05 | 0.55 |
| 1:A:3512:VAL:O | 1:A:3516:HIS:ND1 | 2.34 | 0.54 |
| 1:F:1452:VAL:HA | 1:F:1517:LEU:HD11 | 1.89 | 0.54 |
| 2:G:35:ARG:HH21 | 2:G:80:ARG:HB3 | 1.72 | 0.54 |
| 2:G:166:ILE:HB | 2:G:200:LEU:HA | 1.89 | 0.54 |
| 6:R:195:ILE:HG23 | 6:R:196:GLU:HG3 | 1.88 | 0.54 |
| 1:A:2220:MET:HA | 1:A:2223:VAL:HG12 | 1.89 | 0.54 |
| 1:A:3878:VAL:O | 1:A:3965:ARG:NH1 | 2.39 | 0.54 |
| 1:F:1070:PRO:HG2 | 1:F:3715:TYR:HB2 | 1.88 | 0.54 |
| 1:A:2943:PHE:O | 1:A:2954:GLN:NE2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2986:PRO:O | 1:A:2991:LYS:NZ | 2.40 | 0.54 |
| 2:B:484:GLN:O | 2:B:488:ARG:HG2 | 2.08 | 0.54 |
| 1:F:79:ARG:NH1 | 1:F:119:ARG:HD2 | 2.23 | 0.54 |
| 1:F:1551:ILE:HG13 | 1:F:1552:HIS:H | 1.73 | 0.54 |
| 1:F:1686:LEU:HA | 1:F:1689:LYS:HD2 | 1.90 | 0.54 |
| 2:G:328:ILE:O | 3:H:497:ARG:NE | 2.41 | 0.54 |
| 3:H:641:ALA:O | 3:H:644:GLU:HG3 | 2.06 | 0.54 |
| 5:P:856:LEU:HD11 | 5:P:882:PHE:HZ | 1.72 | 0.54 |
| 1:A:1358:LEU:HA | 1:A:1361:LYS:HE2 | 1.89 | 0.54 |
| 1:A:1878:ASP:OD1 | 1:A:1879:VAL:N | 2.40 | 0.54 |
| 1:A:2402:LEU:HD11 | 1:A:2437:ASP:HB2 | 1.88 | 0.54 |
| 1:A:95:LYS:HD3 | 1:A:97:GLY:H | 1.73 | 0.54 |
| 1:A:1958:GLU:HG2 | 1:A:1959:LEU:H | 1.72 | 0.54 |
| 1:F:863:GLY:HA3 | 1:F:3167:ARG:O | 2.07 | 0.54 |
| 1:F:1268:ASN:HD21 | 1:F:1344:PHE:HA | 1.72 | 0.54 |
| 1:F:1766:LEU:HD23 | 1:F:1822:ARG:HH11 | 1.71 | 0.54 |
| 1:F:2466:SER:OG | 1:F:2469:CYS:SG | 2.65 | 0.54 |
| 1:F:3808:ASN:ND2 | 1:F:3933:GLU:OE1 | 2.40 | 0.54 |
| 1:F:3831:ASP:HB3 | 1:F:3832:PRO:HD3 | 1.90 | 0.54 |
| 1:A:542:ASP:OD1 | 1:A:543:SER:N | 2.41 | 0.54 |
| 1:A:2290:PRO:O | 1:A:2293:GLY:N | 2.36 | 0.54 |
| 1:A:3035:PHE:HA | 1:A:3038:GLU:HB2 | 1.90 | 0.54 |
| 1:A:3701:ILE:HB | 1:A:3704:GLN:NE2 | 2.23 | 0.54 |
| 1:F:762:TYR:HD2 | 1:F:765:LEU:HB2 | 1.71 | 0.54 |
| 1:F:3142:ILE:HA | 1:F:3145:ILE:HG12 | 1.89 | 0.54 |
| 1:F:3183:ILE:HD12 | 1:F:3238:MET:HB3 | 1.89 | 0.54 |
| 6:R:41:LEU:HD11 | 6:R:139:LEU:HD21 | 1.89 | 0.54 |
| 1:A:582:THR:HA | 1:A:660:LEU:HD21 | 1.90 | 0.54 |
| 1:A:1420:ARG:NH1 | 1:A:1467:ILE:O | 2.39 | 0.54 |
| 1:A:1675:TYR:OH | 1:A:1692:ALA:O | 2.22 | 0.54 |
| 1:A:1686:LEU:HA | 1:A:1689:LYS:HD2 | 1.90 | 0.54 |
| 1:F:862:LEU:HD23 | 1:F:866:ILE:HG21 | 1.90 | 0.54 |
| 1:F:2940:ARG:O | 1:F:2944:THR:HB | 2.08 | 0.54 |
| 1:F:3126:LEU:O | 1:F:3130:GLN:NE2 | 2.41 | 0.54 |
| 1:F:3639:GLU:HG3 | 1:F:3643:HIS:HE1 | 1.72 | 0.54 |
| 2:G:85:VAL:HG23 | 2:G:105:LEU:HB3 | 1.90 | 0.54 |
| 4:N:5:ILE:HG13 | 4:N:126:LEU:HD21 | 1.90 | 0.54 |
| 1:A:172:GLU:HG3 | 1:A:220:LEU:HD13 | 1.89 | 0.54 |
| 1:A:759:GLY:HA3 | 1:A:766:ALA:HB2 | 1.90 | 0.54 |
| 1:A:1204:PRO:HB2 | 1:A:1206:LEU:H | 1.72 | 0.54 |
| 1:A:1389:VAL:HG23 | 1:A:1391:VAL:HG22 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2587:GLN:O | 1:A:2777:HIS:N | 2.38 | 0.54 |
| 1:A:3008:TRP:HA | 1:A:3011:LEU:HD12 | 1.90 | 0.54 |
| 1:A:3882:LEU:HA | 1:A:3885:ARG:HE | 1.72 | 0.54 |
| 1:A:3981:TYR:HE1 | 1:A:4105:LYS:HB2 | 1.73 | 0.54 |
| 1:F:3112:GLN:O | 1:F:3115:SER:OG | 2.23 | 0.54 |
| 1:F:3269:ARG:HE | 1:F:3272:TRP:HB2 | 1.73 | 0.54 |
| 1:F:3385:LEU:HB3 | 1:F:3416:LEU:HD12 | 1.89 | 0.54 |
| 4:L:162:PHE:HE2 | 5:M:843:LEU:HB3 | 1.72 | 0.54 |
| 5:M:713:ILE:HG12 | 5:M:745:HIS:HB2 | 1.90 | 0.54 |
| 1:F:305:ASN:O | 1:F:308:LEU:N | 2.40 | 0.54 |
| 1:F:2414:GLN:OE1 | 1:F:2414:GLN:N | 2.40 | 0.54 |
| 1:F:3065:ILE:O | 1:F:3069:MET:N | 2.40 | 0.54 |
| 2:G:163:HIS:HE1 | 2:G:165:ARG:HB2 | 1.72 | 0.54 |
| 1:A:2589:TYR:H | 1:A:2776:ARG:HA | 1.73 | 0.54 |
| 5:P:747:CYS:SG | 5:P:749:SER:OG | 2.62 | 0.54 |
| 1:A:1115:HIS:CE1 | 1:A:1183:CYS:H | 2.26 | 0.53 |
| 1:A:1406:LEU:HA | 1:A:1409:SER:HB3 | 1.90 | 0.53 |
| 2:B:515:ASN:O | 2:B:519:GLY:N | 2.41 | 0.53 |
| 1:F:348:ILE:HG21 | 1:F:362:ALA:HB2 | 1.90 | 0.53 |
| 1:F:3700:GLU:OE1 | 1:F:3705:TYR:OH | 2.24 | 0.53 |
| 5:P:725:TRP:HB2 | 5:P:742:PHE:CD2 | 2.44 | 0.53 |
| 1:A:175:TYR:O | 1:A:227:LEU:HD12 | 2.08 | 0.53 |
| 1:A:977:ASP:OD1 | 1:A:980:THR:N | 2.37 | 0.53 |
| 1:A:1605:PHE:HE2 | 1:A:6013:UNK:HA | 1.73 | 0.53 |
| 1:A:3485:LYS:O | 1:A:3489:SER:OG | 2.25 | 0.53 |
| 2:B:40:PHE:HB2 | 2:B:85:VAL:HG12 | 1.90 | 0.53 |
| 1:F:135:LEU:HD21 | 1:F:177:LEU:HA | 1.90 | 0.53 |
| 1:F:1849:ASP:OD1 | 1:F:1850:VAL:N | 2.42 | 0.53 |
| 1:F:3506:LEU:HG | 1:F:3515:GLN:HG3 | 1.88 | 0.53 |
| 3:H:81:ARG:HD2 | 3:H:90:LEU:HD22 | 1.90 | 0.53 |
| 1:A:1169:VAL:HG11 | 1:A:1198:LEU:HD11 | 1.91 | 0.53 |
| 1:A:3901:ARG:NH1 | 1:A:3971:MET:HG2 | 2.24 | 0.53 |
| 2:B:74:LYS:HG3 | 2:B:83:LEU:HD11 | 1.91 | 0.53 |
| 2:B:426:GLN:NE2 | 2:B:427:VAL:O | 2.42 | 0.53 |
| 1:F:266:ALA:O | 1:F:269:SER:OG | 2.21 | 0.53 |
| 1:F:3179:TRP:HE3 | 1:F:3242:MET:SD | 2.31 | 0.53 |
| 1:F:3278:GLN:HB3 | 1:F:3282:ARG:HH12 | 1.72 | 0.53 |
| 5:P:813:PHE:H | 5:P:848:HIS:CB | 2.21 | 0.53 |
| 6:Q:159:MET:SD | 6:Q:160:LYS:HG3 | 2.48 | 0.53 |
| 8:I:27:DC:H2' | 9:J:30:DT:C2 | 2.43 | 0.53 |
| 1:A:938:VAL:HA | 1:A:941:MET:HG3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1833:LEU:HD11 | 1:A:1883:ARG:HD2 | 1.90 | 0.53 |
| 1:A:2271:SER:HA | 1:A:2274:ILE:HD12 | 1.91 | 0.53 |
| 1:A:3502:MET:HG3 | 1:A:3518:VAL:HG11 | 1.89 | 0.53 |
| 3:C:497:ARG:HH22 | 3:C:504:PRO:HA | 1.73 | 0.53 |
| 1:F:67:VAL:HA | 1:F:71:LYS:HE2 | 1.90 | 0.53 |
| 1:F:651:TYR:CZ | 1:F:655:LEU:HD11 | 2.44 | 0.53 |
| 1:F:959:TYR:CZ | 1:F:963:LYS:HD2 | 2.43 | 0.53 |
| 1:F:3820:MET:HB3 | 1:F:3885:ARG:HH22 | 1.72 | 0.53 |
| 2:G:348:MET:HG3 | 2:G:410:PHE:CE1 | 2.44 | 0.53 |
| 4:L:51:GLU:OE1 | 4:L:112:ASN:ND2 | 2.33 | 0.53 |
| 1:A:886:TRP:O | 1:A:888:ARG:NH1 | 2.41 | 0.53 |
| 1:A:1238:GLN:HA | 1:A:1296:PHE:CZ | 2.43 | 0.53 |
| 1:A:2244:CYS:SG | 1:A:2245:TRP:N | 2.82 | 0.53 |
| 1:F:993:HIS:NE2 | 1:F:1035:GLU:OE2 | 2.32 | 0.53 |
| 1:F:1058:SER:O | 1:F:1062:ARG:HG2 | 2.08 | 0.53 |
| 2:G:318:ARG:HB3 | 3:H:276:TRP:HB3 | 1.90 | 0.53 |
| 4:K:187:LYS:HA | 4:K:190:LYS:HD2 | 1.90 | 0.53 |
| 4:L:56:ALA:HB1 | 4:L:63:LYS:HG2 | 1.90 | 0.53 |
| 1:F:36:ARG:HD3 | 1:F:2426:HIS:CG | 2.44 | 0.53 |
| 1:F:880:MET:O | 1:F:881:LYS:HG2 | 2.08 | 0.53 |
| 1:F:2346:ALA:HB2 | 1:F:2377:ARG:HH11 | 1.74 | 0.53 |
| 2:G:329:LEU:HD12 | 3:H:497:ARG:HH21 | 1.73 | 0.53 |
| 3:H:33:GLN:HA | 3:H:36:LYS:HG2 | 1.90 | 0.53 |
| 4:N:28:LEU:HD23 | 4:N:70:LEU:HD13 | 1.90 | 0.53 |
| 8:I:27:DC:H1' | 9:J:31:DT:C2 | 2.43 | 0.53 |
| 1:A:10:CYS:SG | 1:A:11:SER:N | 2.81 | 0.53 |
| 1:A:992:ILE:HG23 | 1:A:1036:PHE:HD1 | 1.72 | 0.53 |
| 1:A:1864:ASP:OD1 | 1:A:1864:ASP:N | 2.42 | 0.53 |
| 1:A:2283:ASN:HB2 | 1:A:2285:LEU:HG | 1.91 | 0.53 |
| 1:A:3994:ASP:HB3 | 1:A:3998:LEU:HG | 1.91 | 0.53 |
| 2:B:88:TYR:HB3 | 2:B:146:VAL:HG11 | 1.90 | 0.53 |
| 1:F:1238:GLN:HA | 1:F:1296:PHE:CZ | 2.43 | 0.53 |
| 3:H:44:ARG:CZ | 3:H:234:LEU:HA | 2.38 | 0.53 |
| 8:I:30:DA:H3' | 8:I:32:DA:N6 | 2.24 | 0.53 |
| 1:A:1633:TRP:HA | 1:A:1678:LEU:HD21 | 1.90 | 0.53 |
| 3:C:199:GLU:OE2 | 3:C:202:LYS:NZ | 2.42 | 0.53 |
| 3:H:76:ASN:ND2 | 3:H:104:GLN:O | 2.35 | 0.53 |
| 6:R:95:PHE:HE2 | 6:R:108:VAL:HG13 | 1.74 | 0.53 |
| 1:A:651:TYR:CZ | 1:A:655:LEU:HD11 | 2.44 | 0.53 |
| 1:A:1475:LEU:HD23 | 1:A:1527:ARG:HD2 | 1.91 | 0.53 |
| 1:A:2439:ILE:HD12 | 1:A:2454:LEU:HD21 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3479:THR:HA | 1:A:3482:LEU:HB2 | 1.91 | 0.53 |
| 2:G:178:ASN:HD21 | 2:G:182:LYS:HD2 | 1.74 | 0.53 |
| 4:N:99:LYS:NZ | 4:N:100:ASN:O | 2.42 | 0.53 |
| 1:A:1418:HIS:O | 1:A:1422:LYS:HG2 | 2.09 | 0.53 |
| 1:A:3172:LYS:HD3 | 1:A:3248:LYS:HB3 | 1.89 | 0.53 |
| 1:A:3915:HIS:HB2 | 1:A:3920:ILE:HB | 1.91 | 0.53 |
| 2:B:400:TYR:N | 2:B:409:TYR:O | 2.30 | 0.53 |
| 1:F:1601:LEU:HD13 | 1:F:1651:LYS:HB3 | 1.91 | 0.53 |
| 1:F:2160:TYR:HD2 | 1:F:2164:TRP:CD1 | 2.26 | 0.53 |
| 1:F:2287:PRO:HG3 | 1:F:2330:VAL:HA | 1.90 | 0.53 |
| 1:F:3566:GLY:O | 1:F:3570:ASP:N | 2.37 | 0.53 |
| 1:F:3974:MET:SD | 1:F:3976:GLU:N | 2.82 | 0.53 |
| 2:G:327:ILE:HG23 | 3:H:497:ARG:HG2 | 1.90 | 0.53 |
| 5:P:826:ILE:HG13 | 5:P:856:LEU:HD22 | 1.90 | 0.53 |
| 1:A:880:MET:O | 1:A:881:LYS:HG2 | 2.09 | 0.52 |
| 1:A:1805:PHE:HZ | 1:A:1869:LYS:HA | 1.73 | 0.52 |
| 1:A:2271:SER:HB3 | 1:A:2315:VAL:HG22 | 1.91 | 0.52 |
| 1:A:3930:VAL:HB | 1:A:3937:VAL:HG12 | 1.90 | 0.52 |
| 1:F:175:TYR:O | 1:F:227:LEU:HD12 | 2.08 | 0.52 |
| 1:F:2157:PHE:HB2 | 1:F:2160:TYR:HB3 | 1.92 | 0.52 |
| 1:F:3428:GLU:OE1 | 1:F:3474:ARG:NH2 | 2.42 | 0.52 |
| 1:F:4115:ASN:O | 1:F:4119:ARG:N | 2.40 | 0.52 |
| 1:A:4055:ASN:HD22 | 1:A:4058:VAL:HG23 | 1.74 | 0.52 |
| 2:B:357:LYS:HE2 | 2:B:359:HIS:CE1 | 2.43 | 0.52 |
| 3:C:529:PRO:HA | 3:C:532:LYS:HG2 | 1.91 | 0.52 |
| 1:F:440:VAL:HG21 | 1:F:485:GLN:HG3 | 1.91 | 0.52 |
| 1:F:1058:SER:HA | 1:F:1061:LYS:HE2 | 1.92 | 0.52 |
| 1:F:1082:PHE:HA | 1:F:1085:ILE:HG12 | 1.91 | 0.52 |
| 1:F:1790:SER:HG | 1:F:1793:THR:HG1 | 1.55 | 0.52 |
| 1:F:3354:ASP:O | 1:F:3358:ARG:NH1 | 2.42 | 0.52 |
| 1:F:3364:GLY:HA3 | 1:F:3373:VAL:HA | 1.91 | 0.52 |
| 2:G:59:PRO:HA | 2:G:62:MET:SD | 2.49 | 0.52 |
| 2:G:203:MET:HE1 | 2:G:237:SER:HB2 | 1.91 | 0.52 |
| 4:L:4:LYS:HG3 | 4:L:74:LEU:HD22 | 1.92 | 0.52 |
| 5:P:737:PRO:O | 5:P:739:GLN:NE2 | 2.42 | 0.52 |
| 5:P:754:PHE:O | 5:P:758:TYR:N | 2.39 | 0.52 |
| 1:A:79:ARG:HE | 1:A:82:ARG:HD2 | 1.73 | 0.52 |
| 1:A:1086:TYR:CE1 | 1:A:1133:HIS:HB3 | 2.43 | 0.52 |
| 1:A:1590:THR:HG21 | 1:A:1641:THR:HG23 | 1.89 | 0.52 |
| 1:A:4108:MET:O | 1:A:4112:THR:OG1 | 2.25 | 0.52 |
| 2:B:414:VAL:HB | 2:B:433:GLN:HB2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1779:GLN:O | 1:F:1783:ARG:HG2 | 2.10 | 0.52 |
| 2:G:444:ARG:HH11 | 3:H:244:SER:HB2 | 1.74 | 0.52 |
| 7:D:23:DT:H2' | 7:D:24:DT:N3 | 2.24 | 0.52 |
| 1:A:4113:ASP:O | 1:A:4117:LEU:HG | 2.09 | 0.52 |
| 2:B:259:LEU:HD11 | 2:B:400:TYR:HE1 | 1.74 | 0.52 |
| 1:F:56:SER:HA | 1:F:59:PHE:HD2 | 1.74 | 0.52 |
| 1:F:1153:LEU:HD12 | 1:F:1154:PRO:HD2 | 1.92 | 0.52 |
| 1:F:1568:ASN:HD22 | 1:F:1603:GLN:HB2 | 1.74 | 0.52 |
| 1:F:3472:ILE:HA | 1:F:3479:THR:HG21 | 1.91 | 0.52 |
| 1:F:3493:TRP:CD1 | 1:F:3521:ILE:HG12 | 2.42 | 0.52 |
| 2:G:194:ARG:NH1 | 2:G:220:ILE:O | 2.43 | 0.52 |
| 2:G:474:ARG:HB3 | 2:G:477:SER:HB2 | 1.90 | 0.52 |
| 4:L:37:THR:HG22 | 4:L:39:GLY:H | 1.74 | 0.52 |
| 1:A:672:ILE:HG13 | 1:A:676:ASN:HD21 | 1.74 | 0.52 |
| 2:G:348:MET:HG2 | 2:G:398:CYS:HA | 1.90 | 0.52 |
| 5:M:659:PHE:HD2 | 5:M:685:PHE:HB3 | 1.73 | 0.52 |
| 1:A:450:SER:O | 1:A:454:GLN:HG3 | 2.10 | 0.52 |
| 1:A:1867:ILE:HD13 | 1:A:1936:ARG:HB3 | 1.92 | 0.52 |
| 1:A:2948:GLY:HA3 | 1:A:2954:GLN:HE21 | 1.73 | 0.52 |
| 3:C:327:ASP:O | 3:C:331:MET:HG3 | 2.10 | 0.52 |
| 1:F:639:ALA:HA | 1:F:642:PHE:HB3 | 1.91 | 0.52 |
| 2:G:419:GLU:OE1 | 2:G:428:THR:OG1 | 2.26 | 0.52 |
| 1:A:36:ARG:HD3 | 1:A:2426:HIS:HB2 | 1.90 | 0.52 |
| 1:A:1153:LEU:HD12 | 1:A:1154:PRO:HD2 | 1.90 | 0.52 |
| 2:B:85:VAL:HG22 | 2:B:106:GLN:HB3 | 1.92 | 0.52 |
| 1:F:891:ARG:NH1 | 1:F:956:PRO:O | 2.43 | 0.52 |
| 1:F:1348:LEU:O | 1:F:1352:SER:OG | 2.22 | 0.52 |
| 1:F:2312:TYR:CE2 | 1:F:2314:GLU:HB3 | 2.45 | 0.52 |
| 1:F:3011:LEU:HD22 | 1:F:3047:SER:HA | 1.91 | 0.52 |
| 1:F:3781:CYS:HB3 | 1:F:3786:LEU:HB2 | 1.92 | 0.52 |
| 1:A:314:SER:O | 1:A:317:GLU:HG3 | 2.10 | 0.52 |
| 1:A:1727:ARG:HD2 | 1:A:1772:HIS:HB2 | 1.91 | 0.52 |
| 1:A:3503:VAL:HG11 | 1:A:3532:PRO:HB3 | 1.92 | 0.52 |
| 1:A:3921:GLY:H | 1:A:3944:HIS:HB2 | 1.73 | 0.52 |
| 3:C:266:SER:N | 3:C:361:VAL:O | 2.41 | 0.52 |
| 1:F:2847:THR:OG1 | 1:F:2849:SER:O | 2.25 | 0.52 |
| 4:K:150:ARG:O | 4:K:153:ARG:HG3 | 2.10 | 0.52 |
| 4:O:69:GLU:HA | 4:O:72:LYS:HG2 | 1.91 | 0.52 |
| 1:A:1279:LEU:HD22 | 1:A:1356:TRP:HE1 | 1.74 | 0.52 |
| 1:A:3169:PRO:HG2 | 1:A:3179:TRP:CZ2 | 2.45 | 0.52 |
| 1:A:3771:MET:HA | 1:A:3774:ILE:HD12 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:92:LYS:HE2 | 2:B:135:MET:HA | 1.92 | 0.52 |
| 3:C:86:PRO:HA | 3:C:90:LEU:HD12 | 1.92 | 0.52 |
| 3:C:326:VAL:O | 3:C:330:GLN:HG2 | 2.10 | 0.52 |
| 1:F:1438:GLY:O | 1:F:1445:ARG:NH2 | 2.37 | 0.52 |
| 1:F:2201:THR:HG23 | 1:F:2203:THR:HG22 | 1.92 | 0.52 |
| 1:F:2753:ARG:O | 1:F:2757:ILE:HG12 | 2.10 | 0.52 |
| 8:I:24:DA:H5' | 8:I:25:DA:N7 | 2.25 | 0.52 |
| 1:F:98:GLN:NE2 | 1:F:98:GLN:O | 2.42 | 0.52 |
| 1:F:1268:ASN:ND2 | 1:F:1344:PHE:HA | 2.25 | 0.52 |
| 1:F:3575:LEU:HD13 | 1:F:3578:LEU:HD12 | 1.92 | 0.52 |
| 1:A:1016:GLY:O | 1:A:1026:ARG:HG2 | 2.10 | 0.51 |
| 1:A:1281:VAL:HG23 | 1:A:1282:LEU:HG | 1.91 | 0.51 |
| 1:A:1725:GLN:HG3 | 1:A:1728:GLU:H | 1.75 | 0.51 |
| 1:A:1957:ASN:HB2 | 1:A:2103:HIS:NE2 | 2.25 | 0.51 |
| 1:F:214:GLU:OE2 | 8:I:31:DA:N6 | 2.36 | 0.51 |
| 1:F:996:THR:HG23 | 1:F:1043:GLN:NE2 | 2.24 | 0.51 |
| 1:F:1367:HIS:HB2 | 1:F:1370:ARG:NH1 | 2.25 | 0.51 |
| 1:F:3305:SER:OG | 1:F:3308:ASP:OD1 | 2.28 | 0.51 |
| 2:G:515:ASN:O | 2:G:519:GLY:N | 2.42 | 0.51 |
| 1:A:708:VAL:HG22 | 1:A:740:ILE:HG13 | 1.92 | 0.51 |
| 1:A:1452:VAL:HA | 1:A:1517:LEU:HD11 | 1.91 | 0.51 |
| 1:F:72:SER:H | 1:F:82:ARG:NH2 | 2.08 | 0.51 |
| 1:F:860:GLY:HA3 | 1:F:3136:THR:HG21 | 1.91 | 0.51 |
| 1:F:3155:VAL:HG23 | 1:F:3159:ARG:HH12 | 1.75 | 0.51 |
| 2:G:484:GLN:O | 2:G:488:ARG:HG2 | 2.10 | 0.51 |
| 3:H:246:HIS:NE2 | 9:J:36:DG:OP1 | 2.42 | 0.51 |
| 3:H:633:MET:HA | 3:H:636:ILE:HG12 | 1.92 | 0.51 |
| 4:O:34:ILE:HD13 | 4:O:95:PHE:HE2 | 1.75 | 0.51 |
| 8:E:26:DA:C2 | 8:E:27:DC:H2' | 2.44 | 0.51 |
| 1:A:196:LEU:HB3 | 1:A:200:PHE:CZ | 2.45 | 0.51 |
| 1:A:1294:VAL:HA | 1:A:1297:PHE:CD2 | 2.45 | 0.51 |
| 1:A:1649:LEU:HA | 1:A:1652:ILE:HD12 | 1.93 | 0.51 |
| 1:A:1878:ASP:HB3 | 1:A:1947:CYS:HA | 1.92 | 0.51 |
| 1:A:2174:SER:OG | 1:A:2214:ARG:NH1 | 2.43 | 0.51 |
| 2:B:251:THR:O | 3:C:431:ARG:NH1 | 2.42 | 0.51 |
| 1:F:938:VAL:HG21 | 1:F:969:LEU:HD11 | 1.93 | 0.51 |
| 1:F:1010:LEU:HG | 1:F:1014:LEU:HD23 | 1.91 | 0.51 |
| 1:F:1958:GLU:HG2 | 1:F:1959:LEU:N | 2.25 | 0.51 |
| 1:F:3110:PHE:CD2 | 1:F:3135:LEU:HD11 | 2.45 | 0.51 |
| 1:F:3244:ASP:OD1 | 1:F:3247:ARG:NH2 | 2.32 | 0.51 |
| 2:G:407:PRO:HG3 | 3:H:486:ARG:HD3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:H:44:ARG:HH11 | 3:H:236:VAL:H | 1.57 | 0.51 |
| 4:N:165:CYS:HG | 4:O:162:PHE:HZ | 1.59 | 0.51 |
| 1:A:762:TYR:HD2 | 1:A:765:LEU:HD23 | 1.75 | 0.51 |
| 1:A:959:TYR:CE2 | 1:A:963:LYS:HD2 | 2.45 | 0.51 |
| 1:A:2834:GLN:HG3 | 1:A:2838:GLN:HE21 | 1.75 | 0.51 |
| 1:A:3269:ARG:CZ | 1:A:3272:TRP:HB2 | 2.41 | 0.51 |
| 1:A:3619:ASP:OD1 | 1:A:3619:ASP:N | 2.44 | 0.51 |
| 1:F:770:LEU:HD11 | 1:F:858:MET:HG2 | 1.92 | 0.51 |
| 1:F:982:GLN:HE21 | 1:F:2591:ILE:HG23 | 1.75 | 0.51 |
| 1:F:1069:HIS:NE2 | 1:F:3743:HIS:O | 2.44 | 0.51 |
| 1:F:1086:TYR:CE1 | 1:F:1133:HIS:HB3 | 2.45 | 0.51 |
| 2:G:444:ARG:NH2 | 3:H:241:GLU:OE1 | 2.40 | 0.51 |
| 3:H:357:MET:N | 3:H:357:MET:SD | 2.84 | 0.51 |
| 1:A:3263:HIS:HB2 | 1:A:3276:TRP:CE2 | 2.45 | 0.51 |
| 1:A:3965:ARG:HD3 | 1:A:3966:GLN:HE22 | 1.75 | 0.51 |
| 2:B:48:MET:HG3 | 2:B:128:GLN:HE21 | 1.76 | 0.51 |
| 2:B:146:VAL:HA | 2:B:149:VAL:HG12 | 1.93 | 0.51 |
| 2:B:255:ALA:O | 8:E:32:DA:N6 | 2.43 | 0.51 |
| 1:F:1372:LEU:O | 1:F:1376:LEU:HG | 2.11 | 0.51 |
| 1:F:3506:LEU:HD21 | 1:F:3554:PHE:HD2 | 1.76 | 0.51 |
| 1:F:4055:ASN:HB2 | 1:F:4095:GLU:HA | 1.92 | 0.51 |
| 1:F:4107:LEU:O | 1:F:4111:ALA:HB3 | 2.09 | 0.51 |
| 4:N:20:LEU:HD21 | 4:N:74:LEU:HD13 | 1.92 | 0.51 |
| 6:Q:210:PHE:HB2 | 6:R:140:MET:HG3 | 1.93 | 0.51 |
| 1:A:923:ASP:O | 1:A:926:THR:N | 2.44 | 0.51 |
| 2:B:407:PRO:HB3 | 3:C:486:ARG:HG3 | 1.92 | 0.51 |
| 1:F:542:ASP:OD1 | 1:F:543:SER:N | 2.42 | 0.51 |
| 1:F:1086:TYR:CD1 | 1:F:1133:HIS:HB3 | 2.46 | 0.51 |
| 1:F:2746:LYS:O | 1:F:2750:GLU:HG2 | 2.10 | 0.51 |
| 4:L:146:LYS:O | 4:L:149:GLU:HG3 | 2.10 | 0.51 |
| 5:P:812:MET:O | 5:P:850:ALA:HB3 | 2.11 | 0.51 |
| 1:A:1375:THR:HG22 | 1:A:1382:ILE:HD13 | 1.91 | 0.51 |
| 1:A:3295:GLU:O | 1:A:3299:THR:HG22 | 2.11 | 0.51 |
| 2:B:77:SER:HB2 | 2:B:249:LYS:HB3 | 1.92 | 0.51 |
| 1:F:2225:HIS:HB2 | 1:F:2231:PHE:HB2 | 1.93 | 0.51 |
| 1:F:3811:THR:HG23 | 1:F:3814:ASP:H | 1.76 | 0.51 |
| 1:F:3970:LEU:HG | 1:F:3971:MET:HG3 | 1.93 | 0.51 |
| 2:G:101:ASN:ND2 | 2:G:140:ASP:O | 2.43 | 0.51 |
| 3:H:7:LYS:HE2 | 3:H:128:GLU:HG3 | 1.92 | 0.51 |
| 7:D:33:DA:H5" | 7:D:33:DA:C8 | 2.46 | 0.51 |
| 1:A:250:ASN:OD1 | 1:A:254:LYS:NZ | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1611:GLN:HB2 | 1:A:1613:HIS:ND1 | 2.26 | 0.51 |
| 1:A:3500:SER:HA | 1:A:3503:VAL:HG12 | 1.93 | 0.51 |
| 1:A:3992:ARG:NH2 | 1:A:4100:GLU:HG3 | 2.25 | 0.51 |
| 2:B:396:ALA:HB3 | 2:B:413:LEU:HD21 | 1.92 | 0.51 |
| 1:F:1780:SER:HA | 1:F:1783:ARG:HG2 | 1.91 | 0.51 |
| 1:F:2410:GLU:O | 1:F:2414:GLN:NE2 | 2.44 | 0.51 |
| 4:O:150:ARG:NH2 | 4:O:154:ASP:OD2 | 2.44 | 0.51 |
| 6:Q:11:GLN:HG3 | 6:Q:28:PHE:HB2 | 1.92 | 0.51 |
| 7:D:31:DT:H2' | 7:D:32:DT:C2 | 2.45 | 0.51 |
| 1:A:1046:PRO:O | 1:A:1049:GLN:N | 2.43 | 0.51 |
| 1:A:3751:LEU:HD22 | 1:A:3803:ILE:HD11 | 1.92 | 0.51 |
| 1:F:125:ILE:HD12 | 1:F:125:ILE:H | 1.75 | 0.51 |
| 1:F:1746:PHE:HB3 | 1:F:1762:MET:SD | 2.50 | 0.51 |
| 1:F:2357:GLU:HA | 1:F:2360:PHE:HB3 | 1.93 | 0.51 |
| 1:F:2964:ASP:HB2 | 1:F:3252:PHE:HD2 | 1.76 | 0.51 |
| 1:F:4086:ASP:OD1 | 1:F:4087:HIS:N | 2.43 | 0.51 |
| 2:G:317:LYS:NZ | 2:G:330:GLU:OE1 | 2.43 | 0.51 |
| 4:O:67:VAL:HB | 4:O:71:ARG:HH12 | 1.76 | 0.51 |
| 6:Q:128:PRO:HB3 | 6:R:128:PRO:HA | 1.93 | 0.51 |
| 6:R:193:PHE:HD1 | 6:R:197:LYS:HG3 | 1.76 | 0.51 |
| 1:A:2963:SER:OG | 1:A:3250:ASN:O | 2.22 | 0.51 |
| 1:A:3796:MET:H | 1:A:3801:GLY:HA2 | 1.76 | 0.51 |
| 1:F:146:GLU:N | 1:F:146:GLU:OE1 | 2.44 | 0.51 |
| 1:F:1601:LEU:HB3 | 1:F:1655:ILE:HD11 | 1.93 | 0.51 |
| 2:G:355:LEU:HD11 | 3:H:475:ASP:HB2 | 1.92 | 0.51 |
| 4:K:187:LYS:NZ | 4:L:188:LYS:HG3 | 2.26 | 0.51 |
| 6:R:154:ALA:O | 6:R:158:HIS:ND1 | 2.44 | 0.51 |
| 1:A:425:ASP:OD1 | 1:A:425:ASP:N | 2.44 | 0.50 |
| 1:A:1071:ASN:OD1 | 1:A:1073:PHE:N | 2.43 | 0.50 |
| 1:A:1474:ASP:OD1 | 1:A:1474:ASP:N | 2.43 | 0.50 |
| 1:A:1560:TYR:OH | 1:A:1599:GLY:HA3 | 2.11 | 0.50 |
| 1:A:2151:ILE:HG12 | 1:A:2192:THR:HG21 | 1.93 | 0.50 |
| 1:F:2844:LEU:HB3 | 1:F:2875:ALA:HB1 | 1.93 | 0.50 |
| 1:F:2929:LEU:O | 1:F:2932:SER:OG | 2.22 | 0.50 |
| 1:A:440:VAL:HG21 | 1:A:485:GLN:HG3 | 1.94 | 0.50 |
| 1:A:1302:ALA:H | 1:A:1334:LYS:NZ | 2.07 | 0.50 |
| 1:A:1357:LYS:HG3 | 1:A:1361:LYS:HZ3 | 1.76 | 0.50 |
| 1:A:1369:MET:HA | 1:A:1372:LEU:HG | 1.93 | 0.50 |
| 1:A:2571:ASP:O | 1:A:2787:HIS:ND1 | 2.43 | 0.50 |
| 1:A:2833:THR:HG21 | 1:A:2867:ALA:HB1 | 1.91 | 0.50 |
| 1:A:2980:ASP:N | 1:A:2980:ASP:OD1 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3283:LEU:O | 1:A:3287:ARG:HG3 | 2.11 | 0.50 |
| 1:A:4006:VAL:HG11 | 1:A:4009:PRO:HB3 | 1.91 | 0.50 |
| 2:B:261:LEU:HA | 2:B:345:LEU:HB2 | 1.93 | 0.50 |
| 1:F:169:THR:OG1 | 9:J:22:DG:OP1 | 2.22 | 0.50 |
| 1:F:1164:CYS:SG | 1:F:1165:LEU:N | 2.84 | 0.50 |
| 2:G:500:PRO:HD3 | 5:P:707:ILE:HG12 | 1.94 | 0.50 |
| 6:Q:134:HIS:N | 6:R:42:GLN:HB2 | 2.23 | 0.50 |
| 1:A:879:MET:HG2 | 1:A:881:LYS:H | 1.75 | 0.50 |
| 1:A:1058:SER:HA | 1:A:1061:LYS:HE2 | 1.93 | 0.50 |
| 1:A:1261:LEU:HD11 | 1:A:1337:VAL:HA | 1.93 | 0.50 |
| 1:A:3138:ILE:HG22 | 1:A:3189:PHE:HZ | 1.75 | 0.50 |
| 1:A:3831:ASP:HB3 | 1:A:3832:PRO:HD3 | 1.94 | 0.50 |
| 3:C:157:CYS:SG | 3:C:158:ASP:N | 2.84 | 0.50 |
| 3:C:489:ARG:NH1 | 3:C:507:PRO:O | 2.45 | 0.50 |
| 1:F:483:VAL:HG21 | 1:F:567:GLU:HG3 | 1.93 | 0.50 |
| 1:F:2935:GLU:OE2 | 1:F:2938:VAL:N | 2.33 | 0.50 |
| 2:G:163:HIS:CE1 | 2:G:165:ARG:HB2 | 2.46 | 0.50 |
| 4:L:143:HIS:O | 4:L:146:LYS:HG3 | 2.11 | 0.50 |
| 1:A:433:PRO:HA | 1:A:436:GLU:HG2 | 1.93 | 0.50 |
| 1:A:1164:CYS:SG | 1:A:1165:LEU:N | 2.84 | 0.50 |
| 1:A:2353:GLN:HB3 | 1:A:2360:PHE:HB2 | 1.93 | 0.50 |
| 3:C:299:ASP:OD1 | 3:C:303:THR:OG1 | 2.24 | 0.50 |
| 1:F:189:MET:O | 1:F:193:ALA:N | 2.44 | 0.50 |
| 1:F:655:LEU:O | 1:F:659:ARG:HG2 | 2.11 | 0.50 |
| 1:F:1407:LYS:HA | 1:F:1412:LYS:HB3 | 1.93 | 0.50 |
| 1:F:1419:LEU:HG | 1:F:1467:ILE:HD13 | 1.93 | 0.50 |
| 4:N:161:ARG:HH22 | 5:P:837:ARG:HD2 | 1.75 | 0.50 |
| 7:D:15:DA:N6 | 8:E:43:DT:O4 | 2.44 | 0.50 |
| 1:A:237:SER:OG | 1:A:238:MET:N | 2.43 | 0.50 |
| 1:A:2161:ALA:HA | 1:A:2164:TRP:HB2 | 1.94 | 0.50 |
| 1:A:3702:PRO:HB2 | 1:A:3794:VAL:HG11 | 1.94 | 0.50 |
| 1:F:535:LEU:HD23 | 1:F:565:TYR:HD1 | 1.76 | 0.50 |
| 1:F:2921:LEU:O | 1:F:2925:GLU:HG3 | 2.12 | 0.50 |
| 1:F:3294:SER:O | 1:F:3298:LEU:HG | 2.12 | 0.50 |
| 3:H:654:ARG:HA | 3:H:657:ASN:HD21 | 1.75 | 0.50 |
| 4:N:144:LEU:HB3 | 4:O:144:LEU:HB3 | 1.93 | 0.50 |
| 1:A:2428:ASP:HB2 | 1:A:2431:ARG:HB2 | 1.93 | 0.50 |
| 3:C:509:GLN:OE1 | 3:C:511:HIS:ND1 | 2.39 | 0.50 |
| 1:F:19:LEU:HA | 1:F:34:LEU:HD22 | 1.94 | 0.50 |
| 1:F:1373:VAL:HG11 | 1:F:1422:LYS:HG3 | 1.94 | 0.50 |
| 1:F:1583:MET:HG3 | 1:F:1628:LYS:HB2 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1597:LEU:O | 1:F:1601:LEU:HG | 2.12 | 0.50 |
| 1:F:3191:SER:O | 1:F:3194:GLU:N | 2.44 | 0.50 |
| 2:G:364:PRO:HG3 | 3:H:357:MET:HA | 1.94 | 0.50 |
| 2:G:369:TYR:CD1 | 2:G:370:PRO:HD2 | 2.45 | 0.50 |
| 3:H:184:ARG:HG2 | 3:H:519:PRO:HB3 | 1.94 | 0.50 |
| 1:A:1357:LYS:HG3 | 1:A:1361:LYS:NZ | 2.27 | 0.50 |
| 1:A:2331:MET:HG2 | 1:A:2334:LYS:HG2 | 1.92 | 0.50 |
| 1:A:3998:LEU:O | 1:A:4001:THR:HG22 | 2.11 | 0.50 |
| 1:F:1238:GLN:HA | 1:F:1296:PHE:HZ | 1.77 | 0.50 |
| 1:F:1333:SER:O | 1:F:1337:VAL:HG23 | 2.12 | 0.50 |
| 1:F:3714:GLU:OE1 | 1:F:3714:GLU:N | 2.45 | 0.50 |
| 3:H:441:SER:O | 3:H:445:ALA:N | 2.45 | 0.50 |
| 5:M:843:LEU:HA | 5:M:846:ARG:HG2 | 1.92 | 0.50 |
| 4:N:161:ARG:CZ | 5:P:840:ILE:HG21 | 2.42 | 0.50 |
| 4:O:22:VAL:HG23 | 4:O:35:THR:H | 1.77 | 0.50 |
| 4:O:22:VAL:HA | 4:O:35:THR:HB | 1.94 | 0.50 |
| 1:A:406:ARG:HE | 1:A:409:GLN:NE2 | 2.09 | 0.50 |
| 1:A:1018:VAL:HG22 | 1:A:1074:LYS:HG2 | 1.94 | 0.50 |
| 1:A:2847:THR:OG1 | 1:A:2849:SER:O | 2.27 | 0.50 |
| 2:B:350:PHE:HB3 | 2:B:394:VAL:HG12 | 1.94 | 0.50 |
| 3:C:251:LEU:N | 3:C:259:ILE:O | 2.45 | 0.50 |
| 1:F:2101:VAL:HG13 | 1:F:2153:THR:HG22 | 1.93 | 0.50 |
| 6:R:107:ARG:HD3 | 6:R:109:ARG:HH21 | 1.77 | 0.50 |
| 1:A:92:PHE:CD1 | 1:A:96:MET:HG3 | 2.47 | 0.50 |
| 1:A:682:TYR:CZ | 1:A:700:LYS:HD3 | 2.46 | 0.50 |
| 1:A:1626:TRP:HZ2 | 1:A:1674:THR:HG21 | 1.76 | 0.50 |
| 2:B:510:LYS:HG2 | 2:B:513:ALA:HB3 | 1.94 | 0.50 |
| 1:F:908:ASP:HA | 1:F:911:LEU:HD23 | 1.92 | 0.50 |
| 1:F:1713:VAL:O | 1:F:1716:GLN:HG2 | 2.12 | 0.50 |
| 3:H:44:ARG:NH1 | 3:H:236:VAL:H | 2.10 | 0.50 |
| 3:H:250:ARG:NH1 | 3:H:260:ARG:HH21 | 2.10 | 0.50 |
| 4:N:141:ASN:HD21 | 4:O:140:LYS:HD3 | 1.77 | 0.50 |
| 4:O:33:VAL:HG22 | 4:O:47:VAL:H | 1.76 | 0.50 |
| 5:P:743:MET:HE2 | 5:P:743:MET:HA | 1.93 | 0.50 |
| 6:R:57:ARG:HA | 6:R:61:LEU:HB2 | 1.93 | 0.50 |
| 9:J:33:DA:H2" | 9:J:34:DT:C2 | 2.47 | 0.50 |
| 1:A:933:LEU:HD11 | 1:A:2794:LEU:HD23 | 1.93 | 0.49 |
| 1:A:2333:ARG:HH22 | 1:A:2371:PHE:HE1 | 1.60 | 0.49 |
| 1:A:2567:SER:HA | 1:A:2572:TYR:CD2 | 2.47 | 0.49 |
| 1:A:3085:GLU:OE1 | 1:A:3085:GLU:N | 2.38 | 0.49 |
| 1:A:3577:GLN:NE2 | 1:A:3629:ARG:HB3 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3588:TRP:CE2 | 1:A:3613:MET:HG2 | 2.47 | 0.49 |
| 1:F:76:ILE:HA | 1:F:79:ARG:HB2 | 1.93 | 0.49 |
| 1:F:1096:VAL:O | 1:F:1100:VAL:HG13 | 2.12 | 0.49 |
| 1:F:1211:VAL:HG13 | 1:F:1219:PHE:HZ | 1.77 | 0.49 |
| 1:F:1444:ASP:N | 1:F:1444:ASP:OD1 | 2.44 | 0.49 |
| 1:F:1691:GLN:O | 1:F:1694:THR:OG1 | 2.22 | 0.49 |
| 1:F:3034:PRO:O | 1:F:3038:GLU:N | 2.45 | 0.49 |
| 1:F:3930:VAL:HB | 1:F:3937:VAL:HG12 | 1.93 | 0.49 |
| 2:G:64:ILE:HD13 | 2:G:67:ILE:HD11 | 1.93 | 0.49 |
| 2:G:263:LEU:HD22 | 2:G:347:LEU:HD22 | 1.94 | 0.49 |
| 2:G:350:PHE:H | 3:H:463:LEU:HD13 | 1.77 | 0.49 |
| 4:L:145:GLN:HA | 4:L:148:ASN:HD21 | 1.77 | 0.49 |
| 4:O:193:SER:O | 4:O:197:LYS:HG2 | 2.11 | 0.49 |
| 8:I:40:DT:H2” | 8:I:41:DT:O4’ | 2.12 | 0.49 |
| 1:A:111:CYS:HB2 | 1:A:130:LEU:CD2 | 2.42 | 0.49 |
| 1:A:1102:GLU:O | 1:A:1106:ILE:HG12 | 2.12 | 0.49 |
| 1:F:1840:PHE:O | 1:F:1844:VAL:HG23 | 2.12 | 0.49 |
| 1:F:3643:HIS:HB3 | 1:F:3659:PHE:HE2 | 1.76 | 0.49 |
| 7:D:22:DG:H5” | 7:D:23:DT:H73 | 1.93 | 0.49 |
| 1:A:898:PHE:HB2 | 1:A:901:MET:O | 2.12 | 0.49 |
| 1:A:3369:ASP:HB3 | 1:A:3372:LYS:HG2 | 1.94 | 0.49 |
| 1:A:4120:THR:HG21 | 1:A:4126:PRO:HG3 | 1.94 | 0.49 |
| 1:F:4055:ASN:HD21 | 1:F:4057:ALA:HB3 | 1.77 | 0.49 |
| 2:G:469:LEU:HD11 | 2:G:514:MET:HB2 | 1.94 | 0.49 |
| 3:H:251:LEU:HB3 | 3:H:259:ILE:HB | 1.94 | 0.49 |
| 1:A:1565:GLU:OE2 | 1:A:1603:GLN:NE2 | 2.45 | 0.49 |
| 1:A:1603:GLN:HA | 1:A:1606:ARG:HH21 | 1.77 | 0.49 |
| 1:A:3155:VAL:H | 1:A:3159:ARG:HH22 | 1.58 | 0.49 |
| 2:B:317:LYS:N | 3:C:279:VAL:O | 2.34 | 0.49 |
| 2:B:476:ASP:OD1 | 2:B:476:ASP:N | 2.46 | 0.49 |
| 1:F:584:GLU:HB2 | 1:F:613:HIS:HB3 | 1.94 | 0.49 |
| 1:F:1287:GLN:HG3 | 1:F:1289:SER:H | 1.77 | 0.49 |
| 1:F:1921:ASP:OD1 | 1:F:1922:ALA:N | 2.45 | 0.49 |
| 1:F:1934:LEU:HD13 | 1:F:1937:ARG:HH21 | 1.77 | 0.49 |
| 1:F:3658:ASP:OD1 | 1:F:3658:ASP:N | 2.43 | 0.49 |
| 5:P:748:PRO:HA | 5:P:751:LYS:HD2 | 1.95 | 0.49 |
| 6:Q:133:GLN:N | 6:R:43:GLN:H | 2.11 | 0.49 |
| 8:E:40:DT:H4’ | 8:E:41:DT:OP1 | 2.11 | 0.49 |
| 1:A:305:ASN:O | 1:A:308:LEU:N | 2.45 | 0.49 |
| 1:A:1333:SER:O | 1:A:1337:VAL:HG23 | 2.13 | 0.49 |
| 1:A:1921:ASP:OD1 | 1:A:1922:ALA:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:80:ARG:HH22 | 7:D:24:DT:H4' | 1.78 | 0.49 |
| 2:B:173:ASP:HB2 | 2:B:214:SER:N | 2.27 | 0.49 |
| 1:F:1448:LEU:HD11 | 1:F:1514:LEU:HD21 | 1.94 | 0.49 |
| 1:F:1465:HIS:HD2 | 1:F:1468:LEU:HD23 | 1.77 | 0.49 |
| 1:F:1715:GLU:HA | 1:F:1718:ILE:HG12 | 1.94 | 0.49 |
| 3:H:466:LYS:HD2 | 3:H:473:LEU:H | 1.77 | 0.49 |
| 1:A:767:GLU:OE2 | 1:A:771:ASN:ND2 | 2.32 | 0.49 |
| 1:A:3050:LYS:HZ1 | 1:A:3181:ASP:HA | 1.78 | 0.49 |
| 2:B:145:GLU:OE1 | 2:B:145:GLU:N | 2.46 | 0.49 |
| 1:F:73:LEU:O | 1:F:79:ARG:NH2 | 2.45 | 0.49 |
| 1:F:1019:ASP:N | 1:F:1019:ASP:OD1 | 2.46 | 0.49 |
| 1:F:3002:TYR:CD1 | 1:F:3010:SER:HB2 | 2.47 | 0.49 |
| 3:H:81:ARG:HB3 | 3:H:84:MET:SD | 2.52 | 0.49 |
| 3:H:489:ARG:O | 3:H:492:GLN:HG3 | 2.12 | 0.49 |
| 4:L:137:ASN:O | 4:L:141:ASN:ND2 | 2.45 | 0.49 |
| 1:A:1663:THR:HG22 | 1:A:1664:SER:H | 1.77 | 0.49 |
| 1:A:2188:GLU:HG2 | 1:A:2729:ARG:HH12 | 1.77 | 0.49 |
| 1:A:3998:LEU:O | 1:A:4001:THR:N | 2.42 | 0.49 |
| 1:F:3665:MET:HA | 1:F:3668:LEU:HG | 1.94 | 0.49 |
| 1:F:3855:TYR:OH | 1:F:4120:THR:O | 2.30 | 0.49 |
| 4:N:5:ILE:HD11 | 4:N:126:LEU:HD11 | 1.93 | 0.49 |
| 6:Q:15:TRP:HE1 | 6:Q:22:SER:HA | 1.78 | 0.49 |
| 1:A:24:ARG:HH21 | 1:A:70:ARG:HH21 | 1.59 | 0.49 |
| 1:A:1489:LYS:HD2 | 1:A:1492:ALA:HB3 | 1.94 | 0.49 |
| 1:A:3301:LEU:HB3 | 1:A:3304:VAL:HA | 1.94 | 0.49 |
| 1:A:3630:ARG:O | 1:A:3634:GLN:NE2 | 2.40 | 0.49 |
| 3:C:64:THR:HG22 | 3:C:66:ASN:H | 1.78 | 0.49 |
| 1:F:50:VAL:O | 1:F:54:GLN:NE2 | 2.45 | 0.49 |
| 1:F:2138:VAL:HG13 | 1:F:2143:ARG:HE | 1.76 | 0.49 |
| 1:F:3577:GLN:HB3 | 1:F:3683:CYS:SG | 2.53 | 0.49 |
| 1:F:3717:VAL:HA | 1:F:3743:HIS:CE1 | 2.48 | 0.49 |
| 3:H:280:ASP:HB3 | 3:H:283:THR:HG22 | 1.94 | 0.49 |
| 4:L:155:TRP:O | 4:L:159:GLN:HG2 | 2.12 | 0.49 |
| 6:R:50:ASP:OD1 | 6:R:51:THR:N | 2.45 | 0.49 |
| 8:E:28:DT:H6 | 8:E:28:DT:H5" | 1.76 | 0.49 |
| 1:A:716:VAL:HG11 | 1:A:1120:SER:HB2 | 1.94 | 0.49 |
| 1:A:1715:GLU:HA | 1:A:1718:ILE:HG12 | 1.95 | 0.49 |
| 1:A:2301:GLN:HA | 1:A:2304:VAL:HG22 | 1.95 | 0.49 |
| 1:A:2402:LEU:HD12 | 1:A:2438:ILE:HG13 | 1.95 | 0.49 |
| 1:A:3549:HIS:ND1 | 1:A:3553:GLU:OE1 | 2.43 | 0.49 |
| 1:A:3689:ASP:CG | 1:A:3690:PHE:H | 2.16 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:86:VAL:HG22 | 2:B:104:VAL:HG22 | 1.95 | 0.49 |
| 2:B:125:GLN:HG3 | 2:B:129:LYS:HZ1 | 1.77 | 0.49 |
| 1:F:2373:PRO:HA | 1:F:2404:ARG:HH12 | 1.77 | 0.49 |
| 2:G:428:THR:OG1 | 3:H:354:ARG:NH1 | 2.46 | 0.49 |
| 3:H:411:HIS:N | 3:H:418:CYS:O | 2.45 | 0.49 |
| 5:M:668:SER:OG | 5:M:669:GLY:N | 2.46 | 0.49 |
| 1:A:1435:ASN:ND2 | 1:A:1440:ASP:OD2 | 2.46 | 0.49 |
| 2:B:45:SER:HA | 2:B:138:GLY:H | 1.77 | 0.49 |
| 1:F:3169:PRO:HG2 | 1:F:3179:TRP:CH2 | 2.48 | 0.49 |
| 1:F:3266:SER:HA | 1:F:3272:TRP:CD1 | 2.48 | 0.49 |
| 2:G:278:GLN:OE1 | 3:H:431:ARG:NH2 | 2.46 | 0.49 |
| 2:G:318:ARG:HE | 3:H:278:VAL:HG22 | 1.78 | 0.49 |
| 3:H:153:SER:HA | 3:H:156:LYS:HG2 | 1.95 | 0.49 |
| 3:H:413:LYS:NZ | 3:H:416:TYR:O | 2.34 | 0.49 |
| 5:M:654:LYS:N | 5:M:684:GLU:O | 2.46 | 0.49 |
| 4:N:30:SER:OG | 4:N:31:GLY:N | 2.46 | 0.49 |
| 7:D:22:DG:C8 | 7:D:23:DT:H72 | 2.48 | 0.49 |
| 1:A:1298:LEU:HG | 1:A:1367:HIS:CD2 | 2.48 | 0.48 |
| 1:A:1407:LYS:HA | 1:A:1412:LYS:HB3 | 1.95 | 0.48 |
| 1:A:1778:PHE:O | 1:A:1781:SER:OG | 2.25 | 0.48 |
| 1:A:3622:ALA:HB2 | 1:A:3633:ILE:HD11 | 1.93 | 0.48 |
| 2:B:141:TYR:HE2 | 2:B:176:HIS:HD1 | 1.59 | 0.48 |
| 2:B:459:VAL:HA | 2:B:462:MET:SD | 2.53 | 0.48 |
| 3:C:418:CYS:SG | 3:C:419:LEU:N | 2.86 | 0.48 |
| 1:F:430:VAL:HG21 | 1:F:1643:MET:HB3 | 1.94 | 0.48 |
| 1:F:2155:GLU:HA | 1:F:2158:ARG:HG2 | 1.95 | 0.48 |
| 2:G:411:VAL:HG22 | 2:G:436:PHE:HA | 1.94 | 0.48 |
| 3:H:234:LEU:HB3 | 3:H:237:PHE:HB3 | 1.95 | 0.48 |
| 8:I:30:DA:H3' | 8:I:32:DA:H61 | 1.78 | 0.48 |
| 1:A:417:VAL:HA | 1:A:420:VAL:HG12 | 1.94 | 0.48 |
| 1:A:1371:VAL:O | 1:A:1375:THR:HG23 | 2.13 | 0.48 |
| 1:A:2817:LEU:HD23 | 1:A:2865:HIS:CE1 | 2.47 | 0.48 |
| 1:A:3387:GLU:O | 1:A:3390:GLN:HG2 | 2.13 | 0.48 |
| 1:A:3515:GLN:HB3 | 1:A:3554:PHE:CE2 | 2.48 | 0.48 |
| 1:A:3547:THR:HA | 1:A:3550:LYS:HD3 | 1.95 | 0.48 |
| 1:A:3981:TYR:OH | 1:A:4101:GLU:HB2 | 2.13 | 0.48 |
| 2:B:319:SER:N | 3:C:277:THR:O | 2.45 | 0.48 |
| 2:B:351:LYS:O | 2:B:395:ALA:N | 2.46 | 0.48 |
| 3:C:523:THR:O | 3:C:527:GLN:HG2 | 2.12 | 0.48 |
| 1:F:111:CYS:O | 1:F:130:LEU:HD11 | 2.13 | 0.48 |
| 1:F:1196:PRO:HA | 1:F:1202:ARG:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2133:LEU:HD11 | 1:F:2171:LEU:HD13 | 1.94 | 0.48 |
| 1:F:2481:HIS:NE2 | 1:F:2530:ARG:HG2 | 2.27 | 0.48 |
| 1:F:3097:ASP:N | 1:F:3097:ASP:OD1 | 2.45 | 0.48 |
| 1:F:3269:ARG:HG3 | 1:F:3272:TRP:H | 1.77 | 0.48 |
| 1:F:3533:PHE:O | 1:F:3537:SER:N | 2.46 | 0.48 |
| 1:F:3888:VAL:HA | 1:F:3891:SER:HB3 | 1.95 | 0.48 |
| 3:H:319:ASP:OD1 | 3:H:320:ILE:N | 2.43 | 0.48 |
| 3:H:450:GLN:HA | 3:H:537:PHE:HZ | 1.78 | 0.48 |
| 1:A:1058:SER:O | 1:A:1062:ARG:HG2 | 2.13 | 0.48 |
| 1:A:2349:LEU:HB3 | 1:A:2360:PHE:HE1 | 1.77 | 0.48 |
| 1:A:3625:LEU:HB2 | 1:A:3682:GLU:O | 2.13 | 0.48 |
| 1:A:3739:ILE:HA | 1:A:3749:PRO:HA | 1.96 | 0.48 |
| 2:B:299:LYS:HD3 | 3:C:296:CYS:HB2 | 1.94 | 0.48 |
| 1:F:359:LEU:O | 1:F:363:ILE:HG12 | 2.13 | 0.48 |
| 1:F:840:LEU:HD23 | 1:F:840:LEU:H | 1.78 | 0.48 |
| 1:F:2348:GLN:OE1 | 1:F:2352:HIS:NE2 | 2.46 | 0.48 |
| 1:F:3326:GLN:NE2 | 1:F:3326:GLN:O | 2.46 | 0.48 |
| 3:H:233:LYS:HE3 | 3:H:512:ILE:HD12 | 1.95 | 0.48 |
| 4:L:147:GLU:O | 4:L:150:ARG:HD3 | 2.13 | 0.48 |
| 6:Q:57:ARG:HB3 | 6:Q:119:TRP:HH2 | 1.77 | 0.48 |
| 1:A:143:LEU:N | 1:A:146:GLU:OE2 | 2.46 | 0.48 |
| 1:A:848:LEU:HD11 | 1:A:922:SER:HB2 | 1.95 | 0.48 |
| 1:A:1115:HIS:HA | 1:A:1119:LYS:HD3 | 1.95 | 0.48 |
| 1:A:1528:LEU:HD23 | 1:A:1531:LEU:HD12 | 1.96 | 0.48 |
| 1:A:3072:GLU:OE1 | 1:A:3072:GLU:N | 2.44 | 0.48 |
| 1:A:3443:PRO:HA | 1:A:3446:VAL:HG22 | 1.94 | 0.48 |
| 1:A:3927:ASN:O | 1:A:3940:ILE:N | 2.36 | 0.48 |
| 1:F:1354:GLU:HB3 | 1:F:1357:LYS:HD3 | 1.94 | 0.48 |
| 1:F:1881:TYR:CE1 | 1:F:1951:VAL:HA | 2.48 | 0.48 |
| 1:F:3358:ARG:H | 1:F:3358:ARG:HD2 | 1.78 | 0.48 |
| 2:G:262:LYS:HG3 | 2:G:346:MET:HA | 1.96 | 0.48 |
| 2:G:278:GLN:NE2 | 3:H:433:TYR:OH | 2.36 | 0.48 |
| 3:H:484:ASN:HD21 | 3:H:486:ARG:HB3 | 1.76 | 0.48 |
| 3:H:595:ALA:HA | 3:H:598:PHE:CE2 | 2.48 | 0.48 |
| 3:H:605:LYS:HB2 | 3:H:609:PHE:CZ | 2.43 | 0.48 |
| 4:N:155:TRP:HZ3 | 4:O:150:ARG:HH22 | 1.62 | 0.48 |
| 5:P:659:PHE:HB2 | 5:P:685:PHE:O | 2.13 | 0.48 |
| 1:F:175:TYR:HB2 | 1:F:223:CYS:HB3 | 1.94 | 0.48 |
| 1:F:417:VAL:HA | 1:F:420:VAL:HG12 | 1.96 | 0.48 |
| 1:F:2241:LEU:HA | 1:F:2244:CYS:SG | 2.53 | 0.48 |
| 1:F:3007:GLU:O | 1:F:3011:LEU:HG | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:39:ILE:HD11 | 2:G:108:LEU:HD21 | 1.96 | 0.48 |
| 3:H:209:LYS:O | 3:H:213:ILE:HG23 | 2.14 | 0.48 |
| 1:A:460:ALA:O | 1:A:464:VAL:HG13 | 2.14 | 0.48 |
| 1:A:729:CYS:O | 1:A:733:LEU:HD23 | 2.14 | 0.48 |
| 1:A:741:ILE:HA | 1:A:748:TYR:HE2 | 1.79 | 0.48 |
| 1:A:768:VAL:HA | 1:A:771:ASN:HD22 | 1.79 | 0.48 |
| 1:A:2215:LEU:HD23 | 1:A:2219:LEU:HD23 | 1.96 | 0.48 |
| 1:A:3527:GLN:HB2 | 1:A:3705:TYR:CE2 | 2.49 | 0.48 |
| 1:A:3815:LEU:O | 1:A:3819:THR:HG23 | 2.14 | 0.48 |
| 1:A:3930:VAL:HA | 1:A:3937:VAL:HA | 1.95 | 0.48 |
| 2:B:325:ARG:HH12 | 3:C:89:ASP:HB3 | 1.77 | 0.48 |
| 3:C:253:ILE:HG23 | 3:C:342:VAL:HG11 | 1.95 | 0.48 |
| 3:C:363:LYS:HB2 | 3:C:418:CYS:SG | 2.54 | 0.48 |
| 1:F:900:GLU:OE1 | 1:F:900:GLU:N | 2.46 | 0.48 |
| 1:F:2362:VAL:O | 1:F:2366:LYS:HG2 | 2.13 | 0.48 |
| 1:F:2522:ARG:HH22 | 1:F:2564:GLU:HG3 | 1.78 | 0.48 |
| 3:H:531:SER:HA | 3:H:534:LYS:HG2 | 1.96 | 0.48 |
| 4:K:175:ASP:OD1 | 4:K:176:LEU:N | 2.47 | 0.48 |
| 5:M:665:CYS:HB2 | 5:M:697:THR:HG21 | 1.95 | 0.48 |
| 5:P:842:ALA:HA | 5:P:845:LEU:HD12 | 1.94 | 0.48 |
| 1:A:217:LEU:HD23 | 1:A:218:PRO:HD3 | 1.95 | 0.48 |
| 1:A:1444:ASP:HA | 1:A:1447:ARG:HH21 | 1.79 | 0.48 |
| 1:A:1740:VAL:HA | 1:A:1743:MET:HG3 | 1.96 | 0.48 |
| 1:A:3301:LEU:HD23 | 1:A:3304:VAL:HA | 1.95 | 0.48 |
| 1:A:3825:LYS:O | 1:A:3829:LEU:HB2 | 2.14 | 0.48 |
| 2:B:429:PRO:HG2 | 3:C:435:PHE:HD2 | 1.79 | 0.48 |
| 1:F:573:LEU:HD22 | 1:F:649:PHE:HD1 | 1.78 | 0.48 |
| 1:F:758:LEU:HD13 | 1:F:976:VAL:HG21 | 1.96 | 0.48 |
| 1:F:898:PHE:HB2 | 1:F:901:MET:O | 2.14 | 0.48 |
| 1:F:1135:CYS:HB3 | 1:F:1190:LEU:HD11 | 1.95 | 0.48 |
| 1:F:1687:HIS:ND1 | 1:F:1741:ASP:OD2 | 2.46 | 0.48 |
| 1:F:3735:PRO:HB3 | 1:F:3751:LEU:HD21 | 1.95 | 0.48 |
| 1:F:3738:ILE:HD12 | 1:F:3740:ILE:HD11 | 1.96 | 0.48 |
| 1:F:3775:LEU:HD13 | 1:F:3786:LEU:HB3 | 1.96 | 0.48 |
| 3:H:300:ASP:OD1 | 3:H:300:ASP:N | 2.46 | 0.48 |
| 4:L:35:THR:HG22 | 4:L:44:THR:HG23 | 1.94 | 0.48 |
| 1:A:459:ARG:HG2 | 1:A:540:MET:HE2 | 1.96 | 0.48 |
| 1:A:1322:THR:O | 1:A:1326:GLU:N | 2.47 | 0.48 |
| 1:A:1697:PRO:HA | 1:A:1753:SER:HB3 | 1.96 | 0.48 |
| 1:A:3301:LEU:HB2 | 1:A:3333:THR:HG21 | 1.96 | 0.48 |
| 1:A:3700:GLU:HG3 | 1:A:3718:ARG:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:251:LEU:HB3 | 3:C:259:ILE:HG13 | 1.96 | 0.48 |
| 1:F:1803:GLU:HA | 1:F:1806:ARG:HH21 | 1.79 | 0.48 |
| 1:F:3050:LYS:NZ | 1:F:3180:ASP:OD1 | 2.36 | 0.48 |
| 2:G:386:LEU:HD13 | 2:G:430:PRO:HB2 | 1.94 | 0.48 |
| 4:K:7:ARG:HG2 | 4:L:131:LEU:HD13 | 1.95 | 0.48 |
| 1:A:13:LEU:HD21 | 1:A:3069:MET:HB3 | 1.95 | 0.48 |
| 1:A:458:CYS:HG | 1:A:533:HIS:CD2 | 2.32 | 0.48 |
| 1:A:1428:ILE:HA | 1:A:1431:LEU:HB2 | 1.96 | 0.48 |
| 1:A:3262:LEU:HD22 | 1:A:3272:TRP:HZ2 | 1.77 | 0.48 |
| 2:B:249:LYS:NZ | 2:B:250:GLU:O | 2.44 | 0.48 |
| 1:F:866:ILE:HG13 | 1:F:3168:TYR:CD2 | 2.46 | 0.48 |
| 1:F:1069:HIS:ND1 | 1:F:3743:HIS:HD2 | 2.11 | 0.48 |
| 8:E:28:DT:H1' | 8:E:29:DA:H5" | 1.96 | 0.48 |
| 8:I:34:DC:N4 | 9:J:23:DT:H3 | 2.11 | 0.48 |
| 1:A:94:GLU:CD | 1:A:95:LYS:H | 2.16 | 0.48 |
| 1:A:713:GLU:O | 1:A:717:LYS:HG2 | 2.14 | 0.48 |
| 1:A:902:LYS:HG2 | 1:F:2570:PRO:HB2 | 1.96 | 0.48 |
| 1:A:2745:ARG:HH21 | 8:E:45:DG:H2' | 1.78 | 0.48 |
| 1:A:3149:GLY:O | 1:A:3152:SER:OG | 2.31 | 0.48 |
| 2:B:80:ARG:NH2 | 7:D:25:DT:OP1 | 2.47 | 0.48 |
| 1:F:923:ASP:O | 1:F:926:THR:N | 2.47 | 0.48 |
| 1:F:1565:GLU:OE1 | 1:F:1606:ARG:NH1 | 2.47 | 0.48 |
| 1:F:1864:ASP:OD1 | 1:F:1864:ASP:N | 2.47 | 0.48 |
| 1:F:3509:ASP:N | 1:F:3509:ASP:OD1 | 2.46 | 0.48 |
| 3:H:342:VAL:HG12 | 3:H:344:GLY:H | 1.78 | 0.48 |
| 6:R:219:MET:O | 6:R:223:THR:OG1 | 2.31 | 0.48 |
| 9:J:37:DG:H1' | 9:J:38:DG:C2 | 2.48 | 0.48 |
| 1:A:2751:GLN:NE2 | 1:A:2752:LYS:HG2 | 2.29 | 0.47 |
| 1:A:4011:PHE:O | 1:A:4015:ASN:ND2 | 2.46 | 0.47 |
| 3:C:36:LYS:NZ | 3:C:231:LEU:HD11 | 2.29 | 0.47 |
| 1:F:74:ASN:HD21 | 1:F:122:LYS:HB2 | 1.78 | 0.47 |
| 1:F:1249:SER:OG | 1:F:1310:GLU:OE1 | 2.25 | 0.47 |
| 1:F:3679:ASN:HB3 | 1:F:3725:ARG:HA | 1.96 | 0.47 |
| 5:M:716:ASN:ND2 | 5:M:748:PRO:HD3 | 2.29 | 0.47 |
| 6:Q:133:GLN:H | 6:R:42:GLN:N | 2.04 | 0.47 |
| 7:D:15:DA:H2" | 7:D:16:DA:C8 | 2.49 | 0.47 |
| 8:I:27:DC:H2' | 9:J:30:DT:H1' | 1.94 | 0.47 |
| 1:A:734:LEU:HD11 | 1:A:768:VAL:HG13 | 1.96 | 0.47 |
| 1:A:2486:ASP:OD1 | 1:A:2486:ASP:N | 2.45 | 0.47 |
| 3:C:528:ILE:HG22 | 3:C:532:LYS:HZ1 | 1.79 | 0.47 |
| 1:F:144:MET:N | 1:F:146:GLU:OE1 | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:865:GLN:HB2 | 1:F:3168:TYR:CG | 2.49 | 0.47 |
| 1:F:894:PHE:O | 1:F:905:ILE:N | 2.31 | 0.47 |
| 1:F:994:TRP:CG | 1:F:2581:LEU:HD21 | 2.48 | 0.47 |
| 1:F:1725:GLN:NE2 | 1:F:1769:GLU:HG3 | 2.29 | 0.47 |
| 1:F:2428:ASP:O | 1:F:2432:GLN:HG2 | 2.14 | 0.47 |
| 1:F:3088:LEU:HD21 | 1:F:3138:ILE:HG21 | 1.96 | 0.47 |
| 7:D:28:DA:H2 | 8:E:30:DA:N1 | 2.12 | 0.47 |
| 9:J:25:DT:H2' | 9:J:26:DT:C4 | 2.49 | 0.47 |
| 1:A:736:LEU:HB3 | 1:A:740:ILE:HG21 | 1.96 | 0.47 |
| 1:A:4098:LEU:HD11 | 1:A:4103:GLN:HA | 1.96 | 0.47 |
| 2:B:333:GLU:O | 2:B:337:LEU:HG | 2.15 | 0.47 |
| 3:C:165:LEU:HD21 | 3:C:205:LEU:HD11 | 1.95 | 0.47 |
| 1:F:145:ASP:HA | 1:F:147:PHE:CE2 | 2.48 | 0.47 |
| 1:F:396:PHE:CE1 | 1:F:441:MET:HG3 | 2.47 | 0.47 |
| 1:F:425:ASP:OD1 | 1:F:425:ASP:N | 2.48 | 0.47 |
| 1:F:2322:VAL:HA | 1:F:2325:LEU:HD12 | 1.95 | 0.47 |
| 1:F:2335:ASN:ND2 | 1:F:2337:LEU:HD23 | 2.29 | 0.47 |
| 1:F:3669:LYS:HG3 | 1:F:3670:MET:SD | 2.54 | 0.47 |
| 1:F:3680:LEU:HD21 | 1:F:3688:SER:HA | 1.96 | 0.47 |
| 2:G:465:ILE:HG23 | 2:G:518:LEU:HD21 | 1.97 | 0.47 |
| 5:M:708:ARG:O | 5:M:712:ILE:HG12 | 2.14 | 0.47 |
| 1:A:369:PHE:O | 1:A:372:PRO:HD2 | 2.14 | 0.47 |
| 1:A:790:LYS:HA | 1:A:869:ASN:HB3 | 1.96 | 0.47 |
| 1:A:901:MET:N | 1:A:901:MET:SD | 2.87 | 0.47 |
| 1:A:908:ASP:OD1 | 1:A:908:ASP:N | 2.47 | 0.47 |
| 1:A:1099:PHE:CE1 | 1:A:1152:ARG:HD3 | 2.50 | 0.47 |
| 1:A:2548:PRO:HB2 | 1:A:2848:PHE:CD1 | 2.49 | 0.47 |
| 3:C:357:MET:HG2 | 3:C:425:PRO:HB3 | 1.96 | 0.47 |
| 1:F:92:PHE:O | 1:F:96:MET:HG2 | 2.15 | 0.47 |
| 1:F:1474:ASP:OD1 | 1:F:1474:ASP:N | 2.47 | 0.47 |
| 1:F:3569:GLN:HA | 1:F:3572:ILE:HD12 | 1.95 | 0.47 |
| 1:F:4054:ALA:H | 1:F:4103:GLN:NE2 | 2.12 | 0.47 |
| 4:L:134:ILE:HA | 4:L:137:ASN:HD21 | 1.79 | 0.47 |
| 1:A:1424:THR:HA | 1:A:1467:ILE:HD11 | 1.97 | 0.47 |
| 1:A:2205:VAL:HG13 | 1:A:2208:ASP:H | 1.79 | 0.47 |
| 1:A:3825:LYS:HA | 1:A:3829:LEU:HD23 | 1.96 | 0.47 |
| 1:F:168:ASP:H | 1:F:171:LEU:HD12 | 1.79 | 0.47 |
| 1:F:899:ARG:HD3 | 1:F:2568:MET:HB3 | 1.95 | 0.47 |
| 1:F:2938:VAL:O | 1:F:2942:ILE:HG12 | 2.15 | 0.47 |
| 1:F:3443:PRO:HA | 1:F:3446:VAL:HG22 | 1.97 | 0.47 |
| 2:G:166:ILE:O | 2:G:201:ASP:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:366:LEU:HB2 | 2:G:434:LEU:HD12 | 1.97 | 0.47 |
| 3:H:309:ASP:OD1 | 3:H:309:ASP:N | 2.46 | 0.47 |
| 4:O:107:ARG:NH1 | 4:O:108:LEU:O | 2.48 | 0.47 |
| 6:R:176:ARG:NH1 | 6:R:179:LEU:HD23 | 2.29 | 0.47 |
| 1:A:653:LEU:HD21 | 1:A:669:LEU:HB3 | 1.95 | 0.47 |
| 1:A:2584:CYS:HB2 | 1:A:2780:LEU:HD12 | 1.97 | 0.47 |
| 1:A:2866:ALA:HA | 1:A:2869:LEU:HG | 1.97 | 0.47 |
| 2:B:176:HIS:CE1 | 2:B:178:ASN:HD21 | 2.32 | 0.47 |
| 2:B:304:ASN:ND2 | 2:B:307:THR:HB | 2.30 | 0.47 |
| 1:F:3283:LEU:O | 1:F:3287:ARG:HG3 | 2.15 | 0.47 |
| 2:G:206:LYS:HG2 | 2:G:207:LYS:HG3 | 1.96 | 0.47 |
| 4:K:89:SER:OG | 4:K:94:TYR:O | 2.29 | 0.47 |
| 5:P:813:PHE:N | 5:P:850:ALA:H | 2.12 | 0.47 |
| 6:Q:136:ILE:O | 6:Q:140:MET:N | 2.38 | 0.47 |
| 1:A:1833:LEU:HG | 1:A:1836:LEU:HD23 | 1.96 | 0.47 |
| 1:A:4090:ARG:NH2 | 1:A:4109:ASP:OD2 | 2.47 | 0.47 |
| 2:B:100:LYS:HZ3 | 2:B:101:ASN:H | 1.62 | 0.47 |
| 2:B:398:CYS:SG | 2:B:399:ARG:N | 2.87 | 0.47 |
| 2:B:422:ASP:N | 2:B:422:ASP:OD1 | 2.44 | 0.47 |
| 2:B:468:LYS:HG3 | 2:B:518:LEU:HA | 1.95 | 0.47 |
| 3:C:283:THR:HB | 3:C:285:LYS:HE2 | 1.95 | 0.47 |
| 3:C:500:HIS:HB3 | 3:C:503:GLU:HB3 | 1.96 | 0.47 |
| 1:F:58:VAL:HG21 | 1:F:3098:ARG:HD2 | 1.96 | 0.47 |
| 1:F:196:LEU:HB3 | 1:F:200:PHE:CZ | 2.50 | 0.47 |
| 1:F:778:ILE:HD12 | 1:F:3161:LEU:HD11 | 1.97 | 0.47 |
| 1:F:868:LYS:NZ | 1:F:3170:ASP:OD1 | 2.48 | 0.47 |
| 1:F:1181:THR:OG1 | 1:F:1184:ARG:NH2 | 2.47 | 0.47 |
| 1:F:1504:ASP:O | 1:F:1508:LYS:N | 2.41 | 0.47 |
| 1:F:1575:LEU:HD11 | 1:F:1617:LYS:HD2 | 1.97 | 0.47 |
| 1:F:2147:ALA:HB2 | 1:F:2171:LEU:HD21 | 1.95 | 0.47 |
| 1:F:2312:TYR:HD2 | 1:F:2315:VAL:HG23 | 1.80 | 0.47 |
| 1:F:2511:ILE:HD11 | 1:F:2553:HIS:HB2 | 1.96 | 0.47 |
| 1:F:3151:LEU:HD22 | 1:F:3197:LEU:HB2 | 1.97 | 0.47 |
| 1:F:3455:LYS:HE2 | 1:F:3491:PRO:HG3 | 1.97 | 0.47 |
| 1:F:3720:ALA:HB3 | 1:F:3743:HIS:HA | 1.95 | 0.47 |
| 3:H:10:VAL:HG22 | 3:H:131:HIS:HB3 | 1.96 | 0.47 |
| 3:H:662:LEU:HA | 3:H:665:LYS:HG2 | 1.97 | 0.47 |
| 7:D:17:DT:H3 | 8:E:39:DA:H61 | 1.61 | 0.47 |
| 8:I:23:DT:H3' | 8:I:24:DA:C8 | 2.50 | 0.47 |
| 1:A:33:GLN:OE1 | 1:A:2422:GLN:NE2 | 2.39 | 0.47 |
| 1:A:359:LEU:O | 1:A:363:ILE:HG12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:784:VAL:O | 1:A:787:PRO:HD2 | 2.14 | 0.47 |
| 1:A:1722:PHE:HA | 1:A:1729:PHE:HZ | 1.79 | 0.47 |
| 1:A:2723:THR:HA | 1:A:2726:LEU:HD13 | 1.97 | 0.47 |
| 2:B:348:MET:N | 2:B:397:LEU:O | 2.45 | 0.47 |
| 1:F:122:LYS:HD2 | 1:F:122:LYS:HA | 1.79 | 0.47 |
| 1:F:1413:ASP:OD1 | 1:F:1414:ILE:N | 2.48 | 0.47 |
| 1:F:2349:LEU:HB3 | 1:F:2360:PHE:HE1 | 1.79 | 0.47 |
| 1:F:3930:VAL:HA | 1:F:3937:VAL:HA | 1.96 | 0.47 |
| 2:G:36:ASP:OD1 | 2:G:163:HIS:ND1 | 2.35 | 0.47 |
| 3:H:32:GLU:HA | 3:H:35:LYS:HZ3 | 1.79 | 0.47 |
| 5:P:666:VAL:HB | 5:P:689:ILE:HG23 | 1.97 | 0.47 |
| 1:A:50:VAL:HG13 | 1:A:51:LEU:HG | 1.97 | 0.47 |
| 1:A:1196:PRO:HA | 1:A:1202:ARG:O | 2.15 | 0.47 |
| 1:A:2750:GLU:O | 1:A:2754:GLU:HG2 | 2.15 | 0.47 |
| 1:A:3097:ASP:OD1 | 1:A:3098:ARG:N | 2.48 | 0.47 |
| 2:B:509:PRO:HD3 | 3:C:394:ARG:HD3 | 1.97 | 0.47 |
| 3:C:266:SER:HB3 | 3:C:361:VAL:HG12 | 1.95 | 0.47 |
| 1:F:40:GLN:CD | 1:F:2427:ARG:HB2 | 2.35 | 0.47 |
| 1:F:79:ARG:HH22 | 1:F:82:ARG:HD2 | 1.79 | 0.47 |
| 1:F:486:GLY:O | 1:F:490:ILE:HG12 | 2.15 | 0.47 |
| 1:F:1769:GLU:HB2 | 1:F:1772:HIS:CG | 2.49 | 0.47 |
| 1:F:1948:ALA:HA | 1:F:1951:VAL:HG22 | 1.95 | 0.47 |
| 1:F:2353:GLN:HA | 1:F:2356:MET:HG3 | 1.96 | 0.47 |
| 1:F:2584:CYS:HB2 | 1:F:2780:LEU:HD12 | 1.97 | 0.47 |
| 1:F:2821:ASP:N | 1:F:2821:ASP:OD1 | 2.48 | 0.47 |
| 1:F:3165:THR:HG21 | 1:F:3241:LYS:HE2 | 1.96 | 0.47 |
| 1:F:3619:ASP:N | 1:F:3619:ASP:OD1 | 2.48 | 0.47 |
| 3:H:413:LYS:HG2 | 3:H:416:TYR:H | 1.80 | 0.47 |
| 6:Q:135:LEU:N | 6:R:40:ASP:O | 2.47 | 0.47 |
| 6:Q:159:MET:HA | 6:Q:162:LEU:HD12 | 1.97 | 0.47 |
| 8:I:35:DT:C4 | 8:I:36:DA:C6 | 3.03 | 0.47 |
| 1:A:1479:VAL:HG11 | 1:A:1521:PHE:HD2 | 1.79 | 0.47 |
| 1:A:2548:PRO:HB2 | 1:A:2848:PHE:HD1 | 1.80 | 0.47 |
| 2:B:42:VAL:HG12 | 2:B:169:PHE:HB2 | 1.97 | 0.47 |
| 2:B:367:PHE:CE1 | 2:B:431:GLY:HA3 | 2.50 | 0.47 |
| 3:C:9:ALA:HB3 | 3:C:130:ARG:HG3 | 1.97 | 0.47 |
| 3:C:49:GLU:O | 3:C:51:LYS:NZ | 2.48 | 0.47 |
| 3:C:297:LEU:HD13 | 3:C:305:VAL:HG21 | 1.97 | 0.47 |
| 1:F:176:GLU:OE2 | 1:F:226:GLY:HA3 | 2.15 | 0.47 |
| 1:F:2405:VAL:HA | 1:F:2408:MET:HE1 | 1.97 | 0.47 |
| 1:F:3528:ALA:HB2 | 1:F:3705:TYR:HD2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3915:HIS:HB2 | 1:F:3920:ILE:HB | 1.96 | 0.47 |
| 4:K:94:TYR:CZ | 4:K:96:PHE:HB3 | 2.50 | 0.47 |
| 4:L:145:GLN:HA | 4:L:148:ASN:ND2 | 2.29 | 0.47 |
| 5:M:803:TYR:HB2 | 5:M:805:TRP:CE2 | 2.50 | 0.47 |
| 4:N:162:PHE:HD1 | 4:O:162:PHE:HD1 | 1.63 | 0.47 |
| 6:R:13:TRP:HB3 | 6:R:210:PHE:CZ | 2.49 | 0.47 |
| 1:A:865:GLN:HE22 | 1:A:3171:ALA:N | 2.12 | 0.46 |
| 1:A:1635:LYS:HD2 | 1:A:1635:LYS:HA | 1.76 | 0.46 |
| 1:A:3269:ARG:HG3 | 1:A:3272:TRP:H | 1.79 | 0.46 |
| 1:A:3480:LEU:HA | 1:A:3483:MET:HE3 | 1.97 | 0.46 |
| 3:C:250:ARG:HB3 | 3:C:338:LYS:NZ | 2.30 | 0.46 |
| 1:F:2492:ASP:O | 1:F:2496:GLN:HG3 | 2.15 | 0.46 |
| 1:F:2990:GLU:HG2 | 1:F:2994:TRP:CE2 | 2.50 | 0.46 |
| 1:F:3012:GLU:O | 1:F:3015:SER:OG | 2.22 | 0.46 |
| 2:G:413:LEU:HB3 | 2:G:432:PHE:CD1 | 2.50 | 0.46 |
| 4:N:150:ARG:O | 4:N:153:ARG:HD3 | 2.15 | 0.46 |
| 5:P:753:HIS:HA | 5:P:756:ARG:HE | 1.80 | 0.46 |
| 5:P:772:ASN:O | 5:P:776:GLU:HG2 | 2.14 | 0.46 |
| 9:J:24:DT:H2" | 9:J:25:DT:C6 | 2.50 | 0.46 |
| 1:A:38:LEU:CD2 | 1:A:85:ILE:HG13 | 2.45 | 0.46 |
| 1:A:2356:MET:HE1 | 1:A:2359:LYS:H | 1.79 | 0.46 |
| 1:A:3642:LYS:HG3 | 1:A:3643:HIS:ND1 | 2.30 | 0.46 |
| 2:B:38:LEU:HD13 | 2:B:165:ARG:HG3 | 1.96 | 0.46 |
| 2:B:125:GLN:NE2 | 2:B:128:GLN:OE1 | 2.45 | 0.46 |
| 2:B:240:GLU:O | 2:B:244:ARG:N | 2.39 | 0.46 |
| 3:C:251:LEU:HB2 | 3:C:261:ILE:HD13 | 1.96 | 0.46 |
| 1:F:1304:HIS:ND1 | 1:F:1307:ILE:O | 2.34 | 0.46 |
| 1:F:1504:ASP:HB3 | 1:F:1507:CYS:HB2 | 1.96 | 0.46 |
| 1:F:3505:LEU:HD12 | 1:F:3508:LYS:HD2 | 1.97 | 0.46 |
| 3:H:630:PRO:HA | 3:H:633:MET:HG3 | 1.97 | 0.46 |
| 5:P:816:HIS:C | 5:P:851:LYS:H | 2.18 | 0.46 |
| 1:A:1960:LYS:O | 1:A:1962:TYR:N | 2.49 | 0.46 |
| 1:A:2732:PHE:HA | 1:A:2734:ARG:NH1 | 2.31 | 0.46 |
| 1:A:3482:LEU:O | 1:A:3486:GLU:HG3 | 2.16 | 0.46 |
| 2:B:312:LEU:N | 2:B:315:ASP:OD2 | 2.39 | 0.46 |
| 1:F:32:HIS:O | 1:F:35:ILE:HG22 | 2.16 | 0.46 |
| 1:F:406:ARG:HG3 | 1:F:409:GLN:NE2 | 2.31 | 0.46 |
| 1:F:718:MET:HA | 1:F:721:TYR:CD2 | 2.50 | 0.46 |
| 1:F:1783:ARG:HH22 | 1:F:1830:HIS:HB2 | 1.79 | 0.46 |
| 1:F:1867:ILE:HD11 | 1:F:1940:TYR:HB2 | 1.97 | 0.46 |
| 1:F:2826:LEU:HA | 1:F:2829:LYS:HE2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3825:LYS:O | 1:F:3829:LEU:HB2 | 2.16 | 0.46 |
| 1:F:3923:ARG:HA | 1:F:3959:MET:CE | 2.46 | 0.46 |
| 2:G:416:GLN:N | 2:G:431:GLY:O | 2.43 | 0.46 |
| 3:H:364:VAL:HB | 3:H:419:LEU:HB2 | 1.97 | 0.46 |
| 4:O:58:ASP:OD1 | 4:O:58:ASP:N | 2.45 | 0.46 |
| 5:P:690:VAL:HG22 | 5:P:692:ASN:H | 1.79 | 0.46 |
| 1:A:639:ALA:HB2 | 1:A:676:ASN:HB3 | 1.97 | 0.46 |
| 1:A:1366:THR:O | 1:A:1369:MET:HG3 | 2.15 | 0.46 |
| 1:A:1558:TYR:CZ | 1:A:1562:LEU:HD11 | 2.51 | 0.46 |
| 1:A:1745:LYS:HA | 1:A:1748:ASP:OD2 | 2.16 | 0.46 |
| 1:A:2392:VAL:O | 1:A:2396:LEU:HG | 2.14 | 0.46 |
| 1:A:3182:ILE:O | 1:A:3186:ARG:HG2 | 2.15 | 0.46 |
| 1:F:196:LEU:HB3 | 1:F:200:PHE:CE2 | 2.50 | 0.46 |
| 1:F:1154:PRO:HD3 | 1:F:1163:LEU:HD11 | 1.98 | 0.46 |
| 1:F:3980:MET:SD | 1:F:3980:MET:N | 2.87 | 0.46 |
| 2:G:90:THR:HB | 2:G:101:ASN:CA | 2.46 | 0.46 |
| 2:G:244:ARG:HG2 | 2:G:246:VAL:HG13 | 1.98 | 0.46 |
| 2:G:262:LYS:NZ | 2:G:344:GLY:HA3 | 2.31 | 0.46 |
| 3:H:37:VAL:HG12 | 3:H:231:LEU:HD21 | 1.97 | 0.46 |
| 5:P:696:ASP:OD1 | 5:P:696:ASP:N | 2.48 | 0.46 |
| 1:A:787:PRO:O | 1:A:790:LYS:NZ | 2.29 | 0.46 |
| 1:A:1608:ARG:HH21 | 1:A:1612:LYS:NZ | 2.14 | 0.46 |
| 1:A:3158:LYS:HZ3 | 1:A:3186:ARG:NH1 | 2.13 | 0.46 |
| 1:A:3455:LYS:O | 1:A:3455:LYS:NZ | 2.33 | 0.46 |
| 1:A:3835:PRO:HG2 | 1:A:3836:PRO:HD3 | 1.97 | 0.46 |
| 3:C:135:PHE:HD1 | 3:C:227:PHE:CE1 | 2.33 | 0.46 |
| 3:C:147:LEU:HD11 | 3:C:211:VAL:HG21 | 1.96 | 0.46 |
| 3:C:316:TYR:N | 3:C:319:ASP:O | 2.48 | 0.46 |
| 1:F:982:GLN:NE2 | 1:F:2591:ILE:HG23 | 2.30 | 0.46 |
| 1:F:1158:PRO:HG2 | 1:F:1159:PRO:HD3 | 1.96 | 0.46 |
| 1:F:1420:ARG:NE | 1:F:1466:ASN:O | 2.49 | 0.46 |
| 1:F:2731:ARG:O | 1:F:2734:ARG:NH2 | 2.49 | 0.46 |
| 1:F:3267:LYS:H | 1:F:3267:LYS:HG2 | 1.58 | 0.46 |
| 1:A:24:ARG:NH2 | 1:A:70:ARG:HH21 | 2.13 | 0.46 |
| 1:A:32:HIS:O | 1:A:35:ILE:HG22 | 2.16 | 0.46 |
| 1:A:475:LEU:HD22 | 1:A:476:ARG:HD3 | 1.98 | 0.46 |
| 1:A:1101:PHE:HD2 | 1:A:1163:LEU:HD13 | 1.81 | 0.46 |
| 1:A:1663:THR:HG22 | 1:A:1664:SER:N | 2.30 | 0.46 |
| 1:A:3146:SER:C | 1:A:3147:LYS:HD2 | 2.36 | 0.46 |
| 3:C:148:ASP:OD1 | 3:C:148:ASP:N | 2.49 | 0.46 |
| 3:C:297:LEU:HB3 | 3:C:303:THR:OG1 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1148:ALA:HB2 | 1:F:1164:CYS:HB2 | 1.98 | 0.46 |
| 1:F:2310:VAL:HA | 1:F:2316:TYR:CE2 | 2.51 | 0.46 |
| 2:G:367:PHE:CE2 | 2:G:369:TYR:HB2 | 2.51 | 0.46 |
| 6:Q:44:VAL:HG12 | 6:Q:130:LEU:HD11 | 1.98 | 0.46 |
| 1:A:63:PHE:CE2 | 1:A:85:ILE:HG12 | 2.51 | 0.46 |
| 1:A:342:MET:HE3 | 1:A:366:TYR:HE1 | 1.81 | 0.46 |
| 1:A:1086:TYR:CZ | 1:A:1133:HIS:HB3 | 2.51 | 0.46 |
| 1:A:1133:HIS:O | 1:A:1137:ILE:HG12 | 2.15 | 0.46 |
| 1:A:1367:HIS:HB2 | 1:A:1370:ARG:HH12 | 1.79 | 0.46 |
| 1:A:2478:MET:HG2 | 1:A:2524:PHE:CE1 | 2.50 | 0.46 |
| 1:A:3265:GLU:O | 1:A:3268:THR:OG1 | 2.26 | 0.46 |
| 2:B:290:ARG:HH11 | 5:M:690:VAL:HG21 | 1.81 | 0.46 |
| 1:F:3483:MET:HE3 | 1:F:3513:ALA:H | 1.80 | 0.46 |
| 2:G:85:VAL:HG22 | 2:G:106:GLN:HB3 | 1.96 | 0.46 |
| 2:G:362:LEU:HG | 2:G:438:PRO:HG3 | 1.98 | 0.46 |
| 3:H:40:MET:HA | 3:H:43:GLN:HG3 | 1.96 | 0.46 |
| 1:A:1251:GLN:OE1 | 1:A:1251:GLN:N | 2.39 | 0.46 |
| 1:A:1287:GLN:HB3 | 1:A:1290:LEU:HD12 | 1.97 | 0.46 |
| 1:A:1801:VAL:HA | 1:A:1804:MET:HG2 | 1.98 | 0.46 |
| 1:A:3296:GLN:HG3 | 1:A:3337:ILE:HD11 | 1.97 | 0.46 |
| 2:B:89:GLY:HA2 | 2:B:101:ASN:HB3 | 1.98 | 0.46 |
| 2:B:416:GLN:N | 2:B:431:GLY:O | 2.38 | 0.46 |
| 2:B:481:PRO:HG2 | 3:C:403:PRO:HG2 | 1.98 | 0.46 |
| 3:C:265:LYS:NZ | 8:E:23:DT:H5' | 2.31 | 0.46 |
| 3:C:277:THR:HG22 | 3:C:286:LYS:HZ2 | 1.81 | 0.46 |
| 3:C:465:LYS:N | 3:C:474:GLU:O | 2.48 | 0.46 |
| 1:F:75:SER:HB2 | 1:F:77:GLU:HG2 | 1.98 | 0.46 |
| 1:F:2246:LYS:H | 1:F:2249:LEU:HD11 | 1.81 | 0.46 |
| 1:F:2382:VAL:HA | 1:F:2385:LEU:HG | 1.98 | 0.46 |
| 1:F:3008:TRP:HA | 1:F:3011:LEU:HD12 | 1.98 | 0.46 |
| 1:F:3369:ASP:OD1 | 1:F:3370:SER:N | 2.49 | 0.46 |
| 1:F:3499:ILE:HA | 1:F:3502:MET:SD | 2.56 | 0.46 |
| 5:P:811:SER:CB | 5:P:849:GLY:HA3 | 2.37 | 0.46 |
| 8:E:34:DC:H5 | 8:E:35:DT:C2 | 2.32 | 0.46 |
| 1:A:849:GLU:OE1 | 1:A:849:GLU:N | 2.40 | 0.46 |
| 1:A:901:MET:HB2 | 1:A:2819:GLU:HG2 | 1.98 | 0.46 |
| 1:A:3959:MET:HG3 | 1:A:4124:TRP:NE1 | 2.31 | 0.46 |
| 2:B:60:PHE:O | 2:B:63:SER:OG | 2.26 | 0.46 |
| 1:F:935:HIS:CD2 | 1:F:2775:TYR:HE1 | 2.34 | 0.46 |
| 1:F:1046:PRO:HA | 1:F:1049:GLN:HE21 | 1.81 | 0.46 |
| 1:F:1342:MET:O | 1:F:1346:THR:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1580:LEU:HD13 | 1:F:1625:HIS:CD2 | 2.50 | 0.46 |
| 1:F:3583:LEU:HA | 1:F:3586:LYS:HE2 | 1.97 | 0.46 |
| 2:G:419:GLU:N | 2:G:426:GLN:HE22 | 2.13 | 0.46 |
| 3:H:51:LYS:HB3 | 3:H:125:LYS:NZ | 2.31 | 0.46 |
| 4:K:130:CYS:SG | 4:K:131:LEU:N | 2.89 | 0.46 |
| 1:A:163:LYS:NZ | 3:C:291:LYS:HD3 | 2.31 | 0.46 |
| 1:A:459:ARG:HG2 | 1:A:540:MET:CE | 2.46 | 0.46 |
| 1:A:3107:ILE:O | 1:A:3111:MET:HG2 | 2.15 | 0.46 |
| 1:A:3704:GLN:HE22 | 1:A:3717:VAL:HG13 | 1.80 | 0.46 |
| 3:C:242:ARG:HE | 3:C:243:HIS:H | 1.64 | 0.46 |
| 1:F:1048:GLN:HA | 1:F:1051:LYS:HZ2 | 1.81 | 0.46 |
| 1:F:1608:ARG:HE | 1:F:1612:LYS:NZ | 2.14 | 0.46 |
| 1:F:2161:ALA:HA | 1:F:2164:TRP:HB2 | 1.96 | 0.46 |
| 1:F:2427:ARG:HH21 | 1:F:2465:PRO:HD2 | 1.81 | 0.46 |
| 1:F:2443:MET:HA | 1:F:2446:LEU:HB2 | 1.98 | 0.46 |
| 1:F:2510:LEU:O | 1:F:2518:GLN:NE2 | 2.42 | 0.46 |
| 1:F:4121:TRP:HB3 | 1:F:4124:TRP:HB2 | 1.97 | 0.46 |
| 4:N:137:ASN:HB3 | 4:O:137:ASN:HB3 | 1.97 | 0.46 |
| 6:Q:133:GLN:HB2 | 6:R:43:GLN:HB2 | 1.98 | 0.46 |
| 1:A:357:LYS:O | 1:A:361:ILE:HG12 | 2.16 | 0.45 |
| 1:A:1150:LYS:HA | 1:A:1150:LYS:HD2 | 1.79 | 0.45 |
| 1:A:1260:LEU:HD21 | 1:A:1293:ALA:HB1 | 1.97 | 0.45 |
| 1:A:2154:GLU:HA | 1:A:2157:PHE:CZ | 2.51 | 0.45 |
| 1:A:2589:TYR:HB2 | 1:A:2777:HIS:HB2 | 1.98 | 0.45 |
| 1:A:2921:LEU:O | 1:A:2925:GLU:HG3 | 2.16 | 0.45 |
| 1:A:3772:ASN:ND2 | 1:A:3788:LEU:O | 2.44 | 0.45 |
| 3:C:154:LEU:HA | 3:C:159:ILE:HB | 1.98 | 0.45 |
| 1:F:1048:GLN:OE1 | 1:F:1048:GLN:N | 2.49 | 0.45 |
| 2:G:291:GLU:HG3 | 5:P:690:VAL:HG23 | 1.98 | 0.45 |
| 6:R:4:LEU:O | 6:R:8:LEU:HB2 | 2.15 | 0.45 |
| 1:A:251:PHE:HE1 | 1:A:293:LEU:HD11 | 1.80 | 0.45 |
| 1:A:862:LEU:HD12 | 1:A:866:ILE:HG21 | 1.98 | 0.45 |
| 1:A:935:HIS:CE1 | 1:A:987:LEU:HD13 | 2.51 | 0.45 |
| 1:A:3509:ASP:N | 1:A:3509:ASP:OD1 | 2.44 | 0.45 |
| 1:A:3550:LYS:O | 1:A:3553:GLU:HG2 | 2.16 | 0.45 |
| 2:B:90:THR:OG1 | 2:B:135:MET:O | 2.33 | 0.45 |
| 3:C:247:TRP:HD1 | 3:C:263:ALA:HB3 | 1.82 | 0.45 |
| 1:F:237:SER:OG | 1:F:238:MET:N | 2.49 | 0.45 |
| 1:F:913:ARG:O | 1:F:916:GLU:HG3 | 2.16 | 0.45 |
| 1:F:2227:LYS:HB2 | 1:F:2230:VAL:HG22 | 1.98 | 0.45 |
| 1:F:3462:ARG:HG2 | 1:F:3498:TRP:HZ3 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3911:ILE:HD12 | 1:F:3937:VAL:HG23 | 1.98 | 0.45 |
| 2:G:340:PHE:HE2 | 3:H:485:PRO:HB2 | 1.81 | 0.45 |
| 2:G:389:CYS:HA | 2:G:392:LYS:HB3 | 1.98 | 0.45 |
| 2:G:473:TYR:HD2 | 3:H:350:GLN:HB3 | 1.82 | 0.45 |
| 4:K:188:LYS:HZ1 | 5:M:763:ASP:HB3 | 1.81 | 0.45 |
| 5:M:722:LYS:HG3 | 5:M:742:PHE:O | 2.15 | 0.45 |
| 1:A:21:ALA:HA | 1:A:24:ARG:HH12 | 1.81 | 0.45 |
| 1:A:710:PHE:O | 1:A:714:VAL:HG23 | 2.16 | 0.45 |
| 1:A:1773:VAL:O | 1:A:1773:VAL:HG12 | 2.16 | 0.45 |
| 1:A:2420:PHE:CE2 | 1:A:2439:ILE:HD11 | 2.51 | 0.45 |
| 1:A:3308:ASP:N | 1:A:3308:ASP:OD1 | 2.48 | 0.45 |
| 1:A:3915:HIS:CE1 | 1:A:3961:PHE:HB3 | 2.51 | 0.45 |
| 2:B:416:GLN:NE2 | 2:B:433:GLN:OE1 | 2.41 | 0.45 |
| 3:C:363:LYS:HA | 3:C:420:VAL:HA | 1.99 | 0.45 |
| 1:F:642:PHE:HZ | 1:F:673:THR:HG23 | 1.81 | 0.45 |
| 1:F:1217:VAL:HA | 1:F:1285:GLU:OE1 | 2.17 | 0.45 |
| 1:F:2869:LEU:HB2 | 1:F:2899:ARG:NH1 | 2.31 | 0.45 |
| 1:F:3321:LEU:HD13 | 1:F:3324:ARG:HH12 | 1.81 | 0.45 |
| 3:H:626:THR:HG22 | 3:H:628:GLU:H | 1.80 | 0.45 |
| 3:H:661:ALA:HA | 3:H:664:GLU:CD | 2.36 | 0.45 |
| 4:K:3:ARG:NH1 | 4:K:122:VAL:O | 2.50 | 0.45 |
| 4:N:155:TRP:HA | 4:N:158:VAL:HG22 | 1.98 | 0.45 |
| 1:A:145:ASP:HA | 1:A:147:PHE:CE2 | 2.51 | 0.45 |
| 1:A:345:PHE:HB3 | 1:A:366:TYR:CE1 | 2.51 | 0.45 |
| 1:A:1672:PHE:CZ | 1:A:1676:ILE:HD11 | 2.52 | 0.45 |
| 1:A:2257:PHE:O | 1:A:2261:SER:OG | 2.25 | 0.45 |
| 1:A:2430:GLU:OE1 | 1:A:2430:GLU:N | 2.29 | 0.45 |
| 1:A:3988:LEU:HD12 | 1:A:3988:LEU:HA | 1.82 | 0.45 |
| 3:C:247:TRP:CD1 | 3:C:263:ALA:HB3 | 2.52 | 0.45 |
| 1:F:168:ASP:OD1 | 1:F:169:THR:N | 2.43 | 0.45 |
| 1:F:1095:LEU:O | 1:F:1099:PHE:N | 2.48 | 0.45 |
| 1:F:1580:LEU:O | 1:F:1584:GLN:HG2 | 2.17 | 0.45 |
| 1:F:2522:ARG:HH21 | 1:F:2560:ASN:HB3 | 1.81 | 0.45 |
| 1:F:3146:SER:C | 1:F:3147:LYS:HD2 | 2.37 | 0.45 |
| 1:F:3174:ASP:HB3 | 1:F:3178:ILE:HD13 | 1.98 | 0.45 |
| 1:F:3500:SER:HA | 1:F:3503:VAL:HG12 | 1.97 | 0.45 |
| 2:G:480:ASN:OD1 | 2:G:483:LEU:N | 2.33 | 0.45 |
| 3:H:115:MET:O | 3:H:119:GLN:HG2 | 2.17 | 0.45 |
| 3:H:602:VAL:HA | 3:H:609:PHE:CD2 | 2.52 | 0.45 |
| 5:M:843:LEU:HD23 | 5:M:846:ARG:HH11 | 1.82 | 0.45 |
| 7:D:35:DT:H2' | 7:D:36:DG:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:55:THR:O | 1:A:58:VAL:HG12 | 2.16 | 0.45 |
| 1:A:925:GLN:HA | 1:A:2769:VAL:HG13 | 1.99 | 0.45 |
| 1:A:1145:LEU:HD23 | 1:A:1165:LEU:HD13 | 1.97 | 0.45 |
| 1:A:2405:VAL:O | 1:A:2408:MET:HE2 | 2.15 | 0.45 |
| 1:A:3389:VAL:O | 1:A:3393:GLU:HG3 | 2.17 | 0.45 |
| 1:A:3835:PRO:HA | 1:A:3839:TYR:HB2 | 1.98 | 0.45 |
| 2:B:95:ASN:ND2 | 2:B:99:PHE:H | 2.12 | 0.45 |
| 2:B:247:ARG:HG2 | 2:B:247:ARG:O | 2.17 | 0.45 |
| 3:C:259:ILE:HD12 | 3:C:377:LEU:HD21 | 1.98 | 0.45 |
| 1:F:1379:PRO:HB2 | 1:F:1385:ASN:HD22 | 1.81 | 0.45 |
| 1:F:1773:VAL:O | 1:F:1773:VAL:HG12 | 2.16 | 0.45 |
| 1:F:2745:ARG:HG3 | 8:I:45:DG:O4' | 2.16 | 0.45 |
| 1:F:3959:MET:CE | 1:F:4124:TRP:HE1 | 2.29 | 0.45 |
| 2:G:148:TRP:N | 2:G:189:LYS:HZ1 | 2.15 | 0.45 |
| 4:L:144:LEU:O | 4:L:148:ASN:ND2 | 2.50 | 0.45 |
| 4:N:155:TRP:NE1 | 4:O:158:VAL:HG21 | 2.31 | 0.45 |
| 5:P:670:THR:HG23 | 5:P:675:LYS:HB2 | 1.98 | 0.45 |
| 5:P:681:ARG:NH2 | 5:P:730:PHE:HB3 | 2.32 | 0.45 |
| 6:Q:100:VAL:HG12 | 6:Q:101:ALA:H | 1.80 | 0.45 |
| 6:R:80:LEU:HD23 | 6:R:80:LEU:H | 1.82 | 0.45 |
| 1:A:450:SER:N | 1:A:453:MET:SD | 2.89 | 0.45 |
| 1:A:1593:VAL:HA | 1:A:1596:VAL:HG22 | 1.98 | 0.45 |
| 2:B:203:MET:SD | 2:B:238:LYS:N | 2.74 | 0.45 |
| 2:B:361:TYR:OH | 3:C:356:PHE:O | 2.22 | 0.45 |
| 1:F:117:LYS:NZ | 3:H:299:ASP:HA | 2.32 | 0.45 |
| 1:F:241:ASP:O | 1:F:244:THR:HG22 | 2.17 | 0.45 |
| 1:F:1066:LEU:HD12 | 1:F:1074:LYS:HB3 | 1.98 | 0.45 |
| 1:F:2408:MET:HG3 | 1:F:2411:LEU:HD13 | 1.98 | 0.45 |
| 1:F:3128:LYS:HA | 1:F:3128:LYS:HD3 | 1.78 | 0.45 |
| 2:G:200:LEU:HD23 | 2:G:200:LEU:H | 1.82 | 0.45 |
| 3:H:9:ALA:O | 3:H:131:HIS:N | 2.32 | 0.45 |
| 3:H:237:PHE:CE2 | 3:H:239:LYS:HB2 | 2.51 | 0.45 |
| 4:N:179:ARG:O | 4:N:182:LEU:HG | 2.17 | 0.45 |
| 5:P:668:SER:HB3 | 5:P:703:GLY:H | 1.82 | 0.45 |
| 6:Q:29:ILE:HD13 | 6:Q:76:LEU:HB3 | 1.97 | 0.45 |
| 6:R:214:LEU:O | 6:R:218:TYR:HB2 | 2.17 | 0.45 |
| 1:A:371:GLY:HA2 | 1:A:423:TYR:CZ | 2.51 | 0.45 |
| 1:A:525:LYS:HE2 | 1:A:525:LYS:HB2 | 1.71 | 0.45 |
| 1:A:1287:GLN:HG3 | 1:A:1289:SER:H | 1.81 | 0.45 |
| 1:A:1525:CYS:O | 1:A:1529:VAL:HG23 | 2.16 | 0.45 |
| 1:A:3577:GLN:HE21 | 1:A:3629:ARG:HB3 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:100:LYS:HA | 2:B:100:LYS:HD2 | 1.77 | 0.45 |
| 3:C:213:ILE:HB | 3:C:221:LEU:HD22 | 1.99 | 0.45 |
| 3:C:488:GLN:O | 3:C:492:GLN:HG3 | 2.17 | 0.45 |
| 1:F:1101:PHE:HD2 | 1:F:1163:LEU:HD13 | 1.82 | 0.45 |
| 1:F:2264:ASP:N | 1:F:2265:PRO:HD3 | 2.31 | 0.45 |
| 1:F:2404:ARG:HA | 1:F:2404:ARG:HD2 | 1.75 | 0.45 |
| 2:G:171:ASN:HB3 | 2:G:206:LYS:HB2 | 1.98 | 0.45 |
| 2:G:350:PHE:HB3 | 2:G:394:VAL:HG12 | 1.98 | 0.45 |
| 2:G:459:VAL:HG11 | 3:H:382:HIS:ND1 | 2.31 | 0.45 |
| 3:H:496:HIS:NE2 | 3:H:504:PRO:O | 2.48 | 0.45 |
| 1:A:332:GLU:HB2 | 1:A:335:LYS:NZ | 2.32 | 0.45 |
| 1:A:994:TRP:HE1 | 1:A:1000:LYS:HZ3 | 1.62 | 0.45 |
| 1:A:2492:ASP:OD1 | 1:A:2493:ASN:N | 2.50 | 0.45 |
| 2:B:94:LYS:N | 2:B:102:ILE:O | 2.41 | 0.45 |
| 1:F:730:LEU:HD11 | 1:F:765:LEU:HD11 | 1.99 | 0.45 |
| 1:F:1643:MET:SD | 1:F:1688:LEU:HD22 | 2.57 | 0.45 |
| 1:F:3141:PHE:HA | 1:F:3144:PHE:CE1 | 2.52 | 0.45 |
| 1:F:3588:TRP:CD1 | 1:F:3609:MET:SD | 3.10 | 0.45 |
| 1:F:3959:MET:HE3 | 1:F:4124:TRP:HE1 | 1.80 | 0.45 |
| 2:G:254:ARG:NH1 | 8:I:34:DC:O4' | 2.50 | 0.45 |
| 2:G:351:LYS:O | 2:G:395:ALA:N | 2.50 | 0.45 |
| 3:H:461:MET:HG3 | 3:H:526:SER:OG | 2.17 | 0.45 |
| 4:K:73:ALA:HB1 | 4:K:86:PHE:HZ | 1.81 | 0.45 |
| 4:O:20:LEU:HD21 | 4:O:35:THR:O | 2.16 | 0.45 |
| 6:Q:53:VAL:O | 6:Q:56:GLN:HG3 | 2.15 | 0.45 |
| 6:Q:154:ALA:O | 6:Q:158:HIS:ND1 | 2.36 | 0.45 |
| 8:E:31:DA:H2' | 8:E:31:DA:N3 | 2.31 | 0.45 |
| 8:I:33:DA:H2 | 9:J:25:DT:H3 | 1.63 | 0.45 |
| 8:I:41:DT:O3' | 8:I:42:DA:H8 | 2.00 | 0.45 |
| 1:A:1065:SER:O | 1:A:1069:HIS:N | 2.50 | 0.45 |
| 1:A:1867:ILE:O | 1:A:1871:MET:HG2 | 2.17 | 0.45 |
| 1:A:1963:GLN:HA | 1:A:2125:TRP:CH2 | 2.52 | 0.45 |
| 1:A:2142:ILE:O | 1:A:2146:LEU:HG | 2.17 | 0.45 |
| 1:A:3490:VAL:HG21 | 1:A:3495:PHE:CE2 | 2.51 | 0.45 |
| 1:A:3962:ARG:HD2 | 1:A:4124:TRP:CZ2 | 2.52 | 0.45 |
| 3:C:129:LYS:NZ | 3:C:131:HIS:HB2 | 2.32 | 0.45 |
| 1:F:82:ARG:HA | 1:F:85:ILE:HD12 | 1.99 | 0.45 |
| 1:F:1218:SER:O | 1:F:1222:ASN:N | 2.48 | 0.45 |
| 1:F:1603:GLN:OE1 | 1:F:1606:ARG:NH2 | 2.50 | 0.45 |
| 5:P:749:SER:HG | 5:P:750:THR:N | 2.15 | 0.45 |
| 7:D:19:DA:H2 | 8:E:39:DA:C2 | 2.35 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:472:GLY:O | 1:A:475:LEU:HB3 | 2.17 | 0.45 |
| 1:A:652:GLU:HA | 1:A:655:LEU:HD12 | 1.99 | 0.45 |
| 1:A:675:ARG:HG2 | 1:A:678:LYS:HE2 | 1.98 | 0.45 |
| 1:A:1150:LYS:HD2 | 1:A:1162:SER:HA | 1.99 | 0.45 |
| 1:A:2844:LEU:HD21 | 1:A:2858:ILE:HG21 | 1.99 | 0.45 |
| 1:A:3781:CYS:HB3 | 1:A:3786:LEU:HB2 | 1.99 | 0.45 |
| 2:B:85:VAL:HG23 | 2:B:105:LEU:HB3 | 1.99 | 0.45 |
| 2:B:429:PRO:HG2 | 3:C:435:PHE:CD2 | 2.52 | 0.45 |
| 1:F:1169:VAL:HG11 | 1:F:1198:LEU:HD11 | 1.98 | 0.45 |
| 1:F:3577:GLN:HA | 1:F:3629:ARG:CZ | 2.47 | 0.45 |
| 1:F:4125:GLU:HG3 | 1:F:4127:TRP:NE1 | 2.32 | 0.45 |
| 2:G:35:ARG:NH2 | 2:G:80:ARG:HB3 | 2.32 | 0.45 |
| 2:G:367:PHE:HE2 | 2:G:369:TYR:HB2 | 1.82 | 0.45 |
| 2:G:370:PRO:HD3 | 2:G:382:PHE:CD2 | 2.52 | 0.45 |
| 3:H:335:SER:HB3 | 3:H:394:ARG:HH12 | 1.82 | 0.45 |
| 6:R:81:ARG:HD2 | 6:R:81:ARG:O | 2.17 | 0.45 |
| 1:A:242:PRO:O | 1:A:246:ARG:HG2 | 2.16 | 0.44 |
| 1:A:1377:CYS:SG | 1:A:1378:GLU:N | 2.89 | 0.44 |
| 1:A:1667:SER:O | 1:A:1670:GLU:HG2 | 2.16 | 0.44 |
| 1:A:1877:LEU:HA | 1:A:1880:MET:HG2 | 1.98 | 0.44 |
| 1:A:2410:GLU:O | 1:A:2414:GLN:NE2 | 2.50 | 0.44 |
| 1:A:3048:LYS:HD2 | 1:A:3061:LEU:HB2 | 1.99 | 0.44 |
| 1:A:3246:ALA:CB | 1:A:3254:LEU:HD11 | 2.47 | 0.44 |
| 1:F:145:ASP:O | 1:F:148:LYS:NZ | 2.38 | 0.44 |
| 1:F:1069:HIS:CE1 | 1:F:3743:HIS:HD2 | 2.35 | 0.44 |
| 1:F:1353:PRO:HD2 | 1:F:1356:TRP:CE3 | 2.51 | 0.44 |
| 1:F:3387:GLU:O | 1:F:3390:GLN:NE2 | 2.50 | 0.44 |
| 2:G:346:MET:HG2 | 2:G:399:ARG:HH21 | 1.82 | 0.44 |
| 2:G:493:LEU:HD23 | 3:H:323:PHE:CE1 | 2.53 | 0.44 |
| 4:L:175:ASP:OD1 | 4:L:176:LEU:N | 2.50 | 0.44 |
| 5:M:833:ASN:HB3 | 5:M:836:THR:HG21 | 1.99 | 0.44 |
| 4:O:94:TYR:HD2 | 4:O:96:PHE:HB2 | 1.82 | 0.44 |
| 6:R:46:HIS:HB3 | 6:R:126:ALA:HB2 | 1.99 | 0.44 |
| 8:I:25:DA:N6 | 9:J:33:DA:N3 | 2.64 | 0.44 |
| 1:A:475:LEU:O | 1:A:479:ILE:HG12 | 2.16 | 0.44 |
| 1:A:537:SER:O | 1:A:541:MET:HG3 | 2.16 | 0.44 |
| 1:A:1153:LEU:HD11 | 1:A:1157:PHE:HB3 | 1.99 | 0.44 |
| 1:A:2216:LEU:HD13 | 1:A:2241:LEU:HD23 | 2.00 | 0.44 |
| 1:A:2411:LEU:O | 1:A:2415:LEU:HG | 2.16 | 0.44 |
| 1:A:2953:THR:HG1 | 1:A:2994:TRP:HE1 | 1.63 | 0.44 |
| 1:F:992:ILE:HG21 | 1:F:1036:PHE:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1343:GLU:HG2 | 1:F:1398:VAL:HG21 | 1.98 | 0.44 |
| 1:F:1551:ILE:HG13 | 1:F:1552:HIS:N | 2.32 | 0.44 |
| 1:F:1690:GLY:O | 1:F:1694:THR:HG23 | 2.17 | 0.44 |
| 1:F:1740:VAL:HA | 1:F:1743:MET:HG3 | 1.98 | 0.44 |
| 1:F:2091:HIS:HB2 | 1:F:2094:MET:HG3 | 1.99 | 0.44 |
| 1:F:3007:GLU:O | 1:F:3011:LEU:N | 2.50 | 0.44 |
| 1:F:3052:LEU:HA | 1:F:3056:GLU:O | 2.17 | 0.44 |
| 1:F:3118:ASP:OD1 | 1:F:3119:VAL:N | 2.50 | 0.44 |
| 2:G:45:SER:HA | 2:G:138:GLY:H | 1.80 | 0.44 |
| 4:K:96:PHE:HD2 | 4:K:98:GLU:HG3 | 1.83 | 0.44 |
| 4:L:133:THR:O | 4:L:137:ASN:ND2 | 2.51 | 0.44 |
| 4:L:155:TRP:HA | 4:L:158:VAL:HG12 | 1.99 | 0.44 |
| 1:A:122:LYS:HD2 | 1:A:122:LYS:HA | 1.87 | 0.44 |
| 1:A:247:GLU:HG2 | 1:A:251:PHE:CE2 | 2.52 | 0.44 |
| 1:A:827:ASN:HB3 | 1:A:836:LYS:HZ3 | 1.81 | 0.44 |
| 1:A:827:ASN:HB3 | 1:A:836:LYS:NZ | 2.33 | 0.44 |
| 1:A:1526:GLU:OE2 | 1:A:1574:ASN:ND2 | 2.51 | 0.44 |
| 3:C:528:ILE:HG22 | 3:C:532:LYS:NZ | 2.33 | 0.44 |
| 1:F:40:GLN:HA | 1:F:43:VAL:HG22 | 1.97 | 0.44 |
| 1:F:168:ASP:OD2 | 9:J:22:DG:H5" | 2.17 | 0.44 |
| 1:F:754:MET:O | 1:F:758:LEU:HD23 | 2.17 | 0.44 |
| 1:F:1144:SER:O | 1:F:1151:ARG:NH2 | 2.49 | 0.44 |
| 1:F:3686:TRP:CD1 | 1:F:3690:PHE:HD2 | 2.35 | 0.44 |
| 2:G:168:LEU:N | 2:G:201:ASP:O | 2.48 | 0.44 |
| 2:G:458:GLN:O | 2:G:462:MET:HE2 | 2.17 | 0.44 |
| 4:K:51:GLU:O | 4:K:54:GLN:HG3 | 2.17 | 0.44 |
| 1:A:3462:ARG:HG2 | 1:A:3498:TRP:HZ3 | 1.81 | 0.44 |
| 1:A:3775:LEU:HD13 | 1:A:3786:LEU:HB3 | 2.00 | 0.44 |
| 2:B:189:LYS:HE2 | 2:B:189:LYS:HB2 | 1.87 | 0.44 |
| 2:B:416:GLN:HB3 | 2:B:431:GLY:H | 1.81 | 0.44 |
| 3:C:242:ARG:HD3 | 3:C:271:ARG:CZ | 2.47 | 0.44 |
| 1:F:22:ALA:HB3 | 1:F:34:LEU:HD21 | 2.00 | 0.44 |
| 1:F:749:VAL:O | 1:F:753:GLN:HG2 | 2.17 | 0.44 |
| 1:F:889:GLU:HB2 | 1:F:891:ARG:HH21 | 1.82 | 0.44 |
| 1:F:1626:TRP:CZ2 | 1:F:1674:THR:HG21 | 2.51 | 0.44 |
| 1:F:2371:PHE:HD2 | 1:F:2374:LEU:HB2 | 1.82 | 0.44 |
| 1:F:2548:PRO:HB2 | 1:F:2848:PHE:CD1 | 2.53 | 0.44 |
| 1:F:3577:GLN:OE1 | 1:F:3629:ARG:NE | 2.49 | 0.44 |
| 5:M:900:LYS:HB3 | 5:M:900:LYS:HE2 | 1.85 | 0.44 |
| 8:I:33:DA:H2" | 8:I:34:DC:C6 | 2.53 | 0.44 |
| 1:A:1713:VAL:O | 1:A:1716:GLN:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3137:GLU:OE1 | 1:A:3186:ARG:NH2 | 2.51 | 0.44 |
| 1:A:3498:TRP:HD1 | 1:A:3501:HIS:CE1 | 2.36 | 0.44 |
| 2:B:473:TYR:HD2 | 3:C:350:GLN:HB3 | 1.82 | 0.44 |
| 3:C:267:ILE:H | 3:C:361:VAL:HB | 1.83 | 0.44 |
| 1:F:2220:MET:HA | 1:F:2223:VAL:HG12 | 1.99 | 0.44 |
| 1:F:2306:ASN:HA | 1:F:2309:PHE:CD2 | 2.52 | 0.44 |
| 1:F:2331:MET:HG2 | 1:F:2334:LYS:HG2 | 1.98 | 0.44 |
| 1:F:2339:GLU:O | 1:F:2343:GLU:HG2 | 2.17 | 0.44 |
| 2:G:72:ILE:O | 2:G:76:ILE:HG12 | 2.17 | 0.44 |
| 2:G:173:ASP:HB2 | 2:G:215:LEU:HG | 1.99 | 0.44 |
| 2:G:320:GLN:OE1 | 3:H:274:LYS:HE3 | 2.18 | 0.44 |
| 2:G:372:GLU:OE2 | 2:G:379:SER:N | 2.44 | 0.44 |
| 4:K:176:LEU:HD23 | 4:K:176:LEU:HA | 1.86 | 0.44 |
| 4:L:150:ARG:HH12 | 4:L:151:LEU:HG | 1.81 | 0.44 |
| 6:Q:16:LEU:HB3 | 6:Q:23:LEU:HD12 | 1.99 | 0.44 |
| 6:R:50:ASP:HB3 | 6:R:53:VAL:HG12 | 1.99 | 0.44 |
| 6:R:192:GLN:HA | 6:R:195:ILE:HG22 | 2.00 | 0.44 |
| 1:A:164:LYS:HB3 | 1:A:166:ILE:HG12 | 1.99 | 0.44 |
| 1:A:489:ARG:O | 1:A:492:SER:OG | 2.30 | 0.44 |
| 1:A:1186:LYS:HA | 1:A:1186:LYS:HD2 | 1.76 | 0.44 |
| 1:A:2153:THR:O | 1:A:2156:VAL:HG12 | 2.18 | 0.44 |
| 1:A:2306:ASN:HA | 1:A:2309:PHE:CD2 | 2.53 | 0.44 |
| 1:A:3321:LEU:HD13 | 1:A:3324:ARG:NH1 | 2.28 | 0.44 |
| 2:B:350:PHE:HA | 2:B:396:ALA:HA | 1.98 | 0.44 |
| 1:F:278:HIS:HB3 | 1:F:281:GLN:HG3 | 1.98 | 0.44 |
| 1:F:669:LEU:O | 1:F:673:THR:OG1 | 2.29 | 0.44 |
| 1:F:2260:PHE:HB3 | 1:F:2273:GLY:HA3 | 2.00 | 0.44 |
| 1:F:2304:VAL:O | 1:F:2307:MET:HB2 | 2.17 | 0.44 |
| 1:F:3968:ILE:HD12 | 1:F:3976:GLU:HG3 | 1.99 | 0.44 |
| 1:F:3968:ILE:HG23 | 1:F:3976:GLU:HG3 | 2.00 | 0.44 |
| 1:A:1357:LYS:O | 1:A:1360:LYS:HB3 | 2.17 | 0.44 |
| 1:A:2239:LYS:HB2 | 1:A:2279:ILE:HD12 | 2.00 | 0.44 |
| 1:A:3118:ASP:HB3 | 1:A:3121:LEU:HD13 | 2.00 | 0.44 |
| 1:A:4086:ASP:N | 1:A:4086:ASP:OD1 | 2.50 | 0.44 |
| 2:B:288:LEU:HB2 | 3:C:311:ILE:HB | 1.99 | 0.44 |
| 1:F:405:ASP:HB3 | 1:F:406:ARG:H | 1.64 | 0.44 |
| 1:F:539:GLN:N | 1:F:539:GLN:OE1 | 2.46 | 0.44 |
| 1:F:1757:MET:O | 1:F:1760:GLU:HG2 | 2.17 | 0.44 |
| 1:F:1769:GLU:H | 1:F:1772:HIS:CE1 | 2.36 | 0.44 |
| 1:F:2184:TYR:HE1 | 1:F:2734:ARG:HD2 | 1.82 | 0.44 |
| 1:F:2257:PHE:HA | 1:F:2260:PHE:CE2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2928:LYS:HZ2 | 1:F:2996:LEU:HD12 | 1.82 | 0.44 |
| 1:F:3048:LYS:HE2 | 1:F:3061:LEU:HD13 | 1.99 | 0.44 |
| 1:F:3772:ASN:HD21 | 1:F:3788:LEU:HB3 | 1.83 | 0.44 |
| 1:F:3792:SER:N | 1:F:3804:GLU:OE1 | 2.51 | 0.44 |
| 1:F:3992:ARG:HA | 1:F:3992:ARG:HD3 | 1.67 | 0.44 |
| 4:K:3:ARG:HB3 | 4:K:21:GLN:NE2 | 2.32 | 0.44 |
| 4:K:141:ASN:HD21 | 4:L:140:LYS:HE2 | 1.82 | 0.44 |
| 5:M:800:GLU:HG2 | 5:M:805:TRP:HB2 | 1.99 | 0.44 |
| 1:A:990:GLN:HB3 | 1:A:2781:PRO:HD3 | 1.99 | 0.44 |
| 1:A:1066:LEU:HA | 1:A:1069:HIS:HD2 | 1.82 | 0.44 |
| 1:A:2854:PHE:O | 1:A:2858:ILE:HG12 | 2.18 | 0.44 |
| 1:A:2880:CYS:HA | 1:A:2885:GLN:HB2 | 1.99 | 0.44 |
| 1:A:3123:GLN:OE1 | 1:A:3123:GLN:N | 2.40 | 0.44 |
| 1:A:3859:TYR:CE1 | 1:A:4119:ARG:HA | 2.52 | 0.44 |
| 3:C:497:ARG:HA | 3:C:497:ARG:HD3 | 1.79 | 0.44 |
| 1:F:433:PRO:O | 1:F:436:GLU:HG2 | 2.17 | 0.44 |
| 1:F:910:PHE:HE1 | 1:F:2807:GLN:HB3 | 1.83 | 0.44 |
| 1:F:1294:VAL:HA | 1:F:1297:PHE:CD2 | 2.53 | 0.44 |
| 1:F:1778:PHE:O | 1:F:1781:SER:OG | 2.25 | 0.44 |
| 1:F:3243:ILE:HD13 | 1:F:3262:LEU:HD11 | 1.98 | 0.44 |
| 1:F:3700:GLU:OE2 | 1:F:3716:HIS:ND1 | 2.32 | 0.44 |
| 2:G:241:ASP:HA | 2:G:244:ARG:NH1 | 2.33 | 0.44 |
| 3:H:194:LEU:HG | 3:H:195:LYS:HD2 | 1.99 | 0.44 |
| 3:H:667:GLU:HA | 3:H:675:TRP:CZ3 | 2.53 | 0.44 |
| 4:N:170:GLU:O | 4:N:173:GLU:HG2 | 2.17 | 0.44 |
| 8:I:45:DG:H5' | 8:I:45:DG:C8 | 2.51 | 0.44 |
| 1:A:949:PRO:HD3 | 1:F:2579:HIS:HB3 | 1.99 | 0.44 |
| 1:A:1212:LEU:HD12 | 1:A:1216:GLY:HA2 | 1.99 | 0.44 |
| 1:A:1723:PRO:HB2 | 1:A:1724:MET:CE | 2.48 | 0.44 |
| 1:A:1725:GLN:HE22 | 1:A:1727:ARG:HH21 | 1.65 | 0.44 |
| 1:A:2428:ASP:O | 1:A:2432:GLN:HG2 | 2.17 | 0.44 |
| 1:A:2526:SER:O | 1:A:2538:ARG:NH2 | 2.51 | 0.44 |
| 1:A:2919:ASP:OD1 | 1:A:2919:ASP:N | 2.51 | 0.44 |
| 1:A:3019:ILE:HG13 | 1:A:3020:ASP:H | 1.83 | 0.44 |
| 1:A:3967:PHE:O | 1:A:3970:LEU:HD22 | 2.18 | 0.44 |
| 1:A:4065:LEU:HG | 1:A:4069:GLU:HB3 | 1.99 | 0.44 |
| 2:B:93:ASP:OD1 | 2:B:93:ASP:N | 2.51 | 0.44 |
| 2:B:400:TYR:CZ | 2:B:402:PRO:HG3 | 2.53 | 0.44 |
| 2:B:474:ARG:HB3 | 2:B:477:SER:HB3 | 2.00 | 0.44 |
| 3:C:353:ARG:HA | 3:C:356:PHE:CD1 | 2.53 | 0.44 |
| 1:F:1255:CYS:HA | 1:F:1258:ASP:OD2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2274:ILE:HD11 | 1:F:2306:ASN:ND2 | 2.33 | 0.44 |
| 1:F:3959:MET:HG3 | 1:F:4124:TRP:CZ2 | 2.53 | 0.44 |
| 3:H:452:ASN:OD1 | 3:H:453:ALA:N | 2.50 | 0.44 |
| 4:O:32:PHE:HZ | 4:O:109:GLY:HA2 | 1.81 | 0.44 |
| 5:P:708:ARG:O | 5:P:712:ILE:HG12 | 2.18 | 0.44 |
| 5:P:771:LEU:HB3 | 5:P:775:LYS:NZ | 2.33 | 0.44 |
| 7:D:17:DT:H6 | 7:D:17:DT:H2' | 1.68 | 0.44 |
| 1:A:1220:LEU:HA | 1:A:1224:PHE:HD2 | 1.83 | 0.43 |
| 1:A:1439:PRO:HA | 1:A:1445:ARG:HH22 | 1.82 | 0.43 |
| 1:A:1646:LEU:O | 1:A:1649:LEU:HG | 2.18 | 0.43 |
| 1:A:2375:ALA:HB1 | 1:A:2379:MET:HE3 | 1.99 | 0.43 |
| 1:A:3133:GLN:HA | 1:A:3136:THR:HG22 | 1.99 | 0.43 |
| 1:A:3512:VAL:HB | 1:A:3516:HIS:CE1 | 2.53 | 0.43 |
| 1:A:3683:CYS:O | 1:A:3685:PRO:HD3 | 2.17 | 0.43 |
| 3:C:251:LEU:H | 3:C:261:ILE:HG12 | 1.81 | 0.43 |
| 1:F:198:ARG:NH1 | 2:G:315:ASP:OD2 | 2.51 | 0.43 |
| 1:F:393:LYS:HA | 1:F:393:LYS:HD2 | 1.55 | 0.43 |
| 1:F:1133:HIS:O | 1:F:1137:ILE:HG12 | 2.18 | 0.43 |
| 1:F:1725:GLN:OE1 | 1:F:1726:SER:N | 2.51 | 0.43 |
| 1:F:2589:TYR:HB2 | 1:F:2777:HIS:HB2 | 2.00 | 0.43 |
| 1:F:2827:SER:OG | 1:F:2828:GLU:OE2 | 2.36 | 0.43 |
| 1:F:2980:ASP:N | 1:F:2980:ASP:OD1 | 2.50 | 0.43 |
| 2:G:145:GLU:OE1 | 2:G:145:GLU:N | 2.51 | 0.43 |
| 4:K:44:THR:HG23 | 4:K:116:VAL:HG23 | 1.99 | 0.43 |
| 4:K:169:LYS:HE2 | 4:K:169:LYS:HB3 | 1.83 | 0.43 |
| 4:L:176:LEU:HD23 | 4:L:176:LEU:HA | 1.84 | 0.43 |
| 5:P:813:PHE:C | 5:P:849:GLY:H | 2.21 | 0.43 |
| 1:A:899:ARG:HD3 | 1:A:2568:MET:HB3 | 2.00 | 0.43 |
| 1:A:2737:GLU:O | 1:A:2741:LEU:N | 2.41 | 0.43 |
| 1:A:3005:LEU:O | 1:A:3010:SER:OG | 2.28 | 0.43 |
| 2:B:470:ARG:HD2 | 3:C:389:MET:HE1 | 2.00 | 0.43 |
| 1:F:243:GLN:O | 1:F:246:ARG:HG2 | 2.18 | 0.43 |
| 1:F:2184:TYR:CE1 | 1:F:2734:ARG:HD2 | 2.53 | 0.43 |
| 1:F:3823:GLU:HG2 | 1:F:3824:GLU:N | 2.33 | 0.43 |
| 1:F:3919:GLY:HA3 | 1:F:3947:GLY:HA2 | 1.99 | 0.43 |
| 3:H:434:MET:SD | 3:H:436:SER:OG | 2.66 | 0.43 |
| 6:Q:50:ASP:OD1 | 6:Q:51:THR:N | 2.37 | 0.43 |
| 7:D:13:DC:OP1 | 7:D:14:DA:N6 | 2.51 | 0.43 |
| 1:A:1643:MET:HA | 1:A:1646:LEU:HD12 | 2.00 | 0.43 |
| 1:A:1760:GLU:O | 1:A:1764:GLU:HG2 | 2.17 | 0.43 |
| 1:A:2844:LEU:HB3 | 1:A:2875:ALA:HB1 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3165:THR:HB | 1:A:3169:PRO:HG3 | 1.99 | 0.43 |
| 1:A:3353:GLU:HG2 | 1:A:3357:ARG:HG3 | 1.99 | 0.43 |
| 2:B:170:THR:O | 2:B:205:LEU:HD13 | 2.18 | 0.43 |
| 1:F:249:PHE:O | 1:F:252:VAL:HG12 | 2.18 | 0.43 |
| 1:F:460:ALA:O | 1:F:464:VAL:HG13 | 2.18 | 0.43 |
| 1:F:732:PHE:O | 1:F:735:SER:OG | 2.26 | 0.43 |
| 1:F:2162:LYS:HG3 | 1:F:2163:HIS:ND1 | 2.33 | 0.43 |
| 1:F:3419:PHE:O | 1:F:3423:GLN:HG2 | 2.17 | 0.43 |
| 2:G:351:LYS:N | 2:G:395:ALA:O | 2.43 | 0.43 |
| 3:H:65:ASP:O | 3:H:78:THR:HA | 2.18 | 0.43 |
| 3:H:116:ASP:O | 3:H:120:HIS:ND1 | 2.49 | 0.43 |
| 5:M:659:PHE:HB2 | 5:M:685:PHE:O | 2.18 | 0.43 |
| 5:P:788:THR:HG23 | 5:P:791:GLU:H | 1.82 | 0.43 |
| 1:A:1367:HIS:HB2 | 1:A:1370:ARG:NH1 | 2.34 | 0.43 |
| 1:A:3898:LEU:O | 1:A:3901:ARG:HG3 | 2.17 | 0.43 |
| 2:B:360:HIS:HB2 | 2:B:438:PRO:HG2 | 2.00 | 0.43 |
| 1:F:13:LEU:HD21 | 1:F:3069:MET:HG3 | 2.00 | 0.43 |
| 2:G:262:LYS:HB3 | 2:G:268:VAL:HG12 | 1.99 | 0.43 |
| 2:G:276:LEU:HA | 3:H:433:TYR:CE1 | 2.54 | 0.43 |
| 3:H:360:GLN:NE2 | 8:I:24:DA:N1 | 2.65 | 0.43 |
| 4:N:59:MET:SD | 4:N:59:MET:N | 2.87 | 0.43 |
| 6:Q:157:LEU:HD21 | 6:R:157:LEU:HA | 1.99 | 0.43 |
| 1:A:765:LEU:HA | 1:A:768:VAL:HG12 | 2.01 | 0.43 |
| 1:A:1071:ASN:HB3 | 1:A:1074:LYS:HG3 | 2.00 | 0.43 |
| 1:A:1158:PRO:HG2 | 1:A:1159:PRO:HD3 | 2.00 | 0.43 |
| 1:A:4056:PRO:O | 1:A:4060:THR:OG1 | 2.26 | 0.43 |
| 2:B:37:SER:H | 2:B:161:MET:HE1 | 1.84 | 0.43 |
| 2:B:204:HIS:O | 2:B:205:LEU:HD12 | 2.18 | 0.43 |
| 3:C:242:ARG:NE | 3:C:243:HIS:H | 2.16 | 0.43 |
| 1:F:394:GLN:CD | 1:F:1737:ASN:HB3 | 2.39 | 0.43 |
| 1:F:710:PHE:O | 1:F:714:VAL:HG23 | 2.19 | 0.43 |
| 1:F:975:ASP:N | 1:F:981:ARG:HH21 | 2.17 | 0.43 |
| 1:F:1769:GLU:HB2 | 1:F:1772:HIS:CD2 | 2.52 | 0.43 |
| 1:F:2349:LEU:HB3 | 1:F:2360:PHE:CE1 | 2.54 | 0.43 |
| 1:F:2899:ARG:HH21 | 1:F:2900:LEU:HG | 1.84 | 0.43 |
| 1:F:2964:ASP:HB2 | 1:F:3252:PHE:CD2 | 2.54 | 0.43 |
| 1:F:3887:PHE:HA | 1:F:3890:MET:SD | 2.58 | 0.43 |
| 1:F:3962:ARG:HD2 | 1:F:4124:TRP:CZ2 | 2.54 | 0.43 |
| 2:G:325:ARG:HG3 | 3:H:88:PHE:CD2 | 2.54 | 0.43 |
| 3:H:163:PHE:HB3 | 3:H:208:VAL:HG21 | 2.00 | 0.43 |
| 5:P:659:PHE:HD2 | 5:P:685:PHE:HB3 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1300:SER:HA | 1:A:1304:HIS:HB3 | 2.00 | 0.43 |
| 1:A:1372:LEU:O | 1:A:1375:THR:OG1 | 2.25 | 0.43 |
| 1:A:2126:MET:SD | 1:A:2126:MET:N | 2.92 | 0.43 |
| 1:A:2482:ASP:HA | 1:A:2485:ARG:HD2 | 1.99 | 0.43 |
| 1:A:2492:ASP:O | 1:A:2496:GLN:HG3 | 2.19 | 0.43 |
| 1:A:2967:GLU:O | 1:A:2971:GLN:HG2 | 2.18 | 0.43 |
| 1:A:3961:PHE:HE2 | 1:A:4107:LEU:HD21 | 1.83 | 0.43 |
| 2:B:193:LEU:HB2 | 2:B:198:ILE:HD12 | 2.01 | 0.43 |
| 2:B:203:MET:SD | 2:B:237:SER:HB2 | 2.58 | 0.43 |
| 2:B:276:LEU:HD23 | 2:B:276:LEU:H | 1.84 | 0.43 |
| 2:B:403:ARG:NH1 | 8:E:31:DA:O3' | 2.51 | 0.43 |
| 1:F:528:VAL:HA | 1:F:633:ILE:HD11 | 2.00 | 0.43 |
| 1:F:978:GLN:HG2 | 1:F:2597:PHE:HA | 2.01 | 0.43 |
| 1:F:1419:LEU:HD21 | 1:F:1467:ILE:HB | 2.01 | 0.43 |
| 1:F:2238:ILE:O | 1:F:2241:LEU:HG | 2.18 | 0.43 |
| 1:F:3383:GLN:HG3 | 1:F:3387:GLU:OE2 | 2.18 | 0.43 |
| 1:F:4090:ARG:HH22 | 1:F:4106:CYS:HA | 1.82 | 0.43 |
| 3:H:33:GLN:HA | 3:H:36:LYS:HE3 | 2.00 | 0.43 |
| 3:H:400:ARG:HH12 | 9:J:34:DT:P | 2.41 | 0.43 |
| 4:O:95:PHE:HB2 | 4:O:113:LEU:HD13 | 1.98 | 0.43 |
| 6:Q:146:LEU:HD13 | 6:R:147:GLN:HE21 | 1.83 | 0.43 |
| 8:I:43:DT:H2" | 8:I:44:DG:C2 | 2.53 | 0.43 |
| 1:A:168:ASP:OD2 | 7:D:22:DG:H5' | 2.19 | 0.43 |
| 1:A:767:GLU:HB2 | 1:A:851:ILE:HD11 | 2.01 | 0.43 |
| 1:A:894:PHE:O | 1:A:905:ILE:N | 2.40 | 0.43 |
| 1:A:1046:PRO:O | 1:A:1049:GLN:HB2 | 2.18 | 0.43 |
| 1:A:2450:GLU:O | 1:A:2453:GLU:HG2 | 2.19 | 0.43 |
| 1:A:3527:GLN:O | 1:A:3529:ILE:HD12 | 2.19 | 0.43 |
| 1:A:3571:PHE:CE2 | 1:A:3699:LEU:HD22 | 2.53 | 0.43 |
| 1:A:3595:GLU:HB2 | 1:A:3606:ILE:HD11 | 2.00 | 0.43 |
| 1:A:3878:VAL:HG13 | 1:A:3965:ARG:HH11 | 1.83 | 0.43 |
| 3:C:115:MET:O | 3:C:119:GLN:HG2 | 2.18 | 0.43 |
| 3:C:315:ARG:HH11 | 3:C:320:ILE:HG13 | 1.84 | 0.43 |
| 1:F:475:LEU:O | 1:F:479:ILE:HG12 | 2.18 | 0.43 |
| 1:F:1745:LYS:HA | 1:F:1748:ASP:OD2 | 2.19 | 0.43 |
| 1:F:2153:THR:O | 1:F:2156:VAL:HG12 | 2.19 | 0.43 |
| 1:F:2522:ARG:NH2 | 1:F:2564:GLU:HG3 | 2.34 | 0.43 |
| 2:G:388:LYS:HG3 | 3:H:454:VAL:HG11 | 2.00 | 0.43 |
| 2:G:489:ASN:ND2 | 3:H:331:MET:HB2 | 2.34 | 0.43 |
| 4:K:8:ILE:HG21 | 4:K:20:LEU:H | 1.83 | 0.43 |
| 4:N:186:GLU:OE2 | 5:P:803:TYR:OH | 2.26 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:D:19:DA:H2 | 8:E:39:DA:H2 | 1.65 | 0.43 |
| 1:A:264:ARG:HG3 | 8:E:39:DA:H2" | 2.00 | 0.43 |
| 1:A:389:ILE:O | 1:A:393:LYS:HG2 | 2.19 | 0.43 |
| 1:A:535:LEU:O | 1:A:637:LYS:NZ | 2.29 | 0.43 |
| 1:A:536:SER:HB3 | 1:A:637:LYS:HD3 | 2.01 | 0.43 |
| 1:A:1173:LEU:HD12 | 1:A:1191:PHE:CE1 | 2.54 | 0.43 |
| 1:A:2464:HIS:ND1 | 1:A:2466:SER:OG | 2.52 | 0.43 |
| 1:A:2578:GLU:OE1 | 1:A:2578:GLU:N | 2.42 | 0.43 |
| 1:A:2788:SER:HA | 1:A:2791:ILE:HG12 | 2.00 | 0.43 |
| 3:C:497:ARG:NH2 | 3:C:504:PRO:HA | 2.34 | 0.43 |
| 1:F:145:ASP:OD1 | 1:F:145:ASP:N | 2.50 | 0.43 |
| 1:F:1379:PRO:O | 1:F:1382:ILE:HG12 | 2.18 | 0.43 |
| 1:F:1596:VAL:O | 1:F:1600:MET:HG2 | 2.19 | 0.43 |
| 1:F:1959:LEU:HA | 1:F:2123:PRO:HG3 | 1.99 | 0.43 |
| 1:F:2510:LEU:HD12 | 1:F:2521:ILE:HG23 | 2.00 | 0.43 |
| 1:F:3420:CYS:SG | 1:F:3421:ASP:N | 2.92 | 0.43 |
| 2:G:418:GLU:HG2 | 2:G:426:GLN:OE1 | 2.18 | 0.43 |
| 2:G:426:GLN:HG3 | 2:G:429:PRO:HG3 | 2.01 | 0.43 |
| 4:K:107:ARG:O | 4:K:107:ARG:HD3 | 2.19 | 0.43 |
| 5:P:757:GLU:HG3 | 5:P:758:TYR:CD2 | 2.52 | 0.43 |
| 5:P:819:TYR:HA | 5:P:853:VAL:HB | 2.01 | 0.43 |
| 6:Q:98:ASP:OD1 | 6:Q:98:ASP:N | 2.52 | 0.43 |
| 6:R:50:ASP:OD1 | 6:R:52:SER:N | 2.39 | 0.43 |
| 7:D:13:DC:H4' | 7:D:14:DA:H2' | 2.01 | 0.43 |
| 1:A:142:ARG:CZ | 1:A:182:GLY:HA2 | 2.49 | 0.43 |
| 1:A:446:PHE:CD1 | 1:A:530:LEU:HD12 | 2.54 | 0.43 |
| 1:A:715:ALA:O | 1:A:718:MET:HG3 | 2.19 | 0.43 |
| 1:A:935:HIS:HB2 | 1:A:984:TYR:HE1 | 1.83 | 0.43 |
| 1:A:1081:ALA:O | 1:A:1085:ILE:HG23 | 2.19 | 0.43 |
| 1:A:1115:HIS:CD2 | 1:A:1119:LYS:HD3 | 2.53 | 0.43 |
| 1:A:2371:PHE:CD2 | 1:A:2374:LEU:HB2 | 2.53 | 0.43 |
| 1:A:2532:PRO:O | 1:A:2538:ARG:NH1 | 2.50 | 0.43 |
| 2:B:35:ARG:NH2 | 2:B:80:ARG:HB3 | 2.34 | 0.43 |
| 2:B:81:ASP:N | 2:B:81:ASP:OD1 | 2.52 | 0.43 |
| 2:B:126:GLN:O | 2:B:130:ARG:HG2 | 2.17 | 0.43 |
| 2:B:130:ARG:NH1 | 2:B:133:ASP:OD2 | 2.51 | 0.43 |
| 2:B:357:LYS:H | 2:B:360:HIS:CE1 | 2.36 | 0.43 |
| 2:B:488:ARG:O | 2:B:491:GLU:HG2 | 2.19 | 0.43 |
| 3:C:36:LYS:HZ1 | 3:C:231:LEU:HD11 | 1.83 | 0.43 |
| 1:F:356:ASN:HB3 | 1:F:358:GLU:HG2 | 2.00 | 0.43 |
| 1:F:774:GLU:O | 1:F:778:ILE:HG12 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1611:GLN:HB2 | 1:F:1613:HIS:ND1 | 2.34 | 0.43 |
| 1:F:1747:LEU:HD21 | 1:F:1778:PHE:HD1 | 1.82 | 0.43 |
| 1:F:3321:LEU:HD13 | 1:F:3324:ARG:NH1 | 2.34 | 0.43 |
| 3:H:18:PHE:HA | 3:H:101:GLY:HA3 | 2.00 | 0.43 |
| 3:H:219:ASP:OD1 | 3:H:220:GLY:N | 2.52 | 0.43 |
| 3:H:646:ALA:HA | 3:H:651:GLU:HG3 | 2.00 | 0.43 |
| 4:K:187:LYS:HD3 | 4:L:187:LYS:HB3 | 2.01 | 0.43 |
| 4:O:142:GLU:HB3 | 4:O:146:LYS:HZ1 | 1.83 | 0.43 |
| 1:A:525:LYS:O | 1:A:528:VAL:HG22 | 2.19 | 0.43 |
| 1:A:2746:LYS:HD2 | 7:D:12:DC:H3' | 2.00 | 0.43 |
| 1:A:3244:ASP:O | 1:A:3248:LYS:HG2 | 2.19 | 0.43 |
| 1:F:30:ALA:O | 1:F:34:LEU:HG | 2.19 | 0.43 |
| 1:F:275:PHE:CZ | 1:F:319:PHE:HB2 | 2.54 | 0.43 |
| 1:F:294:PHE:CE2 | 1:F:344:GLN:HG2 | 2.54 | 0.43 |
| 1:F:2255:LEU:HA | 1:F:2258:GLU:HG2 | 2.00 | 0.43 |
| 1:F:2486:ASP:N | 1:F:2486:ASP:OD1 | 2.51 | 0.43 |
| 1:F:2869:LEU:HD13 | 1:F:2896:ALA:HA | 1.99 | 0.43 |
| 1:F:3809:THR:OG1 | 1:F:3930:VAL:O | 2.37 | 0.43 |
| 1:F:3912:CYS:HA | 1:F:3915:HIS:CD2 | 2.54 | 0.43 |
| 2:G:330:GLU:HB3 | 2:G:333:GLU:HG2 | 2.01 | 0.43 |
| 3:H:84:MET:SD | 3:H:84:MET:N | 2.92 | 0.43 |
| 3:H:673:HIS:ND1 | 3:H:673:HIS:O | 2.52 | 0.43 |
| 4:L:161:ARG:O | 4:L:164:LYS:HG3 | 2.18 | 0.43 |
| 6:Q:157:LEU:HG | 6:R:157:LEU:HD13 | 2.00 | 0.43 |
| 6:Q:211:VAL:HG23 | 6:Q:212:MET:SD | 2.59 | 0.43 |
| 6:R:24:LEU:HD23 | 6:R:210:PHE:CE1 | 2.53 | 0.43 |
| 7:D:16:DA:H2" | 7:D:17:DT:C5 | 2.53 | 0.43 |
| 1:A:1190:LEU:HD23 | 1:A:1193:LYS:HD3 | 2.01 | 0.42 |
| 1:A:3128:LYS:HD3 | 1:A:3128:LYS:HA | 1.83 | 0.42 |
| 1:A:3981:TYR:CE1 | 1:A:4105:LYS:HB2 | 2.53 | 0.42 |
| 2:B:90:THR:O | 2:B:100:LYS:NZ | 2.52 | 0.42 |
| 2:B:293:ASN:HD21 | 5:M:692:ASN:ND2 | 2.17 | 0.42 |
| 2:B:446:MET:SD | 2:B:446:MET:N | 2.92 | 0.42 |
| 3:C:83:LEU:HD23 | 3:C:83:LEU:H | 1.84 | 0.42 |
| 1:F:12:LEU:HA | 1:F:41:GLU:OE2 | 2.19 | 0.42 |
| 1:F:635:PRO:HB3 | 1:F:672:ILE:HD11 | 2.01 | 0.42 |
| 1:F:1685:ASP:OD1 | 1:F:1686:LEU:N | 2.52 | 0.42 |
| 1:F:3293:CYS:O | 1:F:3297:VAL:HG23 | 2.19 | 0.42 |
| 1:F:4065:LEU:HD12 | 1:F:4069:GLU:HB3 | 2.01 | 0.42 |
| 2:G:154:PHE:CZ | 2:G:166:ILE:HD11 | 2.53 | 0.42 |
| 2:G:353:LEU:O | 2:G:353:LEU:HD23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:O:109:GLY:HA3 | 4:O:111:PHE:CZ | 2.54 | 0.42 |
| 1:A:387:GLU:O | 1:A:391:ARG:HG2 | 2.19 | 0.42 |
| 1:A:567:GLU:HA | 1:A:570:LYS:HE2 | 2.01 | 0.42 |
| 1:A:770:LEU:O | 1:A:774:GLU:HG3 | 2.19 | 0.42 |
| 1:A:2454:LEU:O | 1:A:2458:VAL:HG23 | 2.18 | 0.42 |
| 1:A:3078:LEU:HA | 1:A:3082:TYR:HD2 | 1.84 | 0.42 |
| 1:A:3197:LEU:HD22 | 1:A:3227:ILE:HG21 | 2.00 | 0.42 |
| 1:A:3474:ARG:HE | 1:A:3474:ARG:HB3 | 1.69 | 0.42 |
| 1:A:3499:ILE:HA | 1:A:3502:MET:SD | 2.60 | 0.42 |
| 1:A:3553:GLU:HG3 | 1:A:3557:ARG:NH2 | 2.33 | 0.42 |
| 1:A:4085:LYS:O | 1:A:4089:ILE:HG23 | 2.19 | 0.42 |
| 2:B:332:GLU:O | 2:B:335:GLU:HG2 | 2.18 | 0.42 |
| 1:F:532:ARG:O | 1:F:536:SER:OG | 2.29 | 0.42 |
| 1:F:798:GLY:HA2 | 1:F:801:LYS:NZ | 2.33 | 0.42 |
| 1:F:860:GLY:C | 1:F:3136:THR:HG21 | 2.40 | 0.42 |
| 1:F:1020:PRO:HA | 1:F:1073:PHE:CE1 | 2.54 | 0.42 |
| 1:F:1358:LEU:HA | 1:F:1361:LYS:HE2 | 2.01 | 0.42 |
| 1:F:2365:ASN:ND2 | 1:F:2396:LEU:HG | 2.34 | 0.42 |
| 1:F:3251:ASN:HB2 | 1:F:3254:LEU:HD13 | 2.01 | 0.42 |
| 1:F:3531:TYR:HB2 | 1:F:3532:PRO:HD3 | 2.01 | 0.42 |
| 1:F:4057:ALA:HB1 | 1:F:4082:ARG:HA | 2.01 | 0.42 |
| 2:G:526:LYS:HE2 | 2:G:528:LEU:HB3 | 2.01 | 0.42 |
| 5:M:754:PHE:O | 5:M:758:TYR:N | 2.52 | 0.42 |
| 4:N:8:ILE:HG13 | 4:N:8:ILE:O | 2.19 | 0.42 |
| 5:P:675:LYS:N | 5:P:676:PRO:HD2 | 2.35 | 0.42 |
| 1:A:21:ALA:HA | 1:A:24:ARG:NH1 | 2.35 | 0.42 |
| 1:A:164:LYS:HE3 | 1:A:166:ILE:HG23 | 2.01 | 0.42 |
| 1:A:344:GLN:O | 1:A:348:ILE:HG12 | 2.19 | 0.42 |
| 1:A:959:TYR:CE1 | 1:A:1007:VAL:HG21 | 2.54 | 0.42 |
| 1:A:1006:THR:HG22 | 1:A:1054:VAL:HG21 | 2.01 | 0.42 |
| 1:A:1087:ARG:HA | 1:A:1090:ARG:NH2 | 2.35 | 0.42 |
| 1:A:2295:GLN:HG3 | 1:A:2298:GLU:H | 1.83 | 0.42 |
| 1:A:3569:GLN:NE2 | 1:A:3573:ASN:OD1 | 2.48 | 0.42 |
| 1:A:4083:GLY:HA3 | 1:A:4088:ASN:HB2 | 2.01 | 0.42 |
| 2:B:174:ASN:HB2 | 2:B:215:LEU:HB2 | 2.01 | 0.42 |
| 3:C:53:GLU:HB3 | 3:C:83:LEU:HB2 | 1.99 | 0.42 |
| 3:C:134:ILE:HG21 | 3:C:163:PHE:CE1 | 2.55 | 0.42 |
| 1:F:147:PHE:C | 1:F:148:LYS:HD3 | 2.40 | 0.42 |
| 1:F:1004:GLN:HG2 | 1:F:1005:ASP:N | 2.34 | 0.42 |
| 1:F:1075:ARG:HD3 | 1:F:1113:LEU:HD23 | 2.00 | 0.42 |
| 1:F:1388:ASP:HA | 1:F:1392:MET:HG2 | 1.99 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2173:ALA:HB1 | 1:F:2214:ARG:NH2 | 2.34 | 0.42 |
| 1:F:3148:GLN:NE2 | 1:F:3150:ASN:OD1 | 2.53 | 0.42 |
| 1:F:3285:HIS:NE2 | 1:F:3333:THR:HB | 2.34 | 0.42 |
| 1:F:3506:LEU:HD21 | 1:F:3554:PHE:CD2 | 2.55 | 0.42 |
| 2:G:66:CYS:O | 2:G:70:VAL:HG13 | 2.19 | 0.42 |
| 3:H:677:ILE:HA | 3:H:680:GLN:HG2 | 2.00 | 0.42 |
| 4:L:3:ARG:NE | 4:L:21:GLN:OE1 | 2.51 | 0.42 |
| 6:R:217:LEU:O | 6:R:221:VAL:HG23 | 2.19 | 0.42 |
| 1:A:130:LEU:HA | 1:A:130:LEU:HD23 | 1.73 | 0.42 |
| 1:A:234:PHE:CD2 | 1:A:235:THR:HG23 | 2.53 | 0.42 |
| 1:A:851:ILE:HD13 | 1:A:851:ILE:HA | 1.92 | 0.42 |
| 1:A:1623:LEU:HD12 | 1:A:1623:LEU:HA | 1.88 | 0.42 |
| 1:A:3625:LEU:N | 1:A:3683:CYS:HA | 2.33 | 0.42 |
| 3:C:83:LEU:HD22 | 3:C:121:GLU:HG2 | 2.01 | 0.42 |
| 1:F:36:ARG:HD3 | 1:F:2426:HIS:CD2 | 2.55 | 0.42 |
| 1:F:1296:PHE:HA | 1:F:1299:GLU:HG2 | 2.01 | 0.42 |
| 1:F:1714:LEU:HB3 | 1:F:1761:LEU:HD21 | 2.00 | 0.42 |
| 1:F:2122:LEU:HB2 | 1:F:2126:MET:SD | 2.59 | 0.42 |
| 1:F:2955:SER:O | 1:F:2958:LEU:HG | 2.20 | 0.42 |
| 1:F:3133:GLN:O | 1:F:3136:THR:HG22 | 2.18 | 0.42 |
| 3:H:508:ILE:HG23 | 3:H:509:GLN:N | 2.32 | 0.42 |
| 4:O:158:VAL:HG22 | 4:O:161:ARG:HE | 1.85 | 0.42 |
| 5:P:666:VAL:HG12 | 5:P:675:LYS:HE3 | 2.00 | 0.42 |
| 1:A:156:PHE:HA | 1:A:159:GLU:HG3 | 2.01 | 0.42 |
| 1:A:738:HIS:O | 1:A:742:GLU:HG3 | 2.20 | 0.42 |
| 1:A:1482:GLU:OE1 | 1:A:1482:GLU:N | 2.50 | 0.42 |
| 1:A:1815:THR:OG1 | 1:A:1816:ARG:N | 2.53 | 0.42 |
| 1:A:2102:LYS:HD3 | 1:A:2102:LYS:HA | 1.82 | 0.42 |
| 1:A:2576:MET:HE3 | 1:A:2787:HIS:HA | 2.01 | 0.42 |
| 1:A:2584:CYS:SG | 1:A:2585:GLU:N | 2.93 | 0.42 |
| 1:A:3175:PRO:O | 1:A:3177:ASN:N | 2.53 | 0.42 |
| 1:A:3571:PHE:O | 1:A:3575:LEU:HG | 2.19 | 0.42 |
| 2:B:32:TYR:N | 2:B:253:LYS:HZ2 | 2.17 | 0.42 |
| 2:B:66:CYS:SG | 2:B:242:LEU:HB2 | 2.60 | 0.42 |
| 3:C:198:THR:OG1 | 3:C:199:GLU:N | 2.50 | 0.42 |
| 3:C:200:GLN:HA | 3:C:203:GLU:HG2 | 2.02 | 0.42 |
| 1:F:19:LEU:HD13 | 1:F:34:LEU:HD22 | 2.01 | 0.42 |
| 1:F:296:VAL:HG22 | 1:F:300:TRP:CD1 | 2.54 | 0.42 |
| 1:F:784:VAL:HG13 | 1:F:785:MET:SD | 2.58 | 0.42 |
| 1:F:1018:VAL:HG22 | 1:F:1074:LYS:HG2 | 2.00 | 0.42 |
| 1:F:1403:MET:SD | 1:F:1415:LEU:HD11 | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1598:ASN:HA | 1:F:1601:LEU:HD12 | 2.00 | 0.42 |
| 1:F:1716:GLN:HG3 | 1:F:1717:LEU:HD12 | 2.01 | 0.42 |
| 1:F:1816:ARG:HA | 1:F:1819:PHE:CE2 | 2.54 | 0.42 |
| 1:F:1945:TYR:CE2 | 1:F:1949:ILE:HD11 | 2.54 | 0.42 |
| 1:F:2215:LEU:HD23 | 1:F:2219:LEU:HD23 | 2.00 | 0.42 |
| 1:F:2387:PRO:O | 2:G:158:GLN:NE2 | 2.42 | 0.42 |
| 1:F:2724:ASP:N | 1:F:2724:ASP:OD1 | 2.52 | 0.42 |
| 1:F:3037:GLN:HA | 1:F:3040:TYR:CD2 | 2.54 | 0.42 |
| 2:G:131:PHE:O | 2:G:135:MET:HB3 | 2.18 | 0.42 |
| 4:N:7:ARG:HD3 | 4:O:131:LEU:HD12 | 2.00 | 0.42 |
| 5:P:739:GLN:O | 5:P:741:ARG:N | 2.47 | 0.42 |
| 6:Q:13:TRP:CE3 | 6:Q:24:LEU:HG | 2.55 | 0.42 |
| 6:R:5:GLU:HG3 | 6:R:134:HIS:CE1 | 2.54 | 0.42 |
| 6:R:13:TRP:HB3 | 6:R:210:PHE:CE1 | 2.55 | 0.42 |
| 1:A:380:ASP:O | 1:A:384:MET:HG2 | 2.19 | 0.42 |
| 1:A:1586:SER:OG | 1:A:1593:VAL:HG21 | 2.20 | 0.42 |
| 1:A:2413:PHE:HB3 | 2:B:148:TRP:CH2 | 2.54 | 0.42 |
| 1:A:3472:ILE:HA | 1:A:3479:THR:HG21 | 2.01 | 0.42 |
| 1:A:3588:TRP:CZ2 | 1:A:3613:MET:HG2 | 2.55 | 0.42 |
| 2:B:204:HIS:NE2 | 2:B:237:SER:HB3 | 2.34 | 0.42 |
| 3:C:89:ASP:OD1 | 3:C:90:LEU:N | 2.52 | 0.42 |
| 3:C:469:LYS:HA | 3:C:469:LYS:HD3 | 1.88 | 0.42 |
| 1:F:129:ASP:HA | 1:F:132:ILE:HG12 | 2.00 | 0.42 |
| 1:F:1800:SER:O | 1:F:1803:GLU:HG3 | 2.19 | 0.42 |
| 1:F:3633:ILE:HG13 | 1:F:3634:GLN:N | 2.35 | 0.42 |
| 2:G:204:HIS:CG | 2:G:208:PRO:HA | 2.55 | 0.42 |
| 2:G:321:ILE:H | 3:H:274:LYS:HE2 | 1.85 | 0.42 |
| 3:H:44:ARG:NH2 | 3:H:234:LEU:HA | 2.34 | 0.42 |
| 4:L:4:LYS:HE2 | 4:L:74:LEU:HB3 | 2.02 | 0.42 |
| 1:A:79:ARG:O | 1:A:82:ARG:HG2 | 2.19 | 0.42 |
| 1:A:892:LEU:HD12 | 1:A:892:LEU:HA | 1.83 | 0.42 |
| 1:A:985:GLU:HA | 1:A:988:VAL:HG22 | 2.02 | 0.42 |
| 1:A:1047:GLN:O | 1:A:1051:LYS:HD3 | 2.19 | 0.42 |
| 1:A:1076:LEU:HB3 | 1:A:1123:THR:HG23 | 2.01 | 0.42 |
| 1:F:357:LYS:O | 1:F:361:ILE:HG12 | 2.20 | 0.42 |
| 1:F:1852:LYS:NZ | 1:F:1918:LEU:HB3 | 2.35 | 0.42 |
| 1:F:2256:ILE:O | 1:F:2260:PHE:HD2 | 2.02 | 0.42 |
| 1:F:3980:MET:O | 1:F:3984:MET:HG2 | 2.19 | 0.42 |
| 2:G:204:HIS:ND1 | 2:G:208:PRO:HA | 2.35 | 0.42 |
| 2:G:269:ILE:HG23 | 2:G:378:SER:HB3 | 2.01 | 0.42 |
| 3:H:9:ALA:HB2 | 3:H:127:PHE:CD1 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:M:722:LYS:NZ | 5:M:744:ILE:HD11 | 2.34 | 0.42 |
| 4:N:99:LYS:HD2 | 4:N:99:LYS:HA | 1.82 | 0.42 |
| 4:N:194:LEU:HD11 | 4:O:195:HIS:CE1 | 2.55 | 0.42 |
| 1:A:681:LYS:HD3 | 1:A:681:LYS:HA | 1.84 | 0.42 |
| 1:A:723:ASP:C | 1:A:725:LEU:H | 2.23 | 0.42 |
| 1:A:1102:GLU:H | 1:A:1102:GLU:CD | 2.21 | 0.42 |
| 1:A:1113:LEU:HD12 | 1:A:1113:LEU:HA | 1.91 | 0.42 |
| 1:A:1757:MET:O | 1:A:1760:GLU:HG2 | 2.20 | 0.42 |
| 1:A:1799:GLU:O | 1:A:1802:TYR:HB3 | 2.20 | 0.42 |
| 1:A:2327:LEU:HB3 | 1:A:2371:PHE:CD1 | 2.55 | 0.42 |
| 2:B:76:ILE:HD11 | 2:B:487:PHE:CE1 | 2.55 | 0.42 |
| 2:B:200:LEU:H | 2:B:200:LEU:HD23 | 1.85 | 0.42 |
| 2:B:272:GLY:O | 2:B:369:TYR:N | 2.40 | 0.42 |
| 2:B:488:ARG:HE | 2:B:491:GLU:CD | 2.23 | 0.42 |
| 3:C:132:ILE:HB | 3:C:161:LEU:HB3 | 2.01 | 0.42 |
| 1:F:1729:PHE:HD1 | 1:F:1735:ARG:HH11 | 1.65 | 0.42 |
| 1:F:2335:ASN:OD1 | 1:F:2336:ILE:N | 2.52 | 0.42 |
| 1:F:2578:GLU:HG2 | 1:F:2579:HIS:N | 2.35 | 0.42 |
| 2:G:303:PHE:N | 3:H:290:GLN:O | 2.53 | 0.42 |
| 3:H:41:PHE:HE1 | 3:H:236:VAL:HG11 | 1.85 | 0.42 |
| 3:H:156:LYS:HG3 | 3:H:157:CYS:SG | 2.59 | 0.42 |
| 4:O:131:LEU:HD23 | 4:O:131:LEU:HA | 1.90 | 0.42 |
| 5:P:722:LYS:HG3 | 5:P:742:PHE:O | 2.19 | 0.42 |
| 6:R:135:LEU:HD12 | 6:R:135:LEU:HA | 1.91 | 0.42 |
| 7:D:23:DT:H2' | 7:D:24:DT:C4 | 2.55 | 0.42 |
| 1:A:24:ARG:NH2 | 1:A:70:ARG:HE | 2.18 | 0.42 |
| 1:A:296:VAL:HA | 1:A:299:LYS:HG2 | 2.02 | 0.42 |
| 1:A:538:ASP:HA | 1:A:541:MET:HG3 | 2.02 | 0.42 |
| 1:A:1149:LYS:O | 1:A:1163:LEU:N | 2.42 | 0.42 |
| 1:A:1666:GLY:O | 1:A:1669:PRO:HD2 | 2.20 | 0.42 |
| 1:A:2348:GLN:OE1 | 1:A:2353:GLN:NE2 | 2.52 | 0.42 |
| 1:A:3133:GLN:NE2 | 1:A:3137:GLU:OE2 | 2.53 | 0.42 |
| 1:A:3258:LEU:HA | 1:A:3261:GLU:OE1 | 2.20 | 0.42 |
| 1:A:3945:ALA:H | 1:A:3948:SER:HG | 1.64 | 0.42 |
| 1:A:4062:ASP:OD1 | 1:A:4063:GLU:N | 2.52 | 0.42 |
| 2:B:264:ASN:OD1 | 2:B:265:LYS:N | 2.47 | 0.42 |
| 1:F:433:PRO:HB3 | 1:F:6018:UNK:HA | 2.01 | 0.42 |
| 1:F:1560:TYR:CZ | 1:F:1596:VAL:HA | 2.55 | 0.42 |
| 1:F:2130:HIS:NE2 | 1:F:2167:PRO:HG3 | 2.35 | 0.42 |
| 1:F:2938:VAL:HG12 | 1:F:2942:ILE:HG12 | 2.02 | 0.42 |
| 1:F:2978:LYS:HG2 | 1:F:2980:ASP:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3030:ILE:HD12 | 1:F:3030:ILE:H | 1.85 | 0.42 |
| 1:F:3100:LYS:HA | 1:F:3103:ILE:HG22 | 2.02 | 0.42 |
| 1:F:3149:GLY:O | 1:F:3152:SER:OG | 2.30 | 0.42 |
| 1:F:3480:LEU:O | 1:F:3483:MET:HG2 | 2.20 | 0.42 |
| 3:H:265:LYS:HD3 | 3:H:268:LEU:HD22 | 2.02 | 0.42 |
| 3:H:328:GLU:HA | 3:H:331:MET:HG2 | 2.01 | 0.42 |
| 6:Q:100:VAL:HG12 | 6:Q:101:ALA:N | 2.34 | 0.42 |
| 6:R:95:PHE:CE2 | 6:R:108:VAL:HG13 | 2.53 | 0.42 |
| 1:A:966:PHE:HD1 | 1:A:969:LEU:HD12 | 1.84 | 0.42 |
| 1:A:1278:ALA:HB3 | 1:A:1356:TRP:CD1 | 2.55 | 0.42 |
| 1:A:1400:VAL:HG13 | 1:A:1461:ALA:HB2 | 2.02 | 0.42 |
| 1:A:2155:GLU:HA | 1:A:2158:ARG:HD3 | 2.01 | 0.42 |
| 1:A:2260:PHE:HA | 1:A:2270:ASN:HB2 | 2.01 | 0.42 |
| 1:A:2953:THR:OG1 | 1:A:2994:TRP:NE1 | 2.49 | 0.42 |
| 1:A:3460:GLU:OE1 | 1:A:3460:GLU:N | 2.45 | 0.42 |
| 1:A:3859:TYR:OH | 1:A:4120:THR:O | 2.38 | 0.42 |
| 3:C:345:PHE:HB3 | 3:C:389:MET:SD | 2.60 | 0.42 |
| 1:F:63:PHE:CE2 | 1:F:85:ILE:HG12 | 2.54 | 0.42 |
| 1:F:276:ALA:HB2 | 1:F:315:ALA:HA | 2.01 | 0.42 |
| 1:F:718:MET:SD | 1:F:719:LYS:HG3 | 2.60 | 0.42 |
| 1:F:753:GLN:NE2 | 1:F:791:ASP:O | 2.42 | 0.42 |
| 1:F:1484:LEU:HA | 1:F:1487:VAL:HG12 | 2.02 | 0.42 |
| 1:F:1625:HIS:HA | 1:F:1628:LYS:NZ | 2.35 | 0.42 |
| 1:F:1627:LYS:NZ | 1:F:1670:GLU:HB2 | 2.35 | 0.42 |
| 1:F:2142:ILE:O | 1:F:2146:LEU:HG | 2.19 | 0.42 |
| 1:F:2201:THR:HA | 1:F:2202:PRO:HD3 | 1.89 | 0.42 |
| 1:F:2208:ASP:OD1 | 1:F:2209:GLU:N | 2.52 | 0.42 |
| 1:F:3175:PRO:O | 1:F:3177:ASN:N | 2.53 | 0.42 |
| 4:K:137:ASN:HB3 | 4:L:137:ASN:HB2 | 2.02 | 0.42 |
| 4:L:102:LYS:HE3 | 4:L:102:LYS:HB2 | 1.96 | 0.42 |
| 5:P:725:TRP:NE1 | 5:P:736:VAL:O | 2.43 | 0.42 |
| 6:Q:40:ASP:OD1 | 6:Q:40:ASP:N | 2.51 | 0.42 |
| 1:A:82:ARG:O | 1:A:86:LEU:HG | 2.20 | 0.41 |
| 1:A:461:ILE:O | 1:A:464:VAL:HG22 | 2.19 | 0.41 |
| 1:A:1005:ASP:OD1 | 1:A:1005:ASP:N | 2.54 | 0.41 |
| 1:A:1034:ARG:HD2 | 1:A:1084:ASN:O | 2.20 | 0.41 |
| 1:A:1347:THR:O | 1:A:1351:THR:OG1 | 2.31 | 0.41 |
| 1:A:1419:LEU:HG | 1:A:1467:ILE:HD13 | 2.02 | 0.41 |
| 1:A:1506:SER:O | 1:A:1509:GLN:HG3 | 2.19 | 0.41 |
| 1:A:2243:GLU:HA | 1:A:2246:LYS:HE3 | 2.02 | 0.41 |
| 1:A:2312:TYR:CE2 | 1:A:2314:GLU:HB3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2411:LEU:HD21 | 1:A:2442:MET:HG2 | 2.00 | 0.41 |
| 1:F:889:GLU:OE2 | 1:F:3889:ARG:NH2 | 2.53 | 0.41 |
| 1:F:984:TYR:HA | 1:F:987:LEU:HB3 | 2.02 | 0.41 |
| 1:F:1352:SER:HB2 | 1:F:1356:TRP:HB2 | 2.02 | 0.41 |
| 1:F:2216:LEU:O | 1:F:2219:LEU:HG | 2.19 | 0.41 |
| 2:G:90:THR:HG21 | 2:G:93:ASP:HA | 2.02 | 0.41 |
| 2:G:416:GLN:HB2 | 2:G:431:GLY:N | 2.35 | 0.41 |
| 4:L:134:ILE:HA | 4:L:137:ASN:ND2 | 2.35 | 0.41 |
| 5:M:678:LEU:HD23 | 5:M:681:ARG:HH21 | 1.85 | 0.41 |
| 8:E:45:DG:H21 | 8:E:45:DG:P | 2.43 | 0.41 |
| 8:I:26:DA:H2" | 8:I:27:DC:C6 | 2.55 | 0.41 |
| 1:A:962:TYR:HB3 | 1:A:966:PHE:CE2 | 2.55 | 0.41 |
| 1:A:1958:GLU:HG2 | 1:A:1959:LEU:N | 2.35 | 0.41 |
| 1:A:2962:ARG:NH1 | 1:A:2967:GLU:OE2 | 2.32 | 0.41 |
| 1:A:3444:ALA:HB2 | 1:A:3478:GLU:HG3 | 2.02 | 0.41 |
| 2:B:100:LYS:NZ | 2:B:101:ASN:OD1 | 2.40 | 0.41 |
| 2:B:462:MET:HA | 2:B:465:ILE:HB | 2.01 | 0.41 |
| 1:F:42:CYS:SG | 1:F:91:ILE:HD11 | 2.60 | 0.41 |
| 1:F:72:SER:H | 1:F:82:ARG:HH22 | 1.67 | 0.41 |
| 1:F:151:GLU:H | 1:F:151:GLU:HG2 | 1.66 | 0.41 |
| 1:F:860:GLY:CA | 1:F:3136:THR:HG21 | 2.50 | 0.41 |
| 1:F:983:LEU:HD12 | 1:F:984:TYR:CD1 | 2.56 | 0.41 |
| 1:F:2164:TRP:C | 1:F:2167:PRO:HD2 | 2.41 | 0.41 |
| 1:F:3014:CYS:O | 1:F:3016:THR:HG23 | 2.20 | 0.41 |
| 1:F:3281:CYS:HB2 | 1:F:3329:LEU:HD13 | 2.02 | 0.41 |
| 1:F:3462:ARG:HG2 | 1:F:3498:TRP:CZ3 | 2.55 | 0.41 |
| 2:G:67:ILE:HA | 2:G:70:VAL:HG22 | 2.02 | 0.41 |
| 2:G:134:MET:SD | 2:G:135:MET:HB2 | 2.60 | 0.41 |
| 2:G:362:LEU:HD23 | 2:G:362:LEU:HA | 1.84 | 0.41 |
| 2:G:363:ARG:NH2 | 9:J:28:DA:OP2 | 2.33 | 0.41 |
| 4:K:133:THR:O | 4:K:136:GLU:HG3 | 2.20 | 0.41 |
| 5:P:825:VAL:HG23 | 5:P:828:ASP:HB2 | 2.02 | 0.41 |
| 6:R:174:LEU:HB2 | 6:R:179:LEU:HD11 | 2.02 | 0.41 |
| 1:A:35:ILE:HD12 | 1:A:80:GLU:HG3 | 2.02 | 0.41 |
| 1:A:826:PHE:O | 1:A:836:LYS:NZ | 2.51 | 0.41 |
| 1:A:988:VAL:HG21 | 1:A:1028:PHE:HZ | 1.84 | 0.41 |
| 1:A:1268:ASN:HD21 | 1:A:1344:PHE:HB2 | 1.86 | 0.41 |
| 1:A:3037:GLN:HA | 1:A:3040:TYR:CD2 | 2.55 | 0.41 |
| 1:A:3259:LEU:O | 1:A:3276:TRP:NE1 | 2.46 | 0.41 |
| 1:A:3531:TYR:HB2 | 1:A:3532:PRO:HD3 | 2.02 | 0.41 |
| 1:A:3834:ALA:N | 1:A:3835:PRO:HD2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:338:LYS:HE3 | 2:B:407:PRO:HD3 | 2.01 | 0.41 |
| 1:F:337:LYS:HA | 1:F:341:PHE:CD2 | 2.54 | 0.41 |
| 1:F:3231:ILE:HG13 | 1:F:3232:ARG:N | 2.34 | 0.41 |
| 1:F:3856:MET:N | 1:F:3856:MET:SD | 2.93 | 0.41 |
| 1:F:3971:MET:HE1 | 1:F:3973:PRO:HD2 | 2.03 | 0.41 |
| 1:F:4054:ALA:HA | 1:F:4097:GLY:H | 1.85 | 0.41 |
| 2:G:348:MET:HE1 | 3:H:518:PRO:HD3 | 2.02 | 0.41 |
| 3:H:37:VAL:HA | 3:H:40:MET:HG3 | 2.02 | 0.41 |
| 3:H:496:HIS:CG | 3:H:506:PRO:HD3 | 2.55 | 0.41 |
| 4:N:22:VAL:HG23 | 4:N:32:PHE:HB2 | 2.02 | 0.41 |
| 5:P:837:ARG:HG2 | 5:P:840:ILE:HB | 2.02 | 0.41 |
| 6:Q:164:ILE:HA | 6:Q:167:TYR:CD2 | 2.56 | 0.41 |
| 6:R:142:MET:HA | 6:R:221:VAL:HG11 | 2.02 | 0.41 |
| 9:J:17:DT:H6 | 9:J:17:DT:H2' | 1.67 | 0.41 |
| 9:J:27:DT:H6 | 9:J:27:DT:H2' | 1.59 | 0.41 |
| 1:A:392:CYS:O | 1:A:396:PHE:HB3 | 2.20 | 0.41 |
| 1:A:850:GLU:HG3 | 1:A:851:ILE:N | 2.35 | 0.41 |
| 1:A:891:ARG:HD3 | 1:A:957:PRO:HA | 2.01 | 0.41 |
| 1:A:928:VAL:HB | 1:A:2769:VAL:HG11 | 2.02 | 0.41 |
| 1:A:1255:CYS:HA | 1:A:1258:ASP:OD2 | 2.20 | 0.41 |
| 1:A:2133:LEU:HD13 | 1:A:2146:LEU:HD12 | 2.03 | 0.41 |
| 1:A:2525:TRP:CH2 | 1:A:2545:LEU:HD11 | 2.55 | 0.41 |
| 1:A:3444:ALA:HA | 1:A:3482:LEU:HD11 | 2.02 | 0.41 |
| 2:B:532:PRO:HG3 | 3:C:373:ALA:HB2 | 2.03 | 0.41 |
| 1:F:1023:SER:HG | 1:F:1026:ARG:NH2 | 2.18 | 0.41 |
| 1:F:1101:PHE:CD1 | 1:F:1168:LEU:HG | 2.55 | 0.41 |
| 1:F:1131:ILE:HD11 | 1:F:1186:LYS:HG2 | 2.01 | 0.41 |
| 1:F:1372:LEU:HD22 | 1:F:1402:LEU:HD21 | 2.02 | 0.41 |
| 1:F:2224:PHE:O | 1:F:2225:HIS:ND1 | 2.53 | 0.41 |
| 1:F:2376:ASP:OD1 | 1:F:2377:ARG:N | 2.54 | 0.41 |
| 1:F:2773:ARG:HG2 | 1:F:2789:SER:OG | 2.21 | 0.41 |
| 1:F:2965:TYR:O | 1:F:2969:ALA:N | 2.38 | 0.41 |
| 1:F:3234:CYS:O | 1:F:3238:MET:HG2 | 2.20 | 0.41 |
| 1:F:3243:ILE:CD1 | 1:F:3262:LEU:HD11 | 2.50 | 0.41 |
| 1:F:3781:CYS:O | 1:F:3785:ALA:N | 2.53 | 0.41 |
| 3:H:400:ARG:HH22 | 9:J:34:DT:P | 2.42 | 0.41 |
| 6:Q:60:GLU:HG3 | 6:Q:61:LEU:HD12 | 2.02 | 0.41 |
| 6:R:176:ARG:HD2 | 6:R:178:ARG:HB3 | 2.03 | 0.41 |
| 7:D:37:DG:H21 | 8:E:21:DA:H5' | 1.84 | 0.41 |
| 8:I:19:DC:H1' | 8:I:20:DT:C4 | 2.55 | 0.41 |
| 1:A:452:LYS:HB3 | 7:D:12:DC:H41 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:479:ILE:HG13 | 1:A:480:SER:N | 2.35 | 0.41 |
| 1:A:864:GLY:HA3 | 1:A:3170:ASP:CG | 2.41 | 0.41 |
| 1:A:865:GLN:O | 1:A:868:LYS:HG2 | 2.20 | 0.41 |
| 1:A:972:LEU:HB3 | 1:A:984:TYR:CD2 | 2.56 | 0.41 |
| 1:A:1235:ILE:HD12 | 1:A:1238:GLN:OE1 | 2.21 | 0.41 |
| 1:A:1264:LEU:O | 1:A:1268:ASN:ND2 | 2.53 | 0.41 |
| 1:A:1346:THR:HG22 | 1:A:1402:LEU:HB2 | 2.02 | 0.41 |
| 1:A:2097:LEU:HD12 | 1:A:2149:LEU:HD21 | 2.02 | 0.41 |
| 1:A:2257:PHE:HA | 1:A:2260:PHE:CE1 | 2.56 | 0.41 |
| 1:A:2412:TYR:OH | 1:A:2453:GLU:OE2 | 2.29 | 0.41 |
| 1:A:2899:ARG:HH21 | 1:A:2900:LEU:HG | 1.85 | 0.41 |
| 2:B:183:ALA:O | 2:B:187:ARG:HG3 | 2.20 | 0.41 |
| 2:B:244:ARG:HG3 | 2:B:246:VAL:HG23 | 2.02 | 0.41 |
| 2:B:304:ASN:CG | 2:B:307:THR:HB | 2.41 | 0.41 |
| 3:C:41:PHE:O | 3:C:45:GLN:HG2 | 2.21 | 0.41 |
| 3:C:155:LYS:HZ1 | 3:C:215:LEU:HB2 | 1.85 | 0.41 |
| 3:C:236:VAL:HG23 | 3:C:236:VAL:O | 2.19 | 0.41 |
| 1:F:681:LYS:HA | 1:F:681:LYS:HD3 | 1.78 | 0.41 |
| 1:F:1059:LEU:O | 1:F:1063:LEU:HD23 | 2.20 | 0.41 |
| 1:F:1436:LEU:HD23 | 1:F:1436:LEU:H | 1.84 | 0.41 |
| 1:F:1590:THR:HG21 | 1:F:1641:THR:HG23 | 2.02 | 0.41 |
| 1:F:1713:VAL:HA | 1:F:1716:GLN:HG2 | 2.02 | 0.41 |
| 1:F:1878:ASP:OD1 | 1:F:1879:VAL:N | 2.54 | 0.41 |
| 1:F:2154:GLU:HA | 1:F:2157:PHE:CE1 | 2.55 | 0.41 |
| 1:F:2349:LEU:O | 1:F:2353:GLN:HB2 | 2.20 | 0.41 |
| 1:F:2833:THR:HG21 | 1:F:2867:ALA:HB1 | 2.02 | 0.41 |
| 1:F:4012:ASP:HB2 | 1:F:4038:TRP:CE2 | 2.56 | 0.41 |
| 3:H:198:THR:HG22 | 3:H:200:GLN:H | 1.86 | 0.41 |
| 3:H:366:ALA:O | 3:H:368:ARG:NH1 | 2.46 | 0.41 |
| 6:Q:160:LYS:HB3 | 6:R:164:ILE:HD11 | 2.01 | 0.41 |
| 1:A:337:LYS:HE3 | 1:A:337:LYS:HB3 | 1.95 | 0.41 |
| 1:A:860:GLY:HA3 | 1:A:3136:THR:HG21 | 2.03 | 0.41 |
| 1:A:907:LEU:HD23 | 1:A:937:MET:HG3 | 2.02 | 0.41 |
| 1:A:1240:THR:HG22 | 1:A:1310:GLU:HA | 2.01 | 0.41 |
| 1:A:1468:LEU:HD12 | 1:A:1469:PRO:HD2 | 2.02 | 0.41 |
| 1:A:1598:ASN:HA | 1:A:1601:LEU:HD12 | 2.03 | 0.41 |
| 1:A:1935:GLU:O | 1:A:1939:LEU:HG | 2.21 | 0.41 |
| 1:A:2955:SER:O | 1:A:2958:LEU:HG | 2.20 | 0.41 |
| 1:A:3226:ASP:HB3 | 1:A:3227:ILE:H | 1.75 | 0.41 |
| 3:C:463:LEU:O | 3:C:476:LEU:N | 2.25 | 0.41 |
| 1:F:332:GLU:HA | 1:F:334:HIS:CE1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1603:GLN:O | 1:F:1603:GLN:NE2 | 2.54 | 0.41 |
| 1:F:1772:HIS:CD2 | 1:F:1773:VAL:HG23 | 2.55 | 0.41 |
| 1:F:2753:ARG:O | 1:F:2756:GLU:HG3 | 2.20 | 0.41 |
| 1:F:3008:TRP:O | 1:F:3011:LEU:HB2 | 2.20 | 0.41 |
| 1:F:3255:ALA:HB1 | 1:F:3258:LEU:HD23 | 2.03 | 0.41 |
| 1:F:3621:LYS:HA | 1:F:3630:ARG:NH2 | 2.35 | 0.41 |
| 1:F:4090:ARG:NH1 | 1:F:4091:ALA:HB2 | 2.36 | 0.41 |
| 2:G:130:ARG:O | 2:G:134:MET:HG3 | 2.21 | 0.41 |
| 2:G:367:PHE:CE1 | 2:G:431:GLY:HA3 | 2.55 | 0.41 |
| 3:H:125:LYS:HB2 | 3:H:125:LYS:HE3 | 1.89 | 0.41 |
| 3:H:513:TRP:HA | 3:H:516:LEU:HD13 | 2.02 | 0.41 |
| 3:H:643:ARG:HD2 | 3:H:655:PHE:CD2 | 2.55 | 0.41 |
| 5:P:728:GLU:HB3 | 5:P:736:VAL:HG21 | 2.02 | 0.41 |
| 6:Q:158:HIS:O | 6:Q:162:LEU:HG | 2.21 | 0.41 |
| 6:Q:190:LEU:HD23 | 6:Q:190:LEU:HA | 1.94 | 0.41 |
| 6:R:162:LEU:O | 6:R:165:GLN:HG3 | 2.21 | 0.41 |
| 8:I:44:DG:H2' | 8:I:45:DG:H2' | 2.02 | 0.41 |
| 1:A:297:LEU:HD23 | 1:A:316:LEU:HA | 2.03 | 0.41 |
| 1:A:1127:CYS:O | 1:A:1131:ILE:HG12 | 2.20 | 0.41 |
| 1:A:1342:MET:O | 1:A:1346:THR:HG23 | 2.20 | 0.41 |
| 1:A:1747:LEU:HD23 | 1:A:1747:LEU:HA | 1.94 | 0.41 |
| 1:A:3068:ALA:HB1 | 1:A:3074:GLN:HG2 | 2.00 | 0.41 |
| 2:B:172:GLU:HB2 | 2:B:175:PRO:HB3 | 2.03 | 0.41 |
| 2:B:414:VAL:O | 2:B:432:PHE:HA | 2.20 | 0.41 |
| 3:C:324:SER:OG | 3:C:327:ASP:HB2 | 2.20 | 0.41 |
| 1:F:170:VAL:HA | 1:F:219:VAL:HG11 | 2.03 | 0.41 |
| 1:F:292:SER:O | 1:F:295:GLU:HG2 | 2.21 | 0.41 |
| 1:F:2298:GLU:HG2 | 1:F:2301:GLN:HB3 | 2.02 | 0.41 |
| 1:F:2733:MET:SD | 1:F:2733:MET:N | 2.94 | 0.41 |
| 1:F:3244:ASP:HB3 | 1:F:3248:LYS:NZ | 2.35 | 0.41 |
| 1:F:3665:MET:SD | 1:F:3669:LYS:NZ | 2.93 | 0.41 |
| 1:F:3955:VAL:HG11 | 1:F:4121:TRP:CZ3 | 2.56 | 0.41 |
| 2:G:35:ARG:HE | 2:G:80:ARG:HB3 | 1.85 | 0.41 |
| 2:G:295:PRO:O | 3:H:298:ASN:ND2 | 2.53 | 0.41 |
| 2:G:396:ALA:HB3 | 2:G:413:LEU:HB2 | 2.02 | 0.41 |
| 3:H:206:GLU:O | 3:H:209:LYS:HG2 | 2.20 | 0.41 |
| 3:H:604:GLN:HG3 | 3:H:605:LYS:HG3 | 2.02 | 0.41 |
| 1:A:145:ASP:O | 1:A:148:LYS:NZ | 2.33 | 0.41 |
| 1:A:487:LEU:HD23 | 1:A:487:LEU:HA | 1.93 | 0.41 |
| 1:A:762:TYR:CD2 | 1:A:765:LEU:HD23 | 2.55 | 0.41 |
| 1:A:767:GLU:O | 1:A:771:ASN:ND2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:965:THR:HG22 | 1:A:969:LEU:HG | 2.02 | 0.41 |
| 1:A:1220:LEU:HA | 1:A:1224:PHE:HB2 | 2.03 | 0.41 |
| 1:A:1623:LEU:HD11 | 1:A:1671:VAL:HG11 | 2.02 | 0.41 |
| 1:A:1833:LEU:HA | 1:A:1836:LEU:HB3 | 2.03 | 0.41 |
| 1:A:1851:LEU:HD11 | 1:A:1874:TYR:CE1 | 2.56 | 0.41 |
| 1:A:2382:VAL:HA | 1:A:2385:LEU:HG | 2.02 | 0.41 |
| 1:A:3718:ARG:H | 1:A:3743:HIS:HE1 | 1.62 | 0.41 |
| 1:A:3962:ARG:HH21 | 1:A:3964:THR:HB | 1.85 | 0.41 |
| 2:B:259:LEU:HD11 | 2:B:400:TYR:CE1 | 2.54 | 0.41 |
| 1:F:24:ARG:HG3 | 1:F:25:CYS:N | 2.31 | 0.41 |
| 1:F:67:VAL:O | 1:F:82:ARG:NH2 | 2.51 | 0.41 |
| 1:F:386:VAL:O | 1:F:390:GLN:HG2 | 2.21 | 0.41 |
| 1:F:479:ILE:HG13 | 1:F:480:SER:N | 2.36 | 0.41 |
| 1:F:1476:HIS:ND1 | 1:F:1521:PHE:HB3 | 2.35 | 0.41 |
| 1:F:3677:PRO:HG3 | 1:F:3683:CYS:HB2 | 2.02 | 0.41 |
| 1:F:3704:GLN:CD | 1:F:3716:HIS:HE1 | 2.24 | 0.41 |
| 1:F:3994:ASP:O | 1:F:3998:LEU:N | 2.49 | 0.41 |
| 2:G:90:THR:HG23 | 2:G:135:MET:CE | 2.50 | 0.41 |
| 2:G:100:LYS:NZ | 2:G:101:ASN:H | 2.18 | 0.41 |
| 2:G:174:ASN:HB2 | 2:G:215:LEU:HB2 | 2.03 | 0.41 |
| 4:N:20:LEU:HD13 | 4:N:34:ILE:HG13 | 2.02 | 0.41 |
| 4:O:158:VAL:HG22 | 4:O:161:ARG:HH21 | 1.84 | 0.41 |
| 5:P:713:ILE:HG23 | 5:P:745:HIS:HB2 | 2.01 | 0.41 |
| 6:R:4:LEU:O | 6:R:8:LEU:CB | 2.68 | 0.41 |
| 1:A:40:GLN:NE2 | 1:A:2427:ARG:H | 2.19 | 0.41 |
| 1:A:67:VAL:HA | 1:A:71:LYS:HE2 | 2.02 | 0.41 |
| 1:A:127:ALA:O | 1:A:131:LEU:HG | 2.21 | 0.41 |
| 1:A:296:VAL:HG22 | 1:A:300:TRP:CD1 | 2.56 | 0.41 |
| 1:A:430:VAL:HG21 | 1:A:1643:MET:HG2 | 2.02 | 0.41 |
| 1:A:538:ASP:OD1 | 1:A:539:GLN:N | 2.51 | 0.41 |
| 1:A:573:LEU:HD13 | 1:A:649:PHE:HD1 | 1.86 | 0.41 |
| 1:A:834:LEU:HD12 | 1:A:837:THR:HG23 | 2.03 | 0.41 |
| 1:A:1071:ASN:H | 1:A:1075:ARG:NH1 | 2.19 | 0.41 |
| 1:A:1086:TYR:CD1 | 1:A:1133:HIS:HB3 | 2.56 | 0.41 |
| 1:A:1203:SER:N | 1:A:1204:PRO:HD3 | 2.35 | 0.41 |
| 1:A:1264:LEU:HD11 | 1:A:1344:PHE:CG | 2.55 | 0.41 |
| 1:A:1511:ALA:HA | 1:A:1514:LEU:HD12 | 2.03 | 0.41 |
| 1:A:1574:ASN:CG | 1:A:1578:ALA:H | 2.21 | 0.41 |
| 1:A:1588:ASP:OD1 | 1:A:1589:ASN:N | 2.52 | 0.41 |
| 1:A:1731:PRO:HA | 1:A:1736:PHE:CD2 | 2.56 | 0.41 |
| 1:A:1805:PHE:CZ | 1:A:1869:LYS:HA | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2375:ALA:O | 1:A:2379:MET:HG2 | 2.21 | 0.41 |
| 1:A:2478:MET:HG2 | 1:A:2524:PHE:CD1 | 2.56 | 0.41 |
| 1:A:2506:LEU:HD23 | 1:A:2506:LEU:HA | 1.88 | 0.41 |
| 1:A:2567:SER:HA | 1:A:2572:TYR:CE2 | 2.56 | 0.41 |
| 1:A:2773:ARG:NE | 1:A:2775:TYR:HE1 | 2.18 | 0.41 |
| 1:A:3234:CYS:O | 1:A:3238:MET:HG2 | 2.20 | 0.41 |
| 1:A:3912:CYS:HA | 1:A:3915:HIS:NE2 | 2.36 | 0.41 |
| 1:A:3955:VAL:HG11 | 1:A:4121:TRP:CE3 | 2.56 | 0.41 |
| 1:A:4010:SER:O | 1:A:4014:LYS:HG2 | 2.21 | 0.41 |
| 2:B:193:LEU:HB2 | 2:B:198:ILE:HB | 2.03 | 0.41 |
| 2:B:203:MET:SD | 2:B:238:LYS:HB2 | 2.61 | 0.41 |
| 2:B:253:LYS:HD2 | 2:B:253:LYS:HA | 1.82 | 0.41 |
| 2:B:255:ALA:HB1 | 2:B:273:ILE:O | 2.21 | 0.41 |
| 1:F:53:LEU:O | 1:F:57:LEU:HG | 2.21 | 0.41 |
| 1:F:55:THR:O | 1:F:58:VAL:HG12 | 2.20 | 0.41 |
| 1:F:83:GLU:HG2 | 1:F:129:ASP:OD2 | 2.21 | 0.41 |
| 1:F:183:GLU:HG2 | 1:F:184:VAL:H | 1.86 | 0.41 |
| 1:F:204:LEU:HD21 | 1:F:224:LEU:HD22 | 2.03 | 0.41 |
| 1:F:583:LEU:HB2 | 1:F:614:PRO:HA | 2.02 | 0.41 |
| 1:F:1568:ASN:O | 1:F:1572:LEU:HD23 | 2.21 | 0.41 |
| 1:F:1783:ARG:HH12 | 1:F:1830:HIS:HB2 | 1.86 | 0.41 |
| 1:F:2188:GLU:HG2 | 1:F:2728:LEU:HD21 | 2.01 | 0.41 |
| 1:F:2331:MET:O | 1:F:2331:MET:HG2 | 2.20 | 0.41 |
| 1:F:2366:LYS:HA | 1:F:2369:LYS:NZ | 2.35 | 0.41 |
| 1:F:2418:LYS:HA | 1:F:2418:LYS:HD3 | 1.81 | 0.41 |
| 1:F:2526:SER:O | 1:F:2538:ARG:NH2 | 2.53 | 0.41 |
| 1:F:2531:LEU:HD23 | 1:F:2531:LEU:HA | 1.81 | 0.41 |
| 1:F:2820:MET:SD | 1:F:2821:ASP:N | 2.94 | 0.41 |
| 1:F:3447:VAL:HG11 | 1:F:3471:ILE:HD13 | 2.03 | 0.41 |
| 1:F:3922:ASP:HB3 | 1:F:3928:PHE:CE1 | 2.56 | 0.41 |
| 2:G:91:GLU:OE1 | 2:G:136:GLY:HA3 | 2.20 | 0.41 |
| 2:G:286:ILE:N | 3:H:313:GLY:O | 2.37 | 0.41 |
| 2:G:290:ARG:HH12 | 5:P:695:PRO:HD2 | 1.86 | 0.41 |
| 2:G:351:LYS:C | 2:G:394:VAL:HG13 | 2.41 | 0.41 |
| 3:H:406:GLY:HA3 | 3:H:421:TYR:CE1 | 2.55 | 0.41 |
| 4:K:21:GLN:HE22 | 4:K:126:LEU:HD12 | 1.86 | 0.41 |
| 4:L:120:ALA:HA | 4:L:123:ILE:HG22 | 2.03 | 0.41 |
| 7:D:21:DA:H61 | 8:E:36:DA:H61 | 1.68 | 0.41 |
| 1:A:21:ALA:O | 1:A:24:ARG:HG2 | 2.21 | 0.41 |
| 1:A:629:PHE:O | 1:A:633:ILE:HG12 | 2.21 | 0.41 |
| 1:A:900:GLU:OE1 | 1:A:900:GLU:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1353:PRO:HD2 | 1:A:1356:TRP:CE3 | 2.56 | 0.41 |
| 1:A:1484:LEU:HD13 | 1:A:1531:LEU:HD13 | 2.03 | 0.41 |
| 1:A:2216:LEU:O | 1:A:2219:LEU:HG | 2.21 | 0.41 |
| 1:A:2295:GLN:HG3 | 1:A:2298:GLU:CB | 2.49 | 0.41 |
| 1:A:2331:MET:O | 1:A:2331:MET:HG2 | 2.21 | 0.41 |
| 1:A:2379:MET:SD | 1:A:2404:ARG:HG3 | 2.61 | 0.41 |
| 1:A:3050:LYS:NZ | 1:A:3184:THR:OG1 | 2.47 | 0.41 |
| 2:B:58:THR:N | 2:B:59:PRO:HD2 | 2.36 | 0.41 |
| 1:F:1022:ASP:O | 1:F:1025:LEU:HB3 | 2.20 | 0.41 |
| 1:F:1570:GLU:HA | 1:F:1573:LYS:HE2 | 2.03 | 0.41 |
| 1:F:2797:VAL:HG13 | 1:F:2804:ILE:HD12 | 2.03 | 0.41 |
| 1:F:2963:SER:OG | 1:F:3250:ASN:O | 2.21 | 0.41 |
| 1:F:3175:PRO:HA | 1:F:3249:GLN:HE22 | 1.85 | 0.41 |
| 1:F:3558:ILE:O | 1:F:3562:LEU:HG | 2.21 | 0.41 |
| 2:G:112:GLY:O | 2:G:116:ILE:HG12 | 2.20 | 0.41 |
| 2:G:257:SER:OG | 2:G:273:ILE:HB | 2.20 | 0.41 |
| 2:G:327:ILE:HD11 | 3:H:498:ALA:HB2 | 2.03 | 0.41 |
| 4:K:118:ASN:HB3 | 4:K:121:GLU:HG3 | 2.01 | 0.41 |
| 4:K:164:LYS:HZ2 | 5:M:898:ILE:HG23 | 1.86 | 0.41 |
| 4:N:139:ALA:O | 4:N:142:GLU:HG3 | 2.21 | 0.41 |
| 4:O:63:LYS:O | 4:O:67:VAL:HG22 | 2.20 | 0.41 |
| 5:P:816:HIS:N | 5:P:850:ALA:HA | 2.36 | 0.41 |
| 1:A:2097:LEU:HB2 | 1:A:2149:LEU:HD11 | 2.03 | 0.40 |
| 1:A:2187:VAL:HA | 1:A:2190:VAL:HG22 | 2.03 | 0.40 |
| 1:A:2574:ASN:O | 1:A:2787:HIS:ND1 | 2.54 | 0.40 |
| 1:A:6015:UNK:O | 1:A:6019:UNK:N | 2.54 | 0.40 |
| 2:B:340:PHE:CD2 | 2:B:408:PRO:HG3 | 2.56 | 0.40 |
| 2:B:424:LYS:HA | 2:B:424:LYS:HD3 | 1.80 | 0.40 |
| 2:B:493:LEU:HD12 | 2:B:493:LEU:HA | 1.84 | 0.40 |
| 1:F:734:LEU:HD11 | 1:F:768:VAL:HG22 | 2.04 | 0.40 |
| 1:F:1105:VAL:HG21 | 1:F:1154:PRO:HB2 | 2.03 | 0.40 |
| 1:F:1304:HIS:CE1 | 1:F:1307:ILE:HG22 | 2.54 | 0.40 |
| 1:F:1639:LEU:HA | 1:F:1642:LYS:HE3 | 2.02 | 0.40 |
| 1:F:1803:GLU:HA | 1:F:1806:ARG:NH2 | 2.36 | 0.40 |
| 1:F:1818:SER:O | 1:F:1822:ARG:HG3 | 2.21 | 0.40 |
| 1:F:2481:HIS:HD1 | 1:F:2499:PHE:HE1 | 1.68 | 0.40 |
| 1:F:2839:ASP:HA | 1:F:2842:ARG:NH1 | 2.36 | 0.40 |
| 1:F:3445:LEU:O | 1:F:3448:GLU:HG2 | 2.20 | 0.40 |
| 1:F:3534:ILE:HD13 | 1:F:3534:ILE:HA | 1.89 | 0.40 |
| 2:G:143:LEU:O | 2:G:147:LEU:HG | 2.22 | 0.40 |
| 2:G:164:LYS:HE3 | 2:G:164:LYS:HB3 | 1.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:365:SER:OG | 2:G:434:LEU:N | 2.53 | 0.40 |
| 4:L:180:PHE:HA | 4:L:183:VAL:HG12 | 2.02 | 0.40 |
| 5:M:659:PHE:CD2 | 5:M:685:PHE:HB3 | 2.55 | 0.40 |
| 5:M:764:SER:OG | 5:M:767:ILE:O | 2.36 | 0.40 |
| 4:O:97:PHE:HE2 | 4:O:99:LYS:HD3 | 1.85 | 0.40 |
| 4:O:170:GLU:OE2 | 5:P:847:PHE:HA | 2.20 | 0.40 |
| 4:O:176:LEU:HD23 | 4:O:179:ARG:HH11 | 1.86 | 0.40 |
| 5:P:770:ASP:OD1 | 5:P:773:GLN:HG2 | 2.21 | 0.40 |
| 9:J:33:DA:H2" | 9:J:34:DT:O2 | 2.21 | 0.40 |
| 1:A:238:MET:N | 1:A:238:MET:SD | 2.94 | 0.40 |
| 1:A:1012:ALA:HA | 1:A:1015:ASP:OD2 | 2.21 | 0.40 |
| 1:A:1142:HIS:CG | 1:A:1197:LEU:HD12 | 2.56 | 0.40 |
| 1:A:1771:GLN:H | 1:A:1775:GLU:CD | 2.24 | 0.40 |
| 1:A:2356:MET:SD | 1:A:2357:GLU:N | 2.94 | 0.40 |
| 1:A:2464:HIS:O | 1:A:2466:SER:N | 2.53 | 0.40 |
| 1:A:2735:ASP:N | 1:A:2735:ASP:OD1 | 2.50 | 0.40 |
| 1:A:2752:LYS:HD3 | 1:A:2752:LYS:HA | 1.96 | 0.40 |
| 1:A:3183:ILE:HD12 | 1:A:3238:MET:HB3 | 2.03 | 0.40 |
| 1:A:3701:ILE:HG13 | 1:A:3719:ILE:HG13 | 2.03 | 0.40 |
| 1:A:3731:SER:H | 1:A:3734:ARG:HA | 1.85 | 0.40 |
| 1:F:1071:ASN:OD1 | 1:F:1073:PHE:N | 2.52 | 0.40 |
| 1:F:1771:GLN:HA | 1:F:1775:GLU:HG3 | 2.02 | 0.40 |
| 1:F:2356:MET:SD | 1:F:2357:GLU:N | 2.95 | 0.40 |
| 1:F:2517:LEU:HA | 1:F:2520:ILE:HG22 | 2.04 | 0.40 |
| 1:F:3015:SER:O | 1:F:3016:THR:OG1 | 2.33 | 0.40 |
| 1:F:3186:ARG:O | 1:F:3190:LEU:HG | 2.21 | 0.40 |
| 2:G:205:LEU:HD12 | 2:G:205:LEU:HA | 1.95 | 0.40 |
| 2:G:350:PHE:HB2 | 3:H:462:SER:HA | 2.02 | 0.40 |
| 3:H:44:ARG:HD2 | 3:H:236:VAL:HB | 2.04 | 0.40 |
| 3:H:74:TYR:CD2 | 3:H:109:ASP:HB3 | 2.56 | 0.40 |
| 3:H:539:LEU:HD23 | 3:H:539:LEU:HA | 1.88 | 0.40 |
| 6:Q:67:ALA:HB3 | 6:Q:72:PHE:CE1 | 2.56 | 0.40 |
| 6:Q:211:VAL:O | 6:Q:215:GLN:HG2 | 2.21 | 0.40 |
| 6:R:209:PRO:HA | 6:R:212:MET:HG2 | 2.03 | 0.40 |
| 9:J:37:DG:H1' | 9:J:38:DG:N2 | 2.36 | 0.40 |
| 1:A:75:SER:HB2 | 1:A:77:GLU:HG2 | 2.03 | 0.40 |
| 1:A:446:PHE:HB3 | 1:A:527:TYR:HE1 | 1.86 | 0.40 |
| 1:A:1271:ILE:O | 1:A:1274:ARG:HD2 | 2.21 | 0.40 |
| 1:A:1297:PHE:HA | 1:A:1301:ILE:HG12 | 2.03 | 0.40 |
| 1:A:2129:LEU:HD22 | 1:A:2146:LEU:HD21 | 2.02 | 0.40 |
| 1:A:2193:ILE:HA | 1:A:2196:TRP:CH2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2724:ASP:N | 1:A:2724:ASP:OD1 | 2.54 | 0.40 |
| 1:A:2749:ALA:O | 1:A:2753:ARG:HG2 | 2.21 | 0.40 |
| 1:A:2837:LEU:HD21 | 1:A:2868:LEU:HA | 2.03 | 0.40 |
| 1:A:3278:GLN:HB3 | 1:A:3282:ARG:NH1 | 2.31 | 0.40 |
| 1:A:3911:ILE:O | 1:A:3915:HIS:CD2 | 2.75 | 0.40 |
| 2:B:73:SER:O | 2:B:77:SER:HB3 | 2.22 | 0.40 |
| 2:B:367:PHE:HE1 | 2:B:431:GLY:HA3 | 1.86 | 0.40 |
| 2:B:444:ARG:HH21 | 3:C:268:LEU:HD23 | 1.86 | 0.40 |
| 3:C:31:PHE:CZ | 3:C:100:PRO:HG3 | 2.57 | 0.40 |
| 3:C:335:SER:OG | 3:C:394:ARG:NH2 | 2.55 | 0.40 |
| 1:F:38:LEU:CD2 | 1:F:85:ILE:HG13 | 2.51 | 0.40 |
| 1:F:89:LEU:O | 1:F:133:LYS:NZ | 2.54 | 0.40 |
| 1:F:1045:THR:HG22 | 1:F:1047:GLN:H | 1.87 | 0.40 |
| 1:F:1087:ARG:H | 1:F:1087:ARG:HG2 | 1.65 | 0.40 |
| 1:F:1203:SER:N | 1:F:1204:PRO:HD3 | 2.36 | 0.40 |
| 1:F:1622:ILE:HD12 | 1:F:1622:ILE:HA | 1.92 | 0.40 |
| 1:F:2130:HIS:CD2 | 1:F:2167:PRO:HG3 | 2.57 | 0.40 |
| 1:F:2288:TYR:CZ | 1:F:2290:PRO:HA | 2.56 | 0.40 |
| 1:F:2820:MET:HA | 1:F:2823:PHE:CE1 | 2.56 | 0.40 |
| 1:F:2858:ILE:HD13 | 1:F:2858:ILE:HA | 1.91 | 0.40 |
| 1:F:2964:ASP:OD1 | 1:F:2967:GLU:HB3 | 2.22 | 0.40 |
| 1:F:3700:GLU:HG2 | 1:F:3704:GLN:HE21 | 1.87 | 0.40 |
| 1:F:3736:LYS:O | 1:F:3752:VAL:N | 2.44 | 0.40 |
| 1:F:3886:ALA:O | 1:F:3889:ARG:HB3 | 2.22 | 0.40 |
| 3:H:132:ILE:O | 3:H:161:LEU:HA | 2.21 | 0.40 |
| 3:H:236:VAL:O | 3:H:238:LYS:HE3 | 2.22 | 0.40 |
| 4:K:147:GLU:O | 4:K:151:LEU:HD23 | 2.21 | 0.40 |
| 4:K:155:TRP:HD1 | 4:L:158:VAL:HG11 | 1.86 | 0.40 |
| 4:K:158:VAL:HG11 | 4:L:159:GLN:OE1 | 2.21 | 0.40 |
| 6:R:35:ALA:HB1 | 6:R:46:HIS:CE1 | 2.56 | 0.40 |
| 6:R:151:ARG:O | 6:R:155:THR:HG23 | 2.22 | 0.40 |
| 7:D:23:DT:H5" | 7:D:24:DT:O4 | 2.22 | 0.40 |
| 1:A:332:GLU:HB2 | 1:A:335:LYS:HZ2 | 1.85 | 0.40 |
| 1:A:1253:THR:O | 1:A:1257:LEU:HG | 2.21 | 0.40 |
| 1:A:1721:HIS:HB3 | 1:A:1739:TYR:CE1 | 2.57 | 0.40 |
| 1:A:2335:ASN:OD1 | 1:A:2336:ILE:N | 2.51 | 0.40 |
| 1:A:2427:ARG:HG3 | 1:A:2432:GLN:NE2 | 2.37 | 0.40 |
| 1:A:2957:LEU:HD23 | 1:A:2957:LEU:HA | 1.82 | 0.40 |
| 1:A:3996:GLY:O | 1:A:4000:ASN:ND2 | 2.54 | 0.40 |
| 2:B:220:ILE:HG23 | 2:B:221:ILE:HG13 | 2.04 | 0.40 |
| 2:B:300:THR:HB | 3:C:293:THR:HG23 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:246:HIS:HB2 | 3:C:264:TYR:CE2 | 2.57 | 0.40 |
| 3:C:408:ALA:HA | 3:C:421:TYR:HA | 2.04 | 0.40 |
| 1:F:2952:ILE:HD11 | 1:F:2971:GLN:OE1 | 2.21 | 0.40 |
| 1:F:3997:LEU:HD23 | 1:F:3997:LEU:HA | 1.96 | 0.40 |
| 1:F:4011:PHE:HA | 1:F:4014:LYS:NZ | 2.36 | 0.40 |
| 2:G:337:LEU:HD11 | 3:H:493:CYS:SG | 2.61 | 0.40 |
| 3:H:6:ASN:HA | 3:H:128:GLU:OE1 | 2.22 | 0.40 |
| 3:H:16:VAL:O | 3:H:16:VAL:HG12 | 2.21 | 0.40 |
| 5:M:753:HIS:NE2 | 5:M:757:GLU:OE2 | 2.55 | 0.40 |
| 4:O:20:LEU:HD13 | 4:O:37:THR:HG22 | 2.03 | 0.40 |
| 5:P:741:ARG:NH1 | 5:P:742:PHE:HB3 | 2.37 | 0.40 |
| 5:P:878:PHE:O | 5:P:881:THR:OG1 | 2.25 | 0.40 |
| 7:D:22:DG:H8 | 7:D:23:DT:H72 | 1.85 | 0.40 |
| 1:A:76:ILE:HD11 | 1:A:122:LYS:HE2 | 2.04 | 0.40 |
| 1:A:527:TYR:HB2 | 1:A:629:PHE:HE1 | 1.86 | 0.40 |
| 1:A:717:LYS:HB3 | 1:A:721:TYR:OH | 2.22 | 0.40 |
| 1:A:718:MET:HA | 1:A:721:TYR:CD2 | 2.57 | 0.40 |
| 1:A:1487:VAL:HG23 | 1:A:1488:TYR:CD1 | 2.52 | 0.40 |
| 1:A:1769:GLU:HB2 | 1:A:1772:HIS:CG | 2.57 | 0.40 |
| 1:A:2333:ARG:NH2 | 1:A:2371:PHE:HE1 | 2.18 | 0.40 |
| 1:A:3870:SER:O | 1:A:3874:ARG:NE | 2.34 | 0.40 |
| 1:A:3929:MET:N | 1:A:3938:ILE:O | 2.51 | 0.40 |
| 2:B:33:SER:HB2 | 2:B:253:LYS:HZ3 | 1.86 | 0.40 |
| 2:B:102:ILE:HD11 | 2:B:145:GLU:HB3 | 2.04 | 0.40 |
| 2:B:299:LYS:HB3 | 2:B:299:LYS:HE2 | 1.73 | 0.40 |
| 2:B:350:PHE:HB2 | 3:C:461:MET:O | 2.22 | 0.40 |
| 2:B:485:GLN:NE2 | 3:C:333:TYR:H | 2.19 | 0.40 |
| 2:B:514:MET:SD | 2:B:515:ASN:N | 2.94 | 0.40 |
| 3:C:238:LYS:NZ | 3:C:240:ILE:O | 2.55 | 0.40 |
| 3:C:485:PRO:HG2 | 3:C:516:LEU:HD21 | 2.02 | 0.40 |
| 1:F:275:PHE:CE2 | 1:F:319:PHE:HB2 | 2.56 | 0.40 |
| 1:F:363:ILE:HD13 | 1:F:366:TYR:CE2 | 2.57 | 0.40 |
| 1:F:409:GLN:OE1 | 1:F:409:GLN:N | 2.47 | 0.40 |
| 1:F:527:TYR:HB2 | 1:F:629:PHE:CE1 | 2.56 | 0.40 |
| 1:F:637:LYS:HD2 | 1:F:637:LYS:HA | 1.86 | 0.40 |
| 1:F:977:ASP:OD1 | 1:F:978:GLN:N | 2.54 | 0.40 |
| 1:F:1013:ILE:HA | 1:F:1017:ILE:HD13 | 2.04 | 0.40 |
| 1:F:1429:GLU:HB3 | 1:F:1482:GLU:OE2 | 2.21 | 0.40 |
| 1:F:1697:PRO:HA | 1:F:1753:SER:HB3 | 2.04 | 0.40 |
| 1:F:1723:PRO:O | 1:F:1768:ARG:NH1 | 2.53 | 0.40 |
| 1:F:2253:TYR:HA | 1:F:2256:ILE:HD12 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2849:SER:HB3 | 1:F:3080:LEU:HD13 | 2.04 | 0.40 |
| 2:G:189:LYS:HE2 | 2:G:189:LYS:HB3 | 1.85 | 0.40 |
| 2:G:252:ARG:HB2 | 3:H:431:ARG:HD2 | 2.03 | 0.40 |
| 3:H:346:CYS:SG | 3:H:350:GLN:HG3 | 2.61 | 0.40 |
| 4:K:187:LYS:HZ2 | 4:L:187:LYS:HB2 | 1.86 | 0.40 |
| 5:M:787:GLN:OE1 | 5:M:787:GLN:N | 2.54 | 0.40 |
| 4:O:20:LEU:HB2 | 4:O:37:THR:HG22 | 2.02 | 0.40 |
| 7:D:26:DT:H2" | 7:D:27:DT:C6 | 2.56 | 0.40 |
| 9:J:32:DT:H2" | 9:J:33:DA:O4' | 2.20 | 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 | 3474/4148 (84%) | 3222 (93%) | 248 (7%) | 4 (0%) | 51 85 |
| 1 | F | 3467/4148 (84%) | 3198 (92%) | 265 (8%) | 4 (0%) | 51 85 |
| 2 | B | 468/609 (77%) | 430 (92%) | 37 (8%) | 1 (0%) | 47 80 |
| 2 | G | 485/609 (80%) | 460 (95%) | 25 (5%) | 0 | 100 100 |
| 3 | C | 465/732 (64%) | 445 (96%) | 20 (4%) | 0 | 100 100 |
| 3 | H | 636/732 (87%) | 597 (94%) | 39 (6%) | 0 | 100 100 |
| 4 | K | 199/336 (59%) | 195 (98%) | 4 (2%) | 0 | 100 100 |
| 4 | L | 191/336 (57%) | 184 (96%) | 7 (4%) | 0 | 100 100 |
| 4 | N | 199/336 (59%) | 191 (96%) | 8 (4%) | 0 | 100 100 |
| 4 | O | 190/336 (56%) | 182 (96%) | 8 (4%) | 0 | 100 100 |
| 5 | M | 256/911 (28%) | 239 (93%) | 17 (7%) | 0 | 100 100 |
| 5 | P | 242/911 (27%) | 225 (93%) | 16 (7%) | 1 (0%) | 34 71 |
| 6 | Q | 205/299 (69%) | 185 (90%) | 20 (10%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 6 | R | 214/299 (72%) | 200 (94%) | 14 (6%) | 0 | 100 100 |
| All | All | 10691/14742 (72%) | 9953 (93%) | 728 (7%) | 10 (0%) | 54 85 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2291 | GLN |
| 1 | F | 955 | ALA |
| 1 | F | 956 | PRO |
| 1 | F | 2291 | GLN |
| 1 | A | 1550 | VAL |
| 1 | A | 3671 | ASN |
| 2 | B | 213 | ILE |
| 1 | F | 3304 | VAL |
| 1 | A | 841 | SER |
| 5 | P | 849 | GLY |

### 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 | 3054/3671 (83%) | 3040 (100%) | 14 (0%) | 88 93 |
| 1 | F | 3058/3671 (83%) | 3048 (100%) | 10 (0%) | 92 95 |
| 2 | B | 427/548 (78%) | 425 (100%) | 2 (0%) | 88 93 |
| 2 | G | 444/548 (81%) | 444 (100%) | 0 | 100 100 |
| 3 | C | 434/649 (67%) | 432 (100%) | 2 (0%) | 88 93 |
| 3 | H | 575/649 (89%) | 573 (100%) | 2 (0%) | 92 95 |
| 4 | K | 179/303 (59%) | 178 (99%) | 1 (1%) | 86 92 |
| 4 | L | 177/303 (58%) | 174 (98%) | 3 (2%) | 60 78 |
| 4 | N | 179/303 (59%) | 177 (99%) | 2 (1%) | 73 84 |
| 4 | O | 175/303 (58%) | 175 (100%) | 0 | 100 100 |
| 5 | M | 234/808 (29%) | 232 (99%) | 2 (1%) | 78 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 5 | P | 217/808 (27%) | 214 (99%) | 3 (1%) | 67 80 |
| 6 | Q | 187/262 (71%) | 186 (100%) | 1 (0%) | 88 93 |
| 6 | R | 191/262 (73%) | 189 (99%) | 2 (1%) | 76 86 |
| All | All | 9531/13088 (73%) | 9487 (100%) | 44 (0%) | 89 93 |

All (44) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 782 | ARG |
| 1 | A | 802 | THR |
| 1 | A | 946 | THR |
| 1 | A | 1426 | GLN |
| 1 | A | 1539 | SER |
| 1 | A | 1549 | SER |
| 1 | A | 1727 | ARG |
| 1 | A | 1768 | ARG |
| 1 | A | 2263 | LYS |
| 1 | A | 2311 | ARG |
| 1 | A | 2734 | ARG |
| 1 | A | 3621 | LYS |
| 1 | A | 3874 | ARG |
| 1 | A | 4090 | ARG |
| 2 | B | 247 | ARG |
| 2 | B | 252 | ARG |
| 3 | C | 232 | ARG |
| 3 | C | 338 | LYS |
| 1 | F | 442 | GLN |
| 1 | F | 453 | MET |
| 1 | F | 476 | ARG |
| 1 | F | 1727 | ARG |
| 1 | F | 1768 | ARG |
| 1 | F | 2311 | ARG |
| 1 | F | 3621 | LYS |
| 1 | F | 3664 | ASN |
| 1 | F | 3874 | ARG |
| 1 | F | 4090 | ARG |
| 3 | H | 332 | LYS |
| 3 | H | 399 | LYS |
| 4 | K | 107 | ARG |
| 4 | L | 146 | LYS |
| 4 | L | 150 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | L | 164 | LYS |
| 5 | M | 782 | LYS |
| 5 | M | 883 | LYS |
| 4 | N | 107 | ARG |
| 4 | N | 153 | ARG |
| 5 | P | 741 | ARG |
| 5 | P | 817 | THR |
| 5 | P | 890 | LYS |
| 6 | Q | 64 | ARG |
| 6 | R | 63 | LYS |
| 6 | R | 124 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 409 | GLN |
| 1 | A | 676 | ASN |
| 1 | A | 1043 | GLN |
| 1 | A | 1069 | HIS |
| 1 | A | 1201 | ASN |
| 1 | A | 1568 | ASN |
| 1 | A | 1611 | GLN |
| 1 | A | 2291 | GLN |
| 1 | A | 2348 | GLN |
| 1 | A | 2353 | GLN |
| 1 | A | 2751 | GLN |
| 1 | A | 2838 | GLN |
| 1 | A | 2954 | GLN |
| 1 | A | 3148 | GLN |
| 1 | A | 3150 | ASN |
| 1 | A | 3166 | ASN |
| 1 | A | 3515 | GLN |
| 1 | A | 3704 | GLN |
| 1 | A | 3915 | HIS |
| 1 | A | 3966 | GLN |
| 2 | B | 293 | ASN |
| 2 | B | 359 | HIS |
| 1 | F | 344 | GLN |
| 1 | F | 676 | ASN |
| 1 | F | 982 | GLN |
| 1 | F | 1043 | GLN |
| 1 | F | 1268 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 1568 | ASN |
| 1 | F | 2217 | ASN |
| 1 | F | 2291 | GLN |
| 1 | F | 2348 | GLN |
| 1 | F | 2353 | GLN |
| 1 | F | 2365 | ASN |
| 1 | F | 2426 | HIS |
| 1 | F | 2587 | GLN |
| 1 | F | 2834 | GLN |
| 1 | F | 2859 | GLN |
| 1 | F | 3704 | GLN |
| 1 | F | 3743 | HIS |
| 1 | F | 3924 | HIS |
| 1 | F | 3927 | ASN |
| 1 | F | 4055 | ASN |
| 2 | G | 178 | ASN |
| 2 | G | 426 | GLN |
| 3 | H | 496 | HIS |
| 3 | H | 500 | HIS |
| 3 | H | 657 | ASN |
| 3 | H | 680 | GLN |
| 4 | L | 148 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | F | 1 |
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | F | 4128:MET | C | 6004:UNK | N | 90.10 |
| 1 | A | 4128:MET | C | 6004:UNK | N | 89.52 |

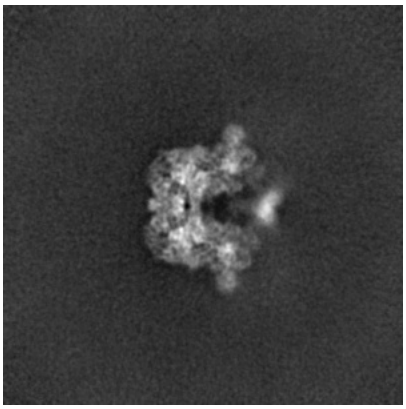
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12299. These allow visual inspection of the internal detail of the map and identification of artifacts.

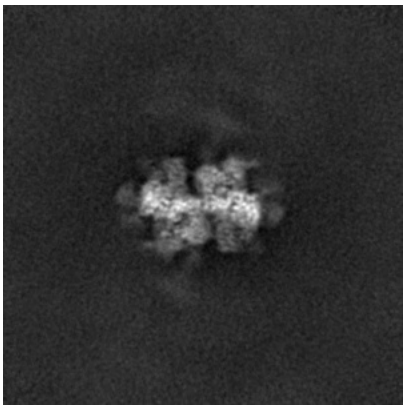
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

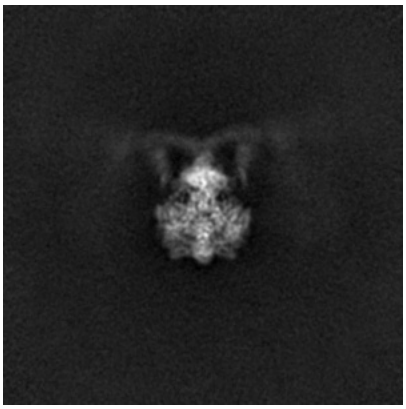
### 6.1.1 Primary map



X

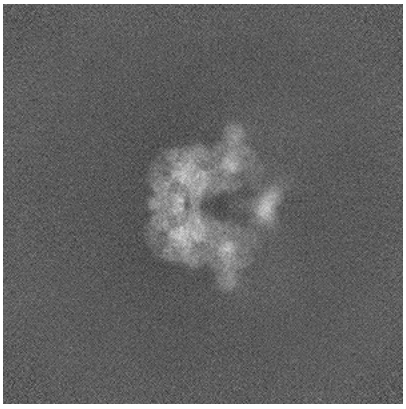


Y

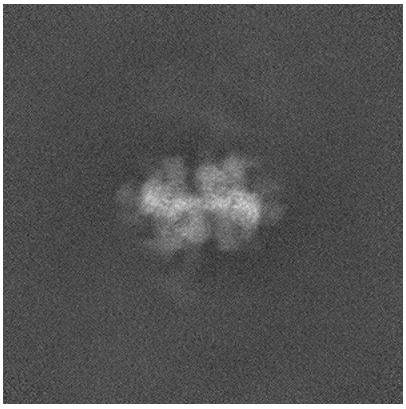


Z

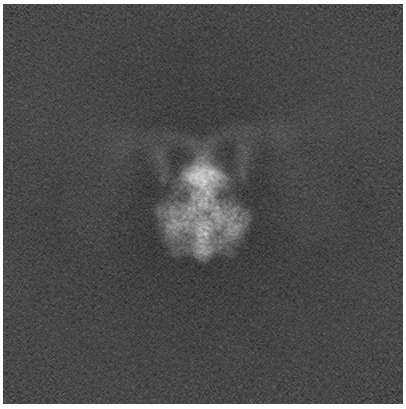
### 6.1.2 Raw map



X



Y

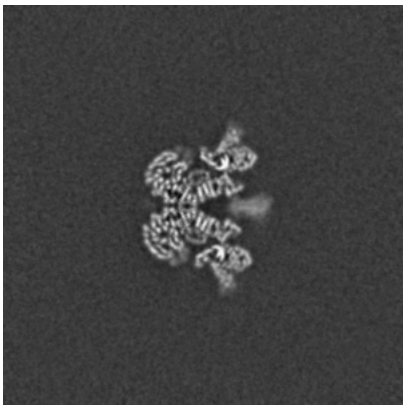


Z

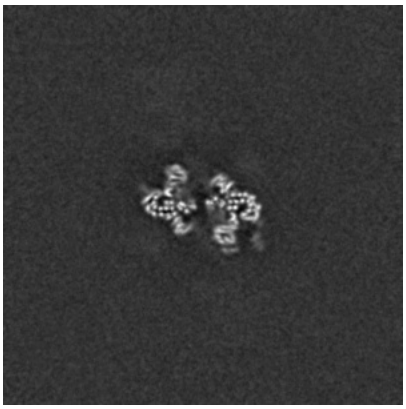
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

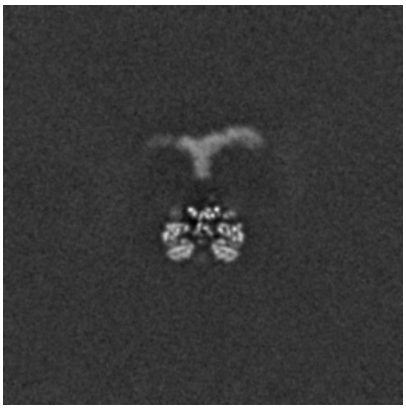
### 6.2.1 Primary map



X Index: 270

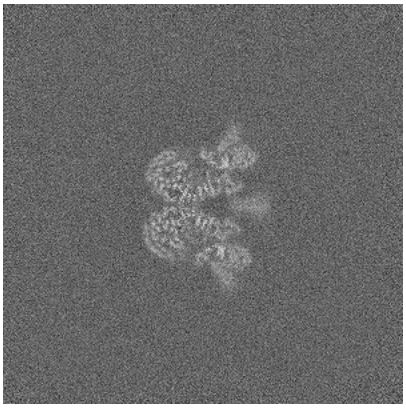


Y Index: 270

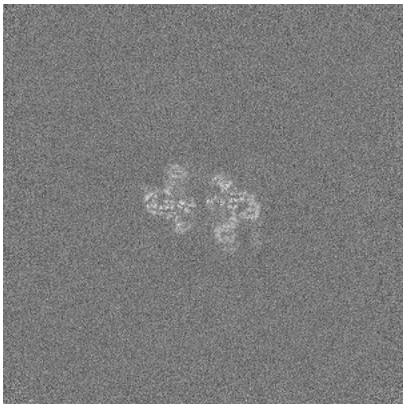


Z Index: 270

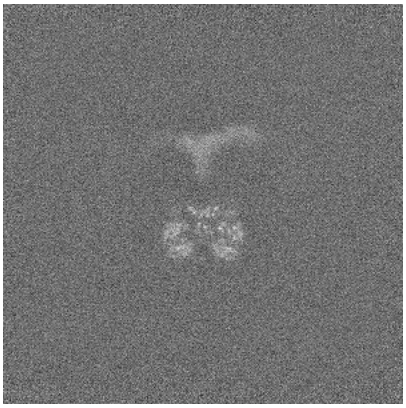
### 6.2.2 Raw map



X Index: 270



Y Index: 270

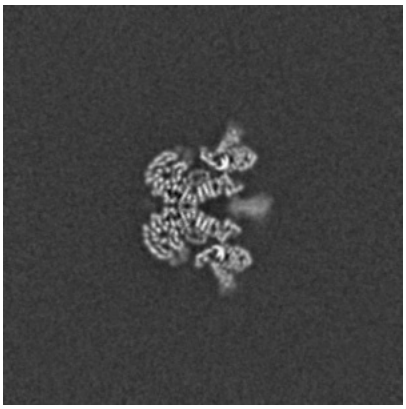


Z Index: 270

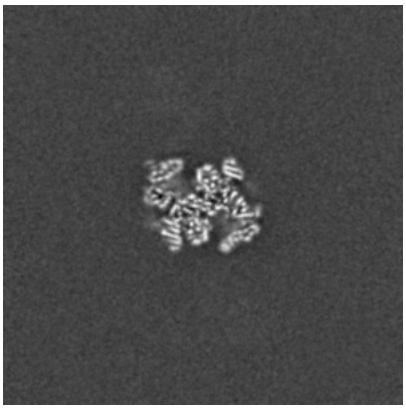
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map



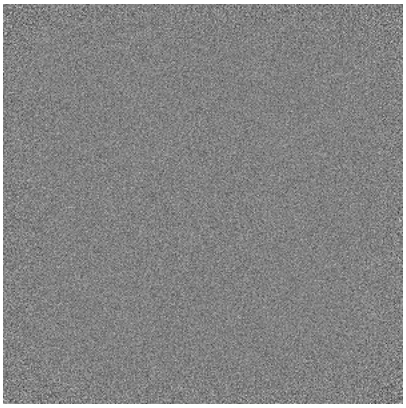
X Index: 270



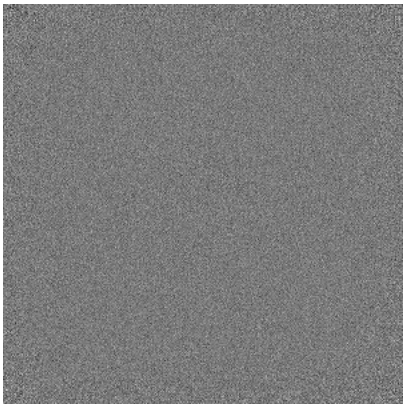
Y Index: 241

Z Index: 313

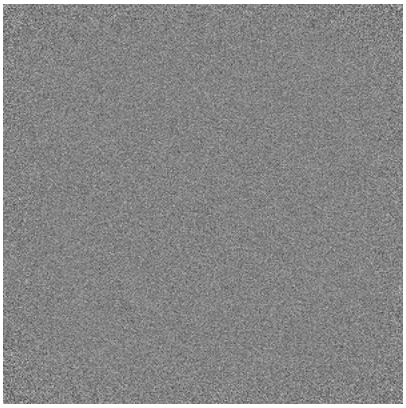
### 6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

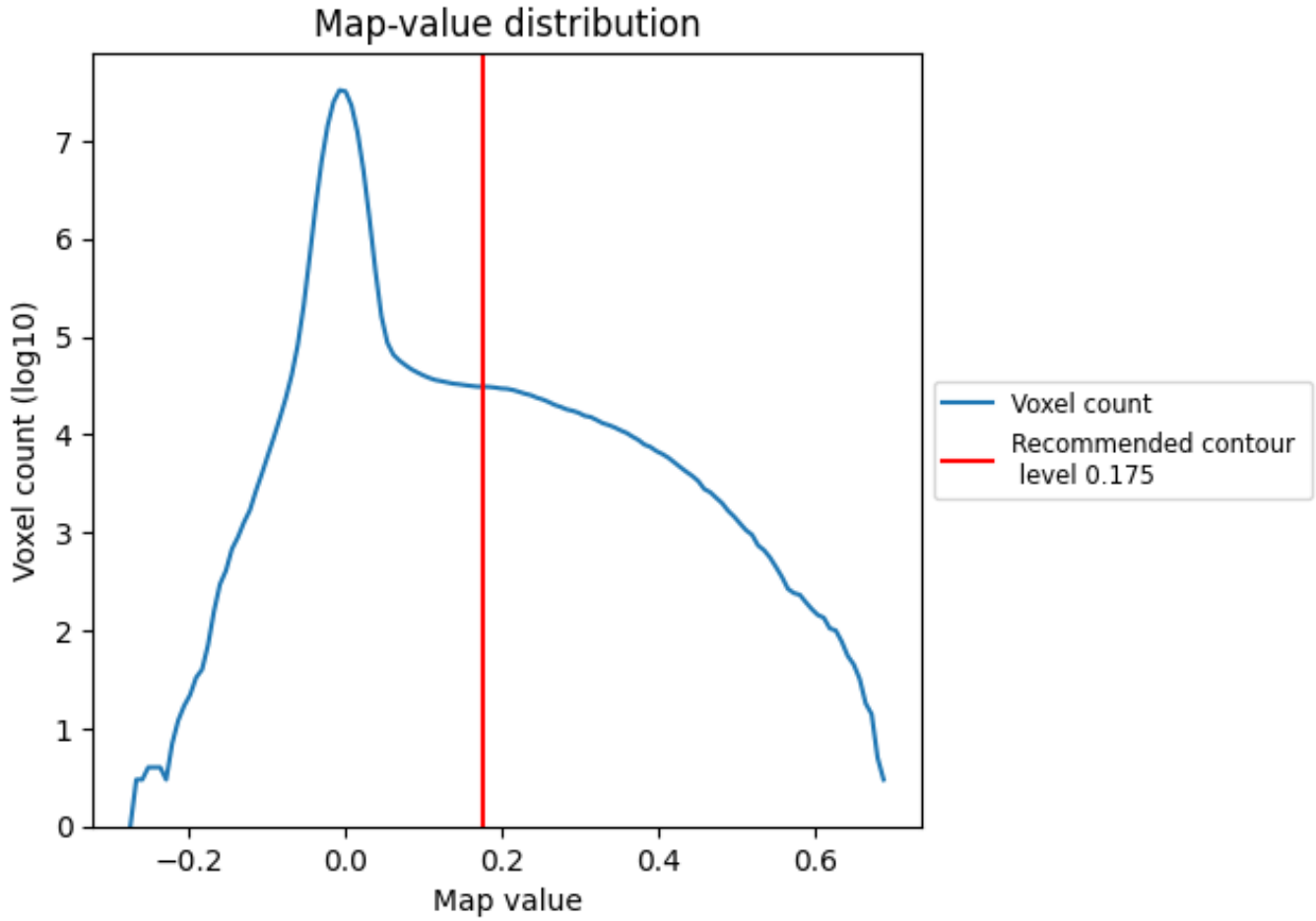
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

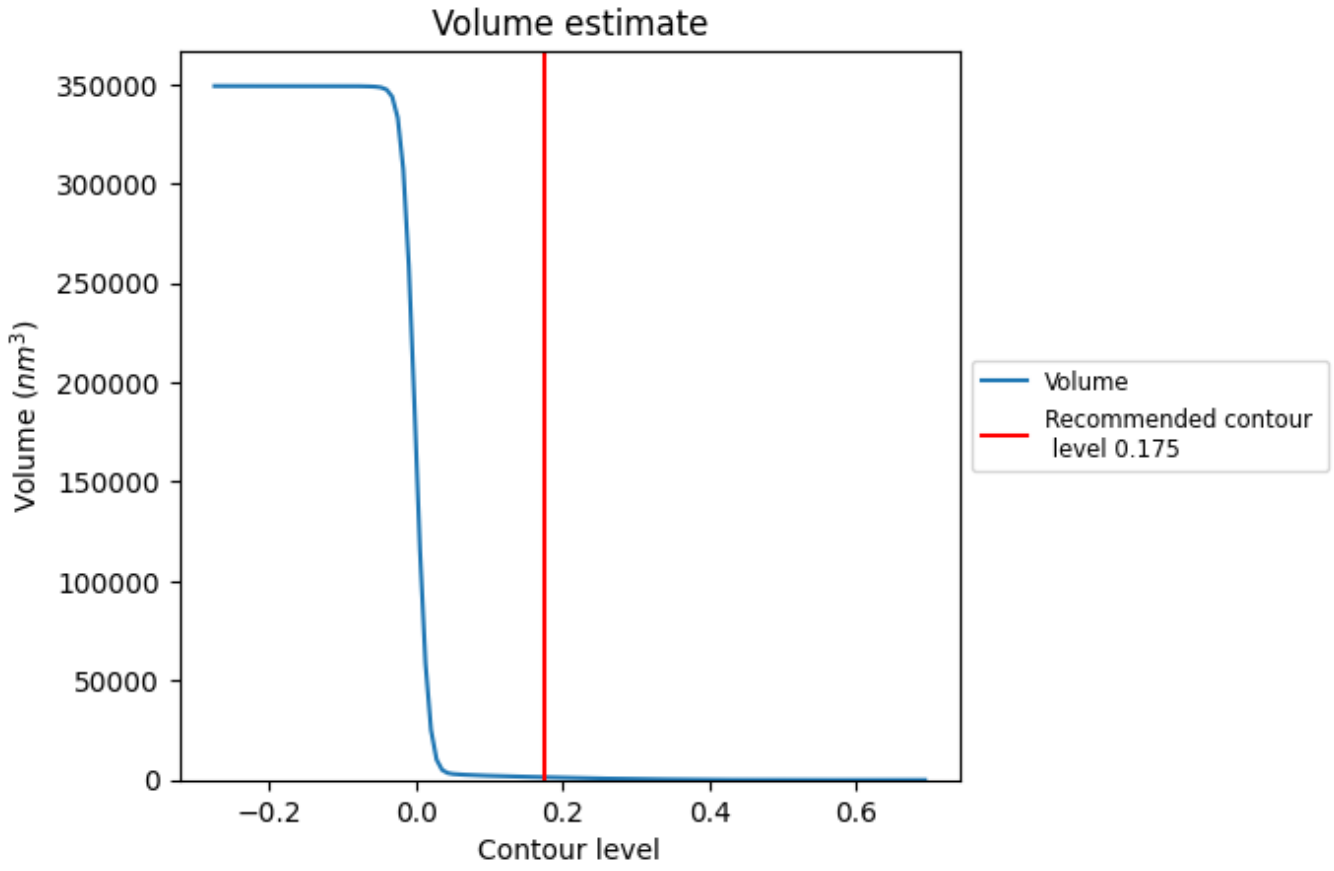
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

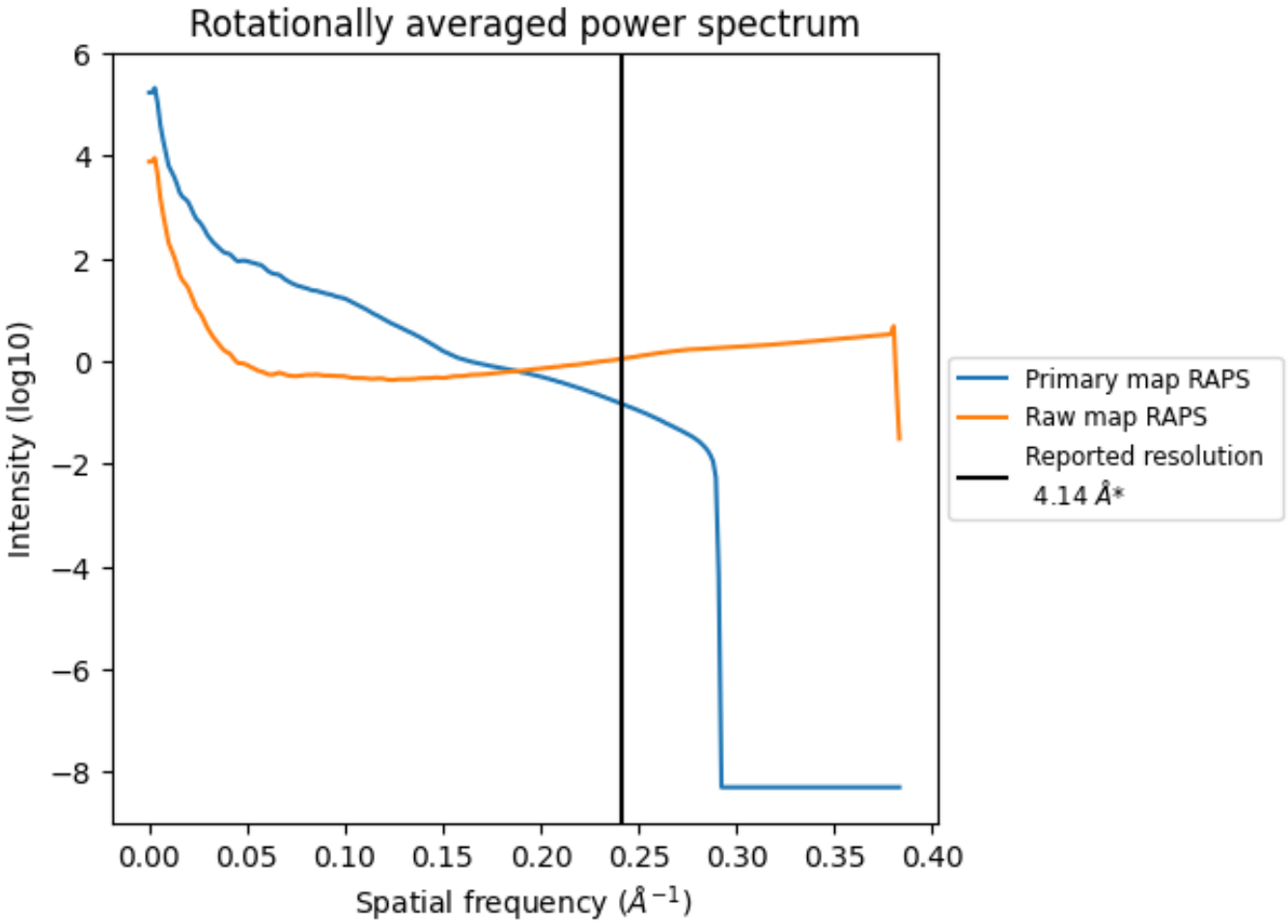
## 7.2 Volume estimate




The volume at the recommended contour level is 1371 $nm^3$; this corresponds to an approximate mass of 1239 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)

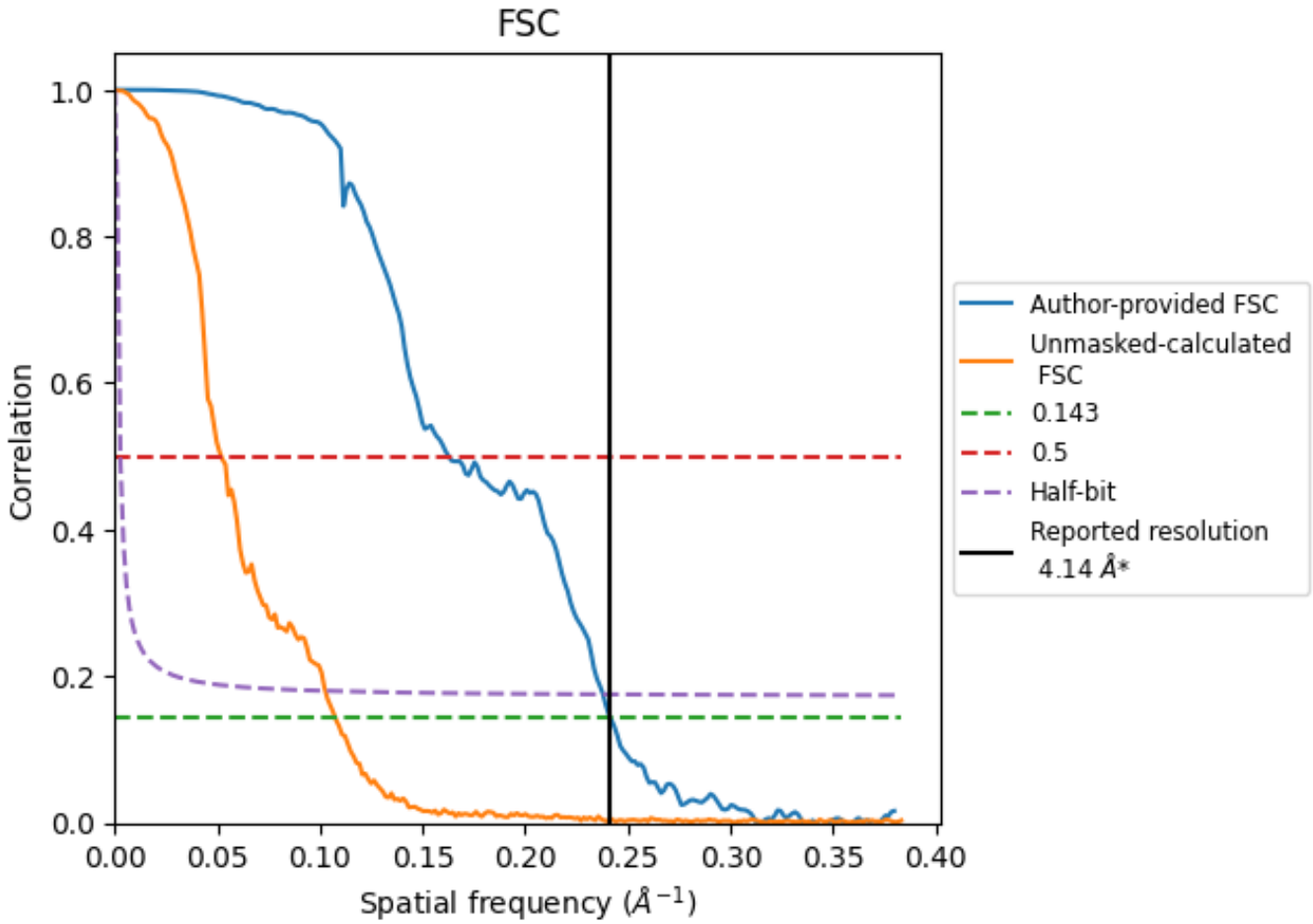



*Reported resolution corresponds to spatial frequency of 0.242 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.242 Å$^{-1}$

## 8.2 Resolution estimates (i)

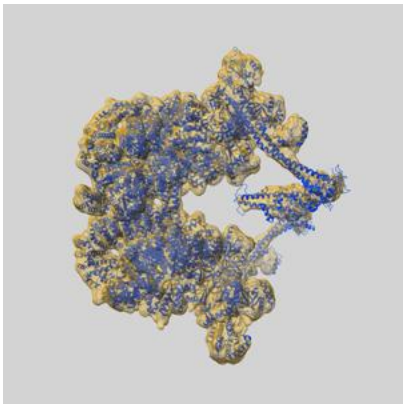
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.14 | - | - |
| Author-provided FSC curve | 4.14 | 6.14 | 4.20 |
| Unmasked-calculated* | 9.30 | 19.27 | 9.74 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.30 differs from the reported value 4.14 by more than 10 %

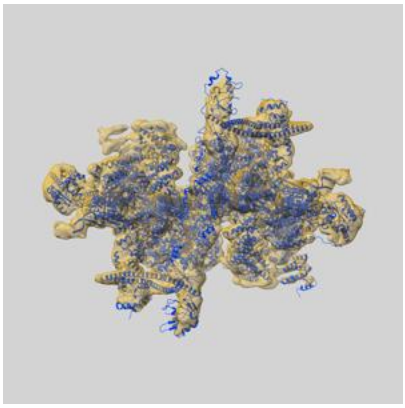
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12299 and PDB model 7NFC. Per-residue inclusion information can be found in section 3 on page 6.

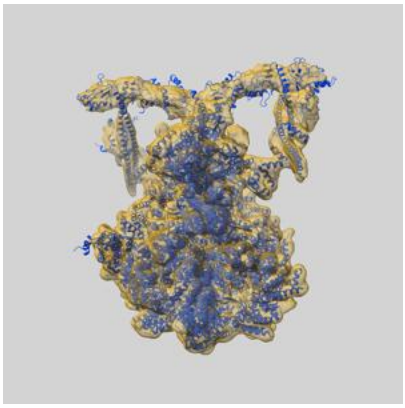
## 9.1 Map-model overlay



X



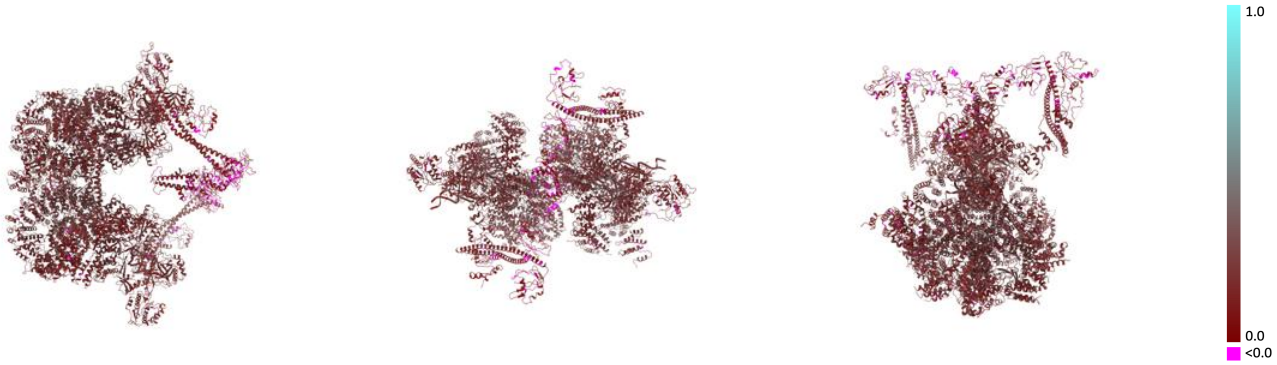
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

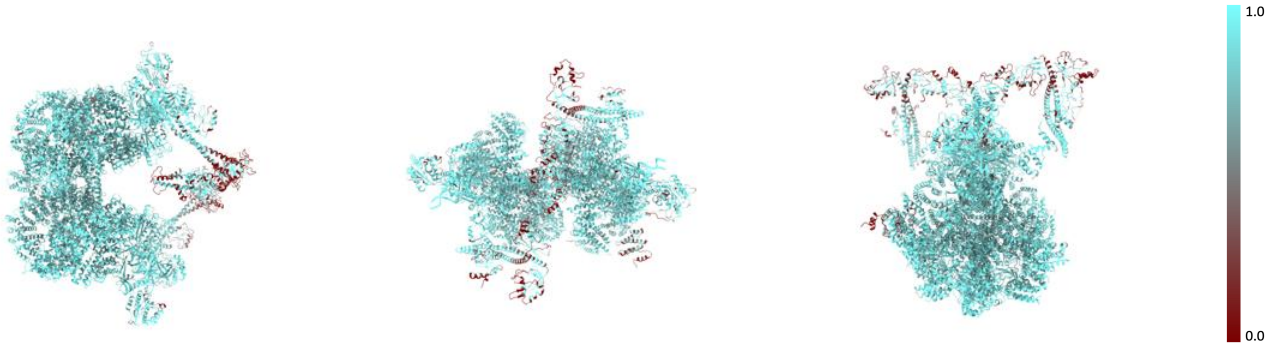
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

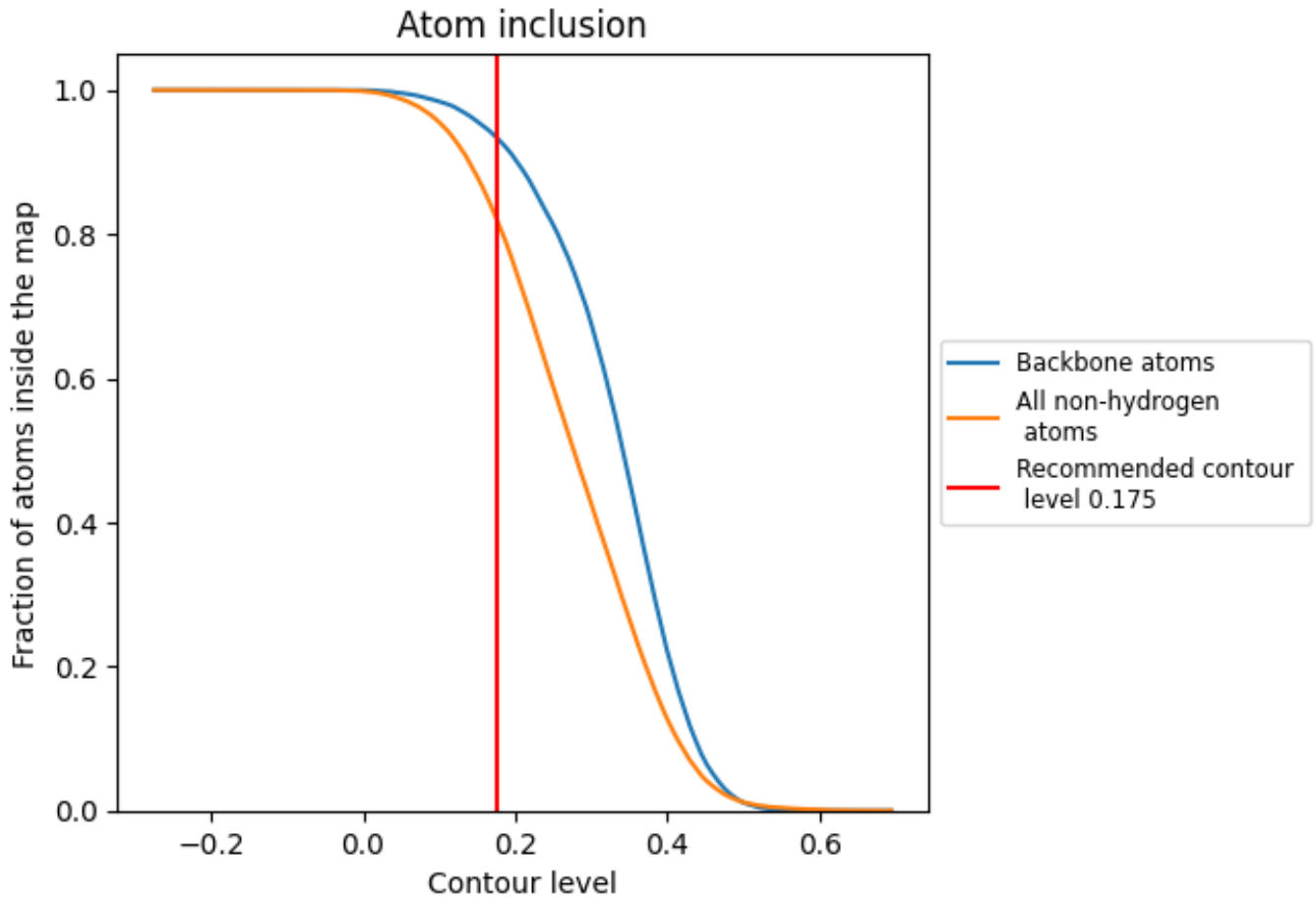
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).

## 9.4 Atom inclusion (i)




At the recommended contour level, 93% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.175) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8224 | 0.2000 |
| A | 0.8612 | 0.2150 |
| B | 0.8785 | 0.2140 |
| C | 0.8575 | 0.2000 |
| D | 0.9191 | 0.2360 |
| E | 0.9288 | 0.2190 |
| F | 0.8628 | 0.2170 |
| G | 0.8787 | 0.2170 |
| H | 0.7593 | 0.1840 |
| I | 0.9288 | 0.2420 |
| J | 0.9318 | 0.2470 |
| K | 0.6287 | 0.1220 |
| L | 0.5850 | 0.1210 |
| M | 0.7294 | 0.1570 |
| N | 0.5899 | 0.1080 |
| O | 0.5000 | 0.1150 |
| P | 0.8410 | 0.1680 |
| Q | 0.5409 | 0.1000 |
| R | 0.5341 | 0.0830 |