



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 07:49 PM UTC

PDB ID : 6YEH / pdb\_00006yeh  
EMDB ID : EMD-10797  
Title : Xenorhabdus nematophila XptA1 in complex with porcine mucosa heparin  
Authors : Roderer, D.; Broecker, F.; Sitsel, O.; Kaplonek, P.; Leidreiter, F.; Seeberger, P.H.; Raunser, S.  
Deposited on : 2020-03-25  
Resolution : 3.70 Å(reported)  
Based on initial model : 6RW8

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

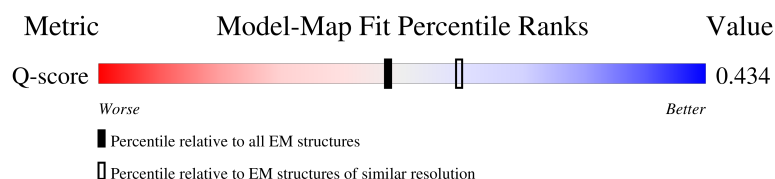
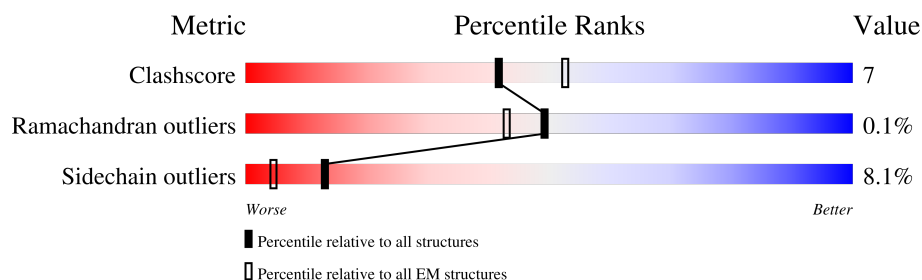
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 2523   |                  |
| 1   | B     | 2523   |                  |
| 1   | C     | 2523   |                  |
| 1   | D     | 2523   |                  |

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| Mol | Chain | Length | Quality of chain                                                                                       |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------|
| 1   | E     | 2523   |  <div>71%20%7%</div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 93500 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.

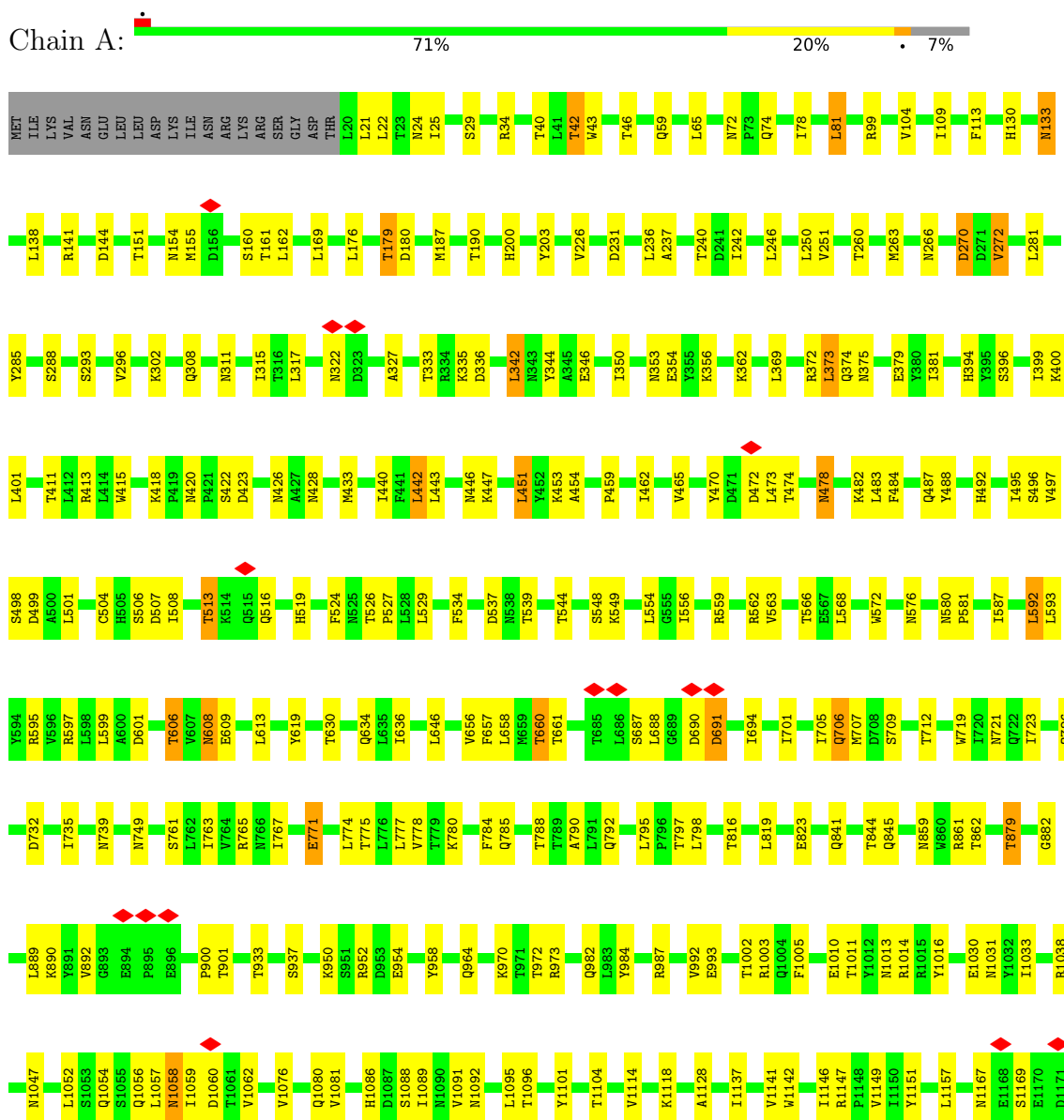
- Molecule 1 is a protein called A component of insecticidal toxin complex (Tc).

| Mol | Chain | Residues | Atoms |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| 1   | A     | 2337     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18700 | 11894 | 3132 | 3607 | 67 |         |       |
| 1   | B     | 2337     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18700 | 11894 | 3132 | 3607 | 67 |         |       |
| 1   | C     | 2337     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18700 | 11894 | 3132 | 3607 | 67 |         |       |
| 1   | D     | 2337     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18700 | 11894 | 3132 | 3607 | 67 |         |       |
| 1   | E     | 2337     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18700 | 11894 | 3132 | 3607 | 67 |         |       |

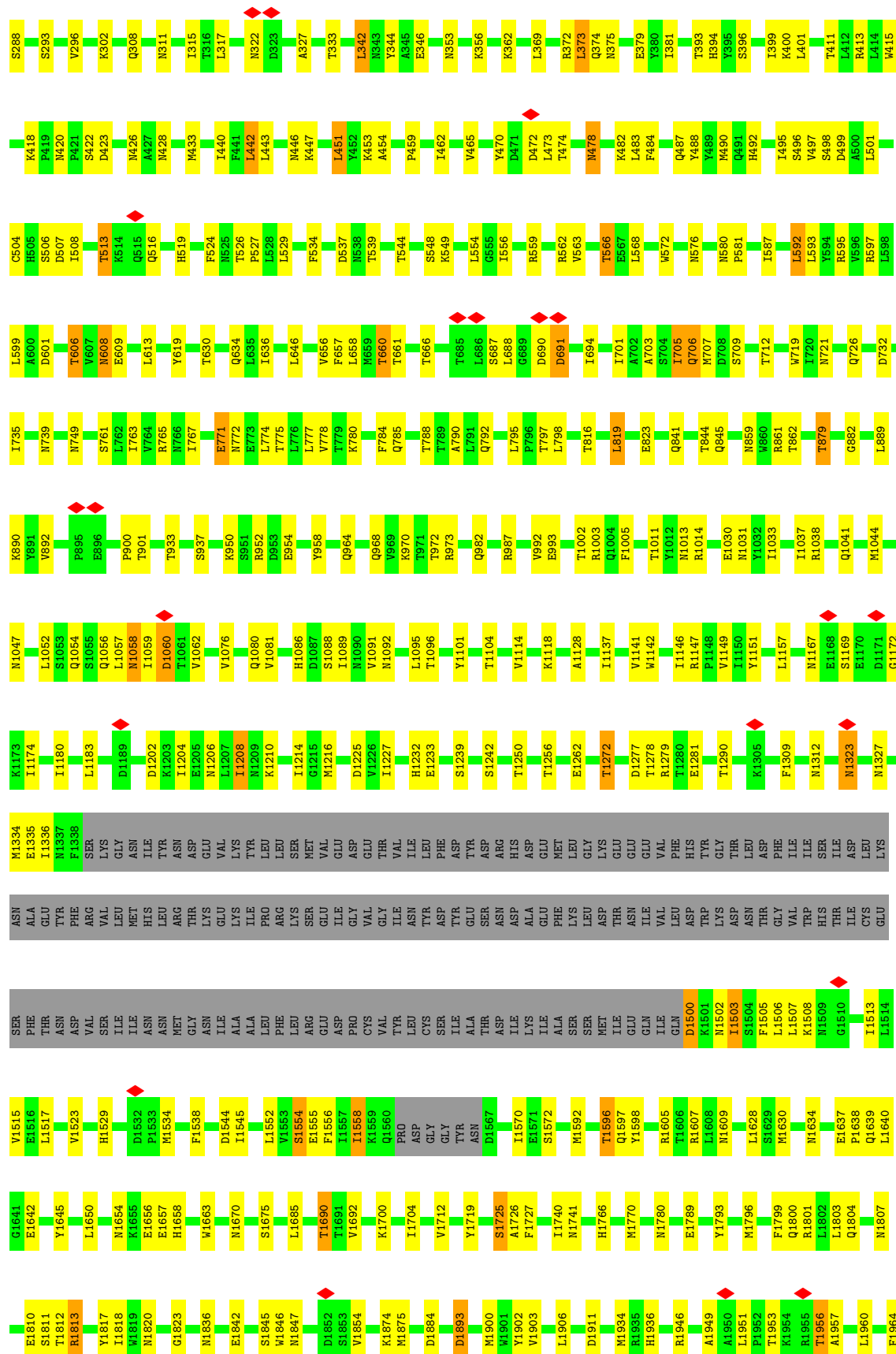
### 3 Residue-property plots

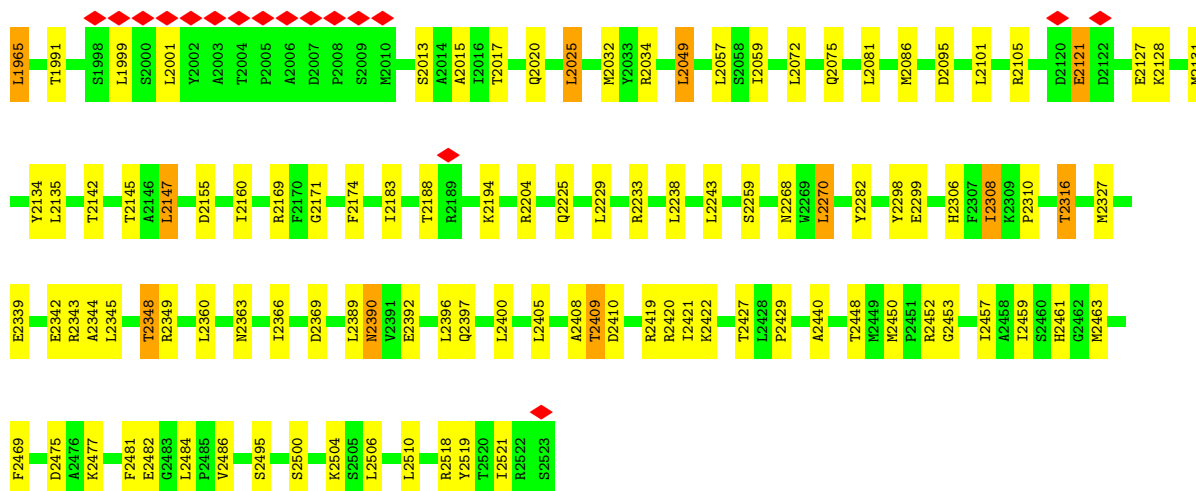
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

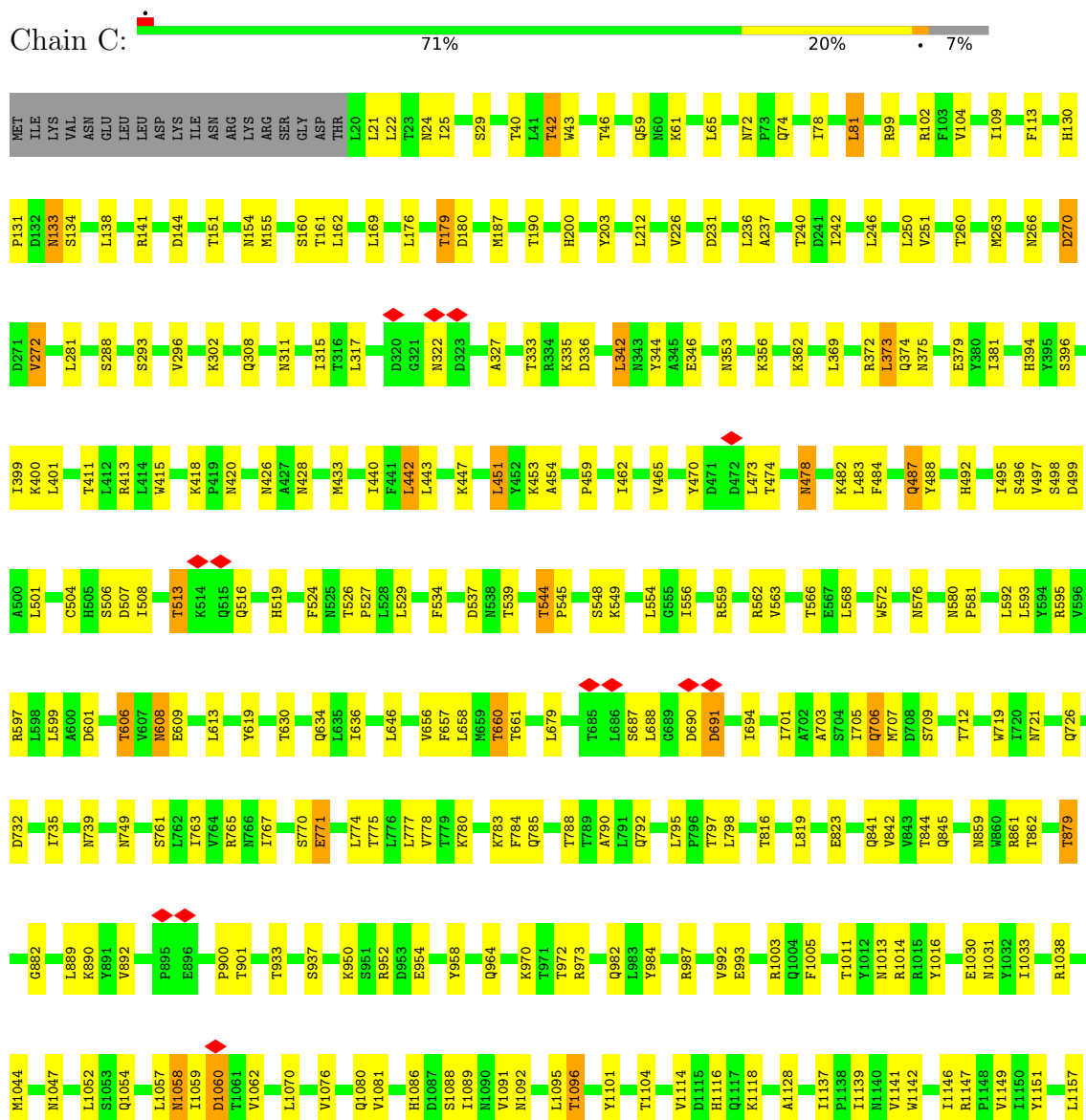




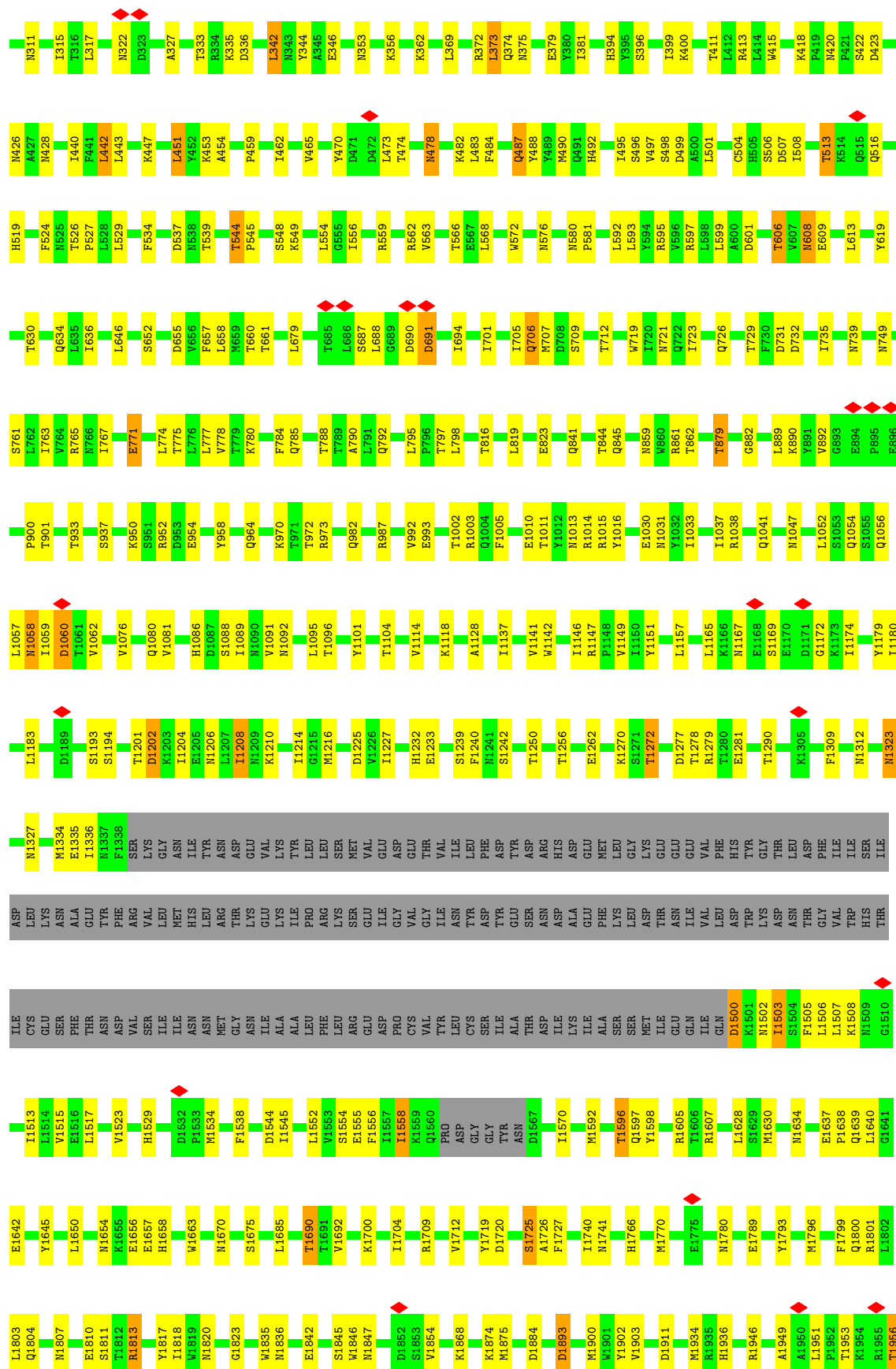


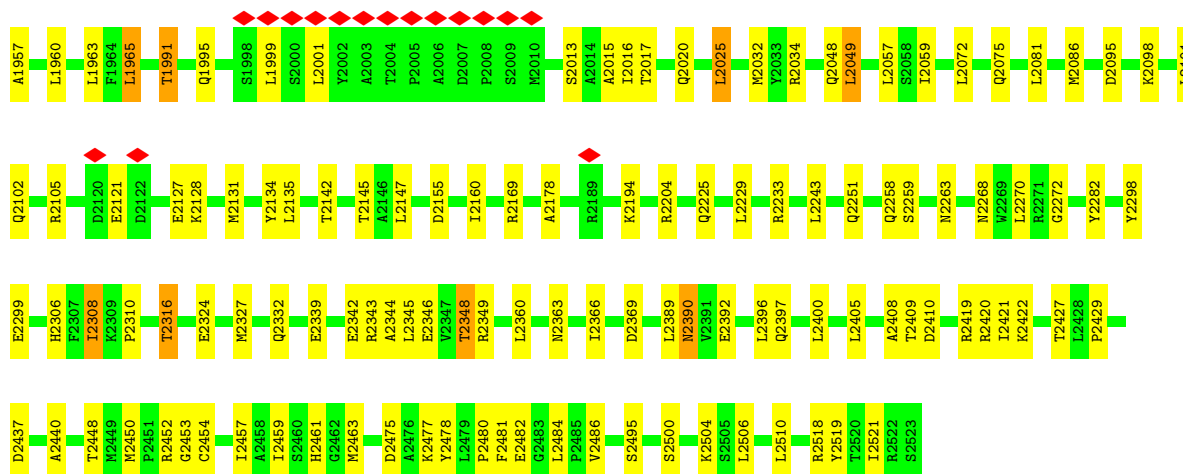


- Molecule 1: A component of insecticidal toxin complex (Tc)



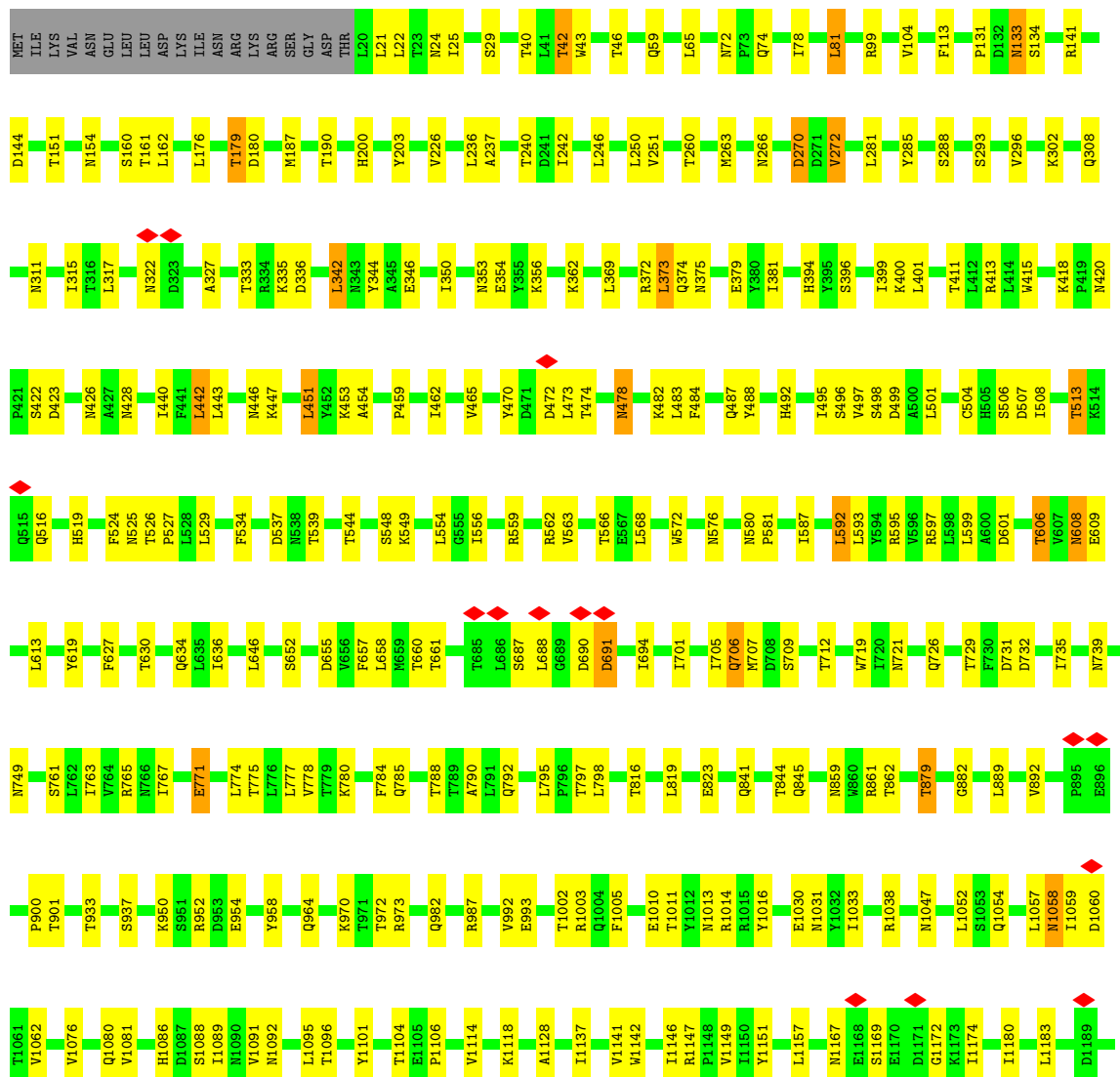






- Molecule 1: A component of insecticidal toxin complex (Tc)

Chain E: 71% 20% 7%



|       |       |       |       |       |       |       |     |       |       |
|-------|-------|-------|-------|-------|-------|-------|-----|-------|-------|
| T2448 | Y2282 | M2086 | F1952 | L1803 | L1640 | V1523 | PHE | E1335 | S1193 |
| M2449 | Y2298 | D2095 | T1953 | Q1804 | G1641 | V1523 | THR | I1336 | S1194 |
| M2450 | E2299 | R1954 | K1954 | E1805 | E1642 | H1529 | ASP | N1337 | D1202 |
| R2451 | H2306 | K2098 | T1955 | Q1806 | Y1645 | E1530 | VAL | F1338 | K1203 |
| G2453 | F2307 | L2101 | A1956 | E1810 | L1650 | S1531 | SER | LYS   | I1204 |
| T2457 | T2308 | Q2102 | L1960 | S1811 | N1654 | D1532 | ILE | GLY   | E1205 |
| D2475 | K2309 | R2105 | F1964 | R1813 | K1655 | P1533 | ILE | ASN   | N1206 |
| A2476 | P2310 | D2120 | L1965 | Y1817 | E1656 | F1538 | ASN | THR   | I1207 |
| K2477 | M2327 | E2121 | L1979 | Y1818 | H1658 | D1544 | ASN | GLY   | N1208 |
| Y2478 | M2327 | D2122 | L1991 | Y1819 | H1658 | I1545 | ASN | ASP   | N1209 |
| F2481 | L2330 | E2127 | G1994 | N1820 | W1663 | I1545 | GLY | THR   | K1210 |
| E2482 | E2339 | K2128 | Q1995 | G1823 | N1670 | L1552 | LYS | GLU   | I1214 |
| L2484 | R2343 | M2131 | L1999 | M1836 | S1675 | V1553 | LYS | VAL   | G1215 |
| F2485 | A2344 | Y2134 | S1998 | E1842 | L1685 | S1554 | ARG | PRO   | M1216 |
| V2486 | T2348 | L2135 | S2000 | S1845 | T1690 | E1555 | LEU | LEU   | D1225 |
| S2495 | R2349 | T2142 | L2001 | W1946 | T1691 | F1556 | LEU | SER   | W1226 |
| S2500 | T2350 | T2145 | Y2002 | M1847 | V1692 | I1557 | ARG | MET   | I1227 |
| K2504 | L2360 | L2145 | A2003 | D1852 | Y1702 | K1559 | GLY | VAL   | H1232 |
| S2505 | N2363 | A2146 | T2004 | V1854 | Y1703 | Q1560 | GLY | GLU   | E1233 |
| L2506 | L2366 | L2147 | P2005 | Y1854 | I1704 | PRO   | THR | THR   | N1242 |
| L2510 | D2369 | D2155 | A2006 | D1863 | R1709 | ASP   | ALA | ASP   | T1250 |
| R2518 | L2389 | T2160 | D2007 | P1864 | V1712 | D1667 | THR | SER   | T1256 |
| T2520 | T2390 | R2169 | P2008 | K1874 | Y1719 | I1570 | ASP | ASN   | E1262 |
| R2521 | V2391 | A2178 | S2009 | M1875 | D1720 | S1572 | LYS | ALA   | K1270 |
| S2523 | E2392 | R2189 | M2010 | R1882 | S1725 | M1692 | ALA | PHE   | S1271 |
|       | L2396 | K2194 | S2013 | G1883 | A1726 | T1596 | SER | LYS   | T1272 |
|       | Q2397 | R2204 | A2014 | D1884 | F1727 | Q1597 | SER | LEU   | D1277 |
|       | L2400 | R2204 | T2016 | D1893 | I1740 | Y1598 | ILE | GLU   | T1278 |
|       | L2405 | Q2225 | T2017 | M1900 | N1741 | R1605 | GLU | GLU   | R1279 |
|       | A2408 | L2229 | Q2020 | Y1901 | K1769 | T1606 | ILE | VAL   | T1280 |
|       | T2409 | R2233 | L2025 | V1902 | M1770 | R1607 | LEU | VAL   | E1281 |
|       | D2410 | L2243 | M2032 | V1903 | M1770 | R1614 | ASP | PHE   | T1290 |
|       | R2419 | Q2251 | Y2033 | D1911 | N1780 | D1625 | TRP | LYS   | L1293 |
|       | R2420 | Q2258 | R2034 | E1923 | E1789 | L1628 | ASP | ASP   | K1305 |
|       | I2421 | S2259 | Q2048 | M1934 | Y1793 | S1829 | THR | THR   | F1309 |
|       | K2422 | Q2268 | L2049 | A1935 | M1796 | M1630 | GLY | ILE   | I1312 |
|       | T2427 | S2269 | L2057 | H1936 | M1796 | M1634 | VAL | TRP   | N1323 |
|       | L2428 | N2268 | S2058 | R1946 | F1799 | L1635 | THR | ILE   | I1327 |
|       | P2429 | W2269 | I2059 | A1949 | Q1800 | P1637 | GLY | ASP   | N1327 |
|       | L2442 | L2270 | L2072 | A1950 | R1801 | P1638 | VAL | LEU   | L1334 |
|       |       |       | Q2075 | L1951 | L1802 | Q1639 | TRP | LYS   |       |
|       |       |       | L2081 |       |       |       | ILE | SER   |       |

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C5                               | Depositor |
| Number of particles used             | 172596                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 52                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.111                                   | Depositor |
| Minimum map value                    | -0.060                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.028                                   | Depositor |
| Map size (Å)                         | 484.0, 484.0, 484.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.21, 1.21, 1.21                        | 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     | 0.28         | 0/19100     | 0.51        | 2/25936 (0.0%)   |
| 1   | B     | 0.28         | 0/19100     | 0.51        | 2/25936 (0.0%)   |
| 1   | C     | 0.28         | 0/19100     | 0.51        | 2/25936 (0.0%)   |
| 1   | D     | 0.28         | 0/19100     | 0.51        | 2/25936 (0.0%)   |
| 1   | E     | 0.28         | 0/19100     | 0.51        | 2/25936 (0.0%)   |
| All | All   | 0.28         | 0/95500     | 0.51        | 10/129680 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 2                   |
| All | All   | 0                   | 10                  |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 161 | THR  | CA-C-N | 5.58 | 132.20      | 121.54   |
| 1   | D     | 161 | THR  | C-N-CA | 5.58 | 132.20      | 121.54   |
| 1   | A     | 161 | THR  | CA-C-N | 5.58 | 132.19      | 121.54   |
| 1   | A     | 161 | THR  | C-N-CA | 5.58 | 132.19      | 121.54   |
| 1   | E     | 161 | THR  | CA-C-N | 5.56 | 132.16      | 121.54   |
| 1   | E     | 161 | THR  | C-N-CA | 5.56 | 132.16      | 121.54   |
| 1   | C     | 161 | THR  | CA-C-N | 5.55 | 132.13      | 121.54   |
| 1   | C     | 161 | THR  | C-N-CA | 5.55 | 132.13      | 121.54   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 161 | THR  | CA-C-N | 5.53 | 132.10      | 121.54   |
| 1   | B     | 161 | THR  | C-N-CA | 5.53 | 132.10      | 121.54   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1558 | ILE  | Peptide |
| 1   | A     | 2344 | ALA  | Peptide |
| 1   | B     | 1558 | ILE  | Peptide |
| 1   | B     | 2344 | ALA  | Peptide |
| 1   | C     | 1558 | ILE  | Peptide |
| 1   | C     | 2344 | ALA  | Peptide |
| 1   | D     | 1558 | ILE  | Peptide |
| 1   | D     | 2344 | ALA  | Peptide |
| 1   | E     | 1558 | ILE  | Peptide |
| 1   | E     | 2344 | ALA  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 18700 | 0        | 18400    | 262     | 0            |
| 1   | B     | 18700 | 0        | 18400    | 264     | 0            |
| 1   | C     | 18700 | 0        | 18400    | 277     | 0            |
| 1   | D     | 18700 | 0        | 18400    | 262     | 0            |
| 1   | E     | 18700 | 0        | 18400    | 260     | 0            |
| All | All   | 93500 | 0        | 92000    | 1258    | 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 7.

All (1258) 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:B:236:LEU:HB2 | 1:B:484:PHE:HB2 | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:236:LEU:HB2   | 1:A:484:PHE:HB2   | 1.74                     | 0.70              |
| 1:C:236:LEU:HB2   | 1:C:484:PHE:HB2   | 1.74                     | 0.70              |
| 1:D:236:LEU:HB2   | 1:D:484:PHE:HB2   | 1.74                     | 0.69              |
| 1:E:236:LEU:HB2   | 1:E:484:PHE:HB2   | 1.74                     | 0.69              |
| 1:C:2048:GLN:HG2  | 1:D:2327:MET:HE2  | 1.75                     | 0.69              |
| 1:C:2258:GLN:HB3  | 1:D:2015:ALA:HB2  | 1.76                     | 0.67              |
| 1:C:2194:LYS:HD2  | 1:E:1054:GLN:HE21 | 1.60                     | 0.67              |
| 1:D:1663:TRP:HA   | 1:D:1685:LEU:H    | 1.62                     | 0.65              |
| 1:E:1663:TRP:HA   | 1:E:1685:LEU:H    | 1.62                     | 0.65              |
| 1:C:1607:ARG:HE   | 1:C:1640:LEU:HD21 | 1.63                     | 0.64              |
| 1:E:1607:ARG:HE   | 1:E:1640:LEU:HD21 | 1.63                     | 0.64              |
| 1:A:1663:TRP:HA   | 1:A:1685:LEU:H    | 1.62                     | 0.64              |
| 1:B:1663:TRP:HA   | 1:B:1685:LEU:H    | 1.62                     | 0.64              |
| 1:C:1663:TRP:HA   | 1:C:1685:LEU:H    | 1.62                     | 0.63              |
| 1:D:1607:ARG:HE   | 1:D:1640:LEU:HD21 | 1.63                     | 0.63              |
| 1:B:1239:SER:HG   | 1:B:1242:SER:HG   | 1.46                     | 0.63              |
| 1:B:1607:ARG:HE   | 1:B:1640:LEU:HD21 | 1.63                     | 0.63              |
| 1:E:534:PHE:HB2   | 1:E:556:ILE:HD13  | 1.81                     | 0.62              |
| 1:A:1607:ARG:HE   | 1:A:1640:LEU:HD21 | 1.63                     | 0.62              |
| 1:D:534:PHE:HB2   | 1:D:556:ILE:HD13  | 1.81                     | 0.62              |
| 1:A:1500:ASP:OD1  | 1:A:1500:ASP:N    | 2.33                     | 0.62              |
| 1:A:534:PHE:HB2   | 1:A:556:ILE:HD13  | 1.81                     | 0.62              |
| 1:B:1500:ASP:OD1  | 1:B:1500:ASP:N    | 2.33                     | 0.61              |
| 1:E:1598:TYR:HB3  | 1:E:1640:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:151:THR:HG23  | 1:A:154:ASN:H     | 1.66                     | 0.61              |
| 1:B:534:PHE:HB2   | 1:B:556:ILE:HD13  | 1.81                     | 0.61              |
| 1:B:1500:ASP:HB2  | 1:B:1502:ASN:H    | 1.66                     | 0.61              |
| 1:C:1598:TYR:HB3  | 1:C:1640:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:1598:TYR:HB3  | 1:A:1640:LEU:HD22 | 1.83                     | 0.61              |
| 1:D:151:THR:HG23  | 1:D:154:ASN:H     | 1.66                     | 0.61              |
| 1:C:374:GLN:HE21  | 1:C:413:ARG:HD2   | 1.66                     | 0.61              |
| 1:C:1052:LEU:HD11 | 1:C:1062:VAL:HG23 | 1.83                     | 0.61              |
| 1:C:1500:ASP:HB2  | 1:C:1502:ASN:H    | 1.66                     | 0.61              |
| 1:C:534:PHE:HB2   | 1:C:556:ILE:HD13  | 1.81                     | 0.61              |
| 1:D:242:ILE:HA    | 1:D:246:LEU:HD23  | 1.83                     | 0.61              |
| 1:E:1500:ASP:HB2  | 1:E:1502:ASN:H    | 1.66                     | 0.61              |
| 1:C:1500:ASP:N    | 1:C:1500:ASP:OD1  | 2.33                     | 0.61              |
| 1:C:242:ILE:HA    | 1:C:246:LEU:HD23  | 1.83                     | 0.60              |
| 1:D:1500:ASP:OD1  | 1:D:1500:ASP:N    | 2.33                     | 0.60              |
| 1:A:374:GLN:HE21  | 1:A:413:ARG:HD2   | 1.66                     | 0.60              |
| 1:C:151:THR:HG23  | 1:C:154:ASN:H     | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1052:LEU:HD11 | 1:D:1062:VAL:HG23 | 1.83                     | 0.60              |
| 1:A:771:GLU:HA    | 1:A:774:LEU:HB3   | 1.84                     | 0.60              |
| 1:B:374:GLN:HE21  | 1:B:413:ARG:HD2   | 1.66                     | 0.60              |
| 1:B:1598:TYR:HB3  | 1:B:1640:LEU:HD22 | 1.82                     | 0.60              |
| 1:D:1500:ASP:HB2  | 1:D:1502:ASN:H    | 1.66                     | 0.60              |
| 1:B:1052:LEU:HD11 | 1:B:1062:VAL:HG23 | 1.83                     | 0.60              |
| 1:E:242:ILE:HA    | 1:E:246:LEU:HD23  | 1.83                     | 0.60              |
| 1:B:242:ILE:HA    | 1:B:246:LEU:HD23  | 1.83                     | 0.60              |
| 1:E:151:THR:HG23  | 1:E:154:ASN:H     | 1.66                     | 0.60              |
| 1:E:374:GLN:HE21  | 1:E:413:ARG:HD2   | 1.66                     | 0.60              |
| 1:B:151:THR:HG23  | 1:B:154:ASN:H     | 1.66                     | 0.60              |
| 1:D:374:GLN:HE21  | 1:D:413:ARG:HD2   | 1.66                     | 0.60              |
| 1:D:1598:TYR:HB3  | 1:D:1640:LEU:HD22 | 1.82                     | 0.60              |
| 1:B:1005:PHE:O    | 1:B:1013:ASN:ND2  | 2.35                     | 0.60              |
| 1:D:889:LEU:HD22  | 1:D:900:PRO:HB3   | 1.84                     | 0.60              |
| 1:A:242:ILE:HA    | 1:A:246:LEU:HD23  | 1.83                     | 0.60              |
| 1:A:1500:ASP:HB2  | 1:A:1502:ASN:H    | 1.66                     | 0.59              |
| 1:B:1505:PHE:HB3  | 1:B:1517:LEU:HB2  | 1.84                     | 0.59              |
| 1:A:889:LEU:HD22  | 1:A:900:PRO:HB3   | 1.84                     | 0.59              |
| 1:C:2284:LEU:HD11 | 1:D:2332:GLN:HG3  | 1.84                     | 0.59              |
| 1:E:1005:PHE:O    | 1:E:1013:ASN:ND2  | 2.35                     | 0.59              |
| 1:B:777:LEU:HD22  | 1:B:784:PHE:HB2   | 1.85                     | 0.59              |
| 1:C:889:LEU:HD22  | 1:C:900:PRO:HB3   | 1.84                     | 0.59              |
| 1:E:1052:LEU:HD11 | 1:E:1062:VAL:HG23 | 1.83                     | 0.59              |
| 1:A:1505:PHE:HB3  | 1:A:1517:LEU:HB2  | 1.84                     | 0.59              |
| 1:C:771:GLU:HA    | 1:C:774:LEU:HB3   | 1.84                     | 0.59              |
| 1:C:1654:ASN:OD1  | 1:C:1658:HIS:NE2  | 2.36                     | 0.59              |
| 1:D:1820:ASN:ND2  | 1:D:1823:GLY:O    | 2.36                     | 0.59              |
| 1:E:777:LEU:HD22  | 1:E:784:PHE:HB2   | 1.85                     | 0.59              |
| 1:A:1052:LEU:HD11 | 1:A:1062:VAL:HG23 | 1.83                     | 0.59              |
| 1:D:771:GLU:HA    | 1:D:774:LEU:HB3   | 1.84                     | 0.59              |
| 1:E:889:LEU:HD22  | 1:E:900:PRO:HB3   | 1.84                     | 0.59              |
| 1:C:657:PHE:O     | 1:C:661:THR:HB    | 2.03                     | 0.59              |
| 1:E:1820:ASN:ND2  | 1:E:1823:GLY:O    | 2.36                     | 0.59              |
| 1:A:1005:PHE:O    | 1:A:1013:ASN:ND2  | 2.35                     | 0.59              |
| 1:A:1820:ASN:ND2  | 1:A:1823:GLY:O    | 2.36                     | 0.59              |
| 1:A:657:PHE:O     | 1:A:661:THR:HB    | 2.03                     | 0.58              |
| 1:B:937:SER:OG    | 1:B:952:ARG:NH1   | 2.36                     | 0.58              |
| 1:C:1505:PHE:HB3  | 1:C:1517:LEU:HB2  | 1.84                     | 0.58              |
| 1:E:1500:ASP:N    | 1:E:1500:ASP:OD1  | 2.33                     | 0.58              |
| 1:B:771:GLU:HA    | 1:B:774:LEU:HB3   | 1.84                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1820:ASN:ND2 | 1:B:1823:GLY:O    | 2.36                     | 0.58              |
| 1:E:771:GLU:HA   | 1:E:774:LEU:HB3   | 1.84                     | 0.58              |
| 1:E:1505:PHE:HB3 | 1:E:1517:LEU:HB2  | 1.84                     | 0.58              |
| 1:C:1820:ASN:ND2 | 1:C:1823:GLY:O    | 2.36                     | 0.58              |
| 1:E:657:PHE:O    | 1:E:661:THR:HB    | 2.03                     | 0.58              |
| 1:A:937:SER:OG   | 1:A:952:ARG:NH1   | 2.36                     | 0.58              |
| 1:A:1650:LEU:HB2 | 1:A:1690:THR:HG23 | 1.86                     | 0.58              |
| 1:A:1654:ASN:OD1 | 1:A:1658:HIS:NE2  | 2.35                     | 0.58              |
| 1:A:2194:LYS:HD2 | 1:C:1054:GLN:HE21 | 1.68                     | 0.58              |
| 1:B:599:LEU:HD21 | 1:B:636:ILE:HG12  | 1.86                     | 0.58              |
| 1:D:1650:LEU:HB2 | 1:D:1690:THR:HG23 | 1.86                     | 0.58              |
| 1:D:1654:ASN:OD1 | 1:D:1658:HIS:NE2  | 2.36                     | 0.58              |
| 1:C:599:LEU:HD21 | 1:C:636:ILE:HG12  | 1.86                     | 0.58              |
| 1:C:1005:PHE:O   | 1:C:1013:ASN:ND2  | 2.35                     | 0.58              |
| 1:D:657:PHE:O    | 1:D:661:THR:HB    | 2.03                     | 0.58              |
| 1:D:777:LEU:HD22 | 1:D:784:PHE:HB2   | 1.85                     | 0.58              |
| 1:A:599:LEU:HD21 | 1:A:636:ILE:HG12  | 1.86                     | 0.58              |
| 1:E:1654:ASN:OD1 | 1:E:1658:HIS:NE2  | 2.35                     | 0.58              |
| 1:A:2348:THR:HB  | 1:A:2518:ARG:HG2  | 1.86                     | 0.58              |
| 1:C:1239:SER:HG  | 1:C:1242:SER:HG   | 1.51                     | 0.58              |
| 1:D:1505:PHE:HB3 | 1:D:1517:LEU:HB2  | 1.84                     | 0.58              |
| 1:E:2348:THR:HB  | 1:E:2518:ARG:HG2  | 1.86                     | 0.58              |
| 1:A:777:LEU:HD22 | 1:A:784:PHE:HB2   | 1.85                     | 0.57              |
| 1:B:889:LEU:HD22 | 1:B:900:PRO:HB3   | 1.84                     | 0.57              |
| 1:B:2348:THR:HB  | 1:B:2518:ARG:HG2  | 1.86                     | 0.57              |
| 1:C:2348:THR:HB  | 1:C:2518:ARG:HG2  | 1.86                     | 0.57              |
| 1:D:1556:PHE:HB2 | 1:D:1570:ILE:HB   | 1.86                     | 0.57              |
| 1:B:657:PHE:O    | 1:B:661:THR:HB    | 2.03                     | 0.57              |
| 1:D:599:LEU:HD21 | 1:D:636:ILE:HG12  | 1.86                     | 0.57              |
| 1:D:1323:ASN:OD1 | 1:D:1323:ASN:N    | 2.38                     | 0.57              |
| 1:D:1725:SER:OG  | 1:D:1726:ALA:N    | 2.38                     | 0.57              |
| 1:E:302:LYS:HG3  | 1:E:308:GLN:HE21  | 1.70                     | 0.57              |
| 1:E:1645:TYR:HB2 | 1:E:1770:MET:HB2  | 1.87                     | 0.57              |
| 1:A:1531:SER:HG  | 1:B:1766:HIS:HE2  | 1.51                     | 0.57              |
| 1:C:777:LEU:HD22 | 1:C:784:PHE:HB2   | 1.85                     | 0.57              |
| 1:C:937:SER:OG   | 1:C:952:ARG:NH1   | 2.37                     | 0.57              |
| 1:D:1005:PHE:O   | 1:D:1013:ASN:ND2  | 2.35                     | 0.57              |
| 1:A:59:GLN:OE1   | 1:A:1946:ARG:NH2  | 2.38                     | 0.57              |
| 1:B:353:ASN:O    | 1:B:400:LYS:NZ    | 2.38                     | 0.57              |
| 1:D:2348:THR:HB  | 1:D:2518:ARG:HG2  | 1.86                     | 0.57              |
| 1:E:353:ASN:O    | 1:E:400:LYS:NZ    | 2.38                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1323:ASN:OD1 | 1:A:1323:ASN:N    | 2.38                     | 0.57              |
| 1:B:1645:TYR:HB2 | 1:B:1770:MET:HB2  | 1.87                     | 0.57              |
| 1:C:302:LYS:HG3  | 1:C:308:GLN:HE21  | 1.70                     | 0.57              |
| 1:E:937:SER:OG   | 1:E:952:ARG:NH1   | 2.37                     | 0.57              |
| 1:A:353:ASN:O    | 1:A:400:LYS:NZ    | 2.38                     | 0.57              |
| 1:C:1323:ASN:OD1 | 1:C:1323:ASN:N    | 2.38                     | 0.57              |
| 1:C:1810:GLU:OE1 | 1:C:1813:ARG:NH1  | 2.38                     | 0.57              |
| 1:D:353:ASN:O    | 1:D:400:LYS:NZ    | 2.38                     | 0.57              |
| 1:D:937:SER:OG   | 1:D:952:ARG:NH1   | 2.36                     | 0.57              |
| 1:E:1556:PHE:HB2 | 1:E:1570:ILE:HB   | 1.86                     | 0.57              |
| 1:B:1810:GLU:OE1 | 1:B:1813:ARG:NH1  | 2.38                     | 0.57              |
| 1:C:1650:LEU:HB2 | 1:C:1690:THR:HG23 | 1.86                     | 0.57              |
| 1:D:1810:GLU:OE1 | 1:D:1813:ARG:NH1  | 2.38                     | 0.57              |
| 1:C:1556:PHE:HB2 | 1:C:1570:ILE:HB   | 1.86                     | 0.57              |
| 1:E:1650:LEU:HB2 | 1:E:1690:THR:HG23 | 1.86                     | 0.57              |
| 1:B:1650:LEU:HB2 | 1:B:1690:THR:HG23 | 1.86                     | 0.57              |
| 1:E:1810:GLU:OE1 | 1:E:1813:ARG:NH1  | 2.38                     | 0.57              |
| 1:A:1810:GLU:OE1 | 1:A:1813:ARG:NH1  | 2.38                     | 0.56              |
| 1:B:59:GLN:OE1   | 1:B:1946:ARG:NH2  | 2.38                     | 0.56              |
| 1:B:1556:PHE:HB2 | 1:B:1570:ILE:HB   | 1.86                     | 0.56              |
| 1:B:1654:ASN:OD1 | 1:B:1658:HIS:NE2  | 2.36                     | 0.56              |
| 1:D:22:LEU:HD23  | 1:D:25:ILE:HD12   | 1.87                     | 0.56              |
| 1:A:1556:PHE:HB2 | 1:A:1570:ILE:HB   | 1.86                     | 0.56              |
| 1:C:22:LEU:HD23  | 1:C:25:ILE:HD12   | 1.87                     | 0.56              |
| 1:C:1645:TYR:HB2 | 1:C:1770:MET:HB2  | 1.87                     | 0.56              |
| 1:E:599:LEU:HD21 | 1:E:636:ILE:HG12  | 1.86                     | 0.56              |
| 1:B:608:ASN:OD1  | 1:B:608:ASN:N     | 2.39                     | 0.56              |
| 1:C:726:GLN:OE1  | 1:C:749:ASN:ND2   | 2.37                     | 0.56              |
| 1:D:719:TRP:HD1  | 1:D:778:VAL:HG22  | 1.70                     | 0.56              |
| 1:E:1725:SER:OG  | 1:E:1726:ALA:N    | 2.38                     | 0.56              |
| 1:A:302:LYS:HG3  | 1:A:308:GLN:HE21  | 1.69                     | 0.56              |
| 1:B:302:LYS:HG3  | 1:B:308:GLN:HE21  | 1.69                     | 0.56              |
| 1:A:719:TRP:HD1  | 1:A:778:VAL:HG22  | 1.70                     | 0.56              |
| 1:A:1645:TYR:HB2 | 1:A:1770:MET:HB2  | 1.87                     | 0.56              |
| 1:B:719:TRP:HD1  | 1:B:778:VAL:HG22  | 1.70                     | 0.56              |
| 1:B:1323:ASN:N   | 1:B:1323:ASN:OD1  | 2.38                     | 0.56              |
| 1:D:726:GLN:OE1  | 1:D:749:ASN:ND2   | 2.37                     | 0.56              |
| 1:A:133:ASN:OD1  | 1:A:133:ASN:N     | 2.39                     | 0.56              |
| 1:A:2390:ASN:ND2 | 1:A:2392:GLU:OE2  | 2.39                     | 0.56              |
| 1:E:1323:ASN:N   | 1:E:1323:ASN:OD1  | 2.38                     | 0.56              |
| 1:D:302:LYS:HG3  | 1:D:308:GLN:HE21  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:608:ASN:OD1  | 1:E:608:ASN:N    | 2.39                     | 0.56              |
| 1:C:353:ASN:O    | 1:C:400:LYS:NZ   | 2.38                     | 0.56              |
| 1:C:719:TRP:HD1  | 1:C:778:VAL:HG22 | 1.70                     | 0.56              |
| 1:C:2390:ASN:ND2 | 1:C:2392:GLU:OE2 | 2.39                     | 0.56              |
| 1:D:133:ASN:OD1  | 1:D:133:ASN:N    | 2.39                     | 0.56              |
| 1:D:1645:TYR:HB2 | 1:D:1770:MET:HB2 | 1.87                     | 0.56              |
| 1:C:59:GLN:OE1   | 1:C:1946:ARG:NH2 | 2.38                     | 0.55              |
| 1:E:719:TRP:HD1  | 1:E:778:VAL:HG22 | 1.70                     | 0.55              |
| 1:A:22:LEU:HD23  | 1:A:25:ILE:HD12  | 1.87                     | 0.55              |
| 1:A:1057:LEU:O   | 1:A:1807:ASN:ND2 | 2.40                     | 0.55              |
| 1:B:22:LEU:HD23  | 1:B:25:ILE:HD12  | 1.87                     | 0.55              |
| 1:B:133:ASN:N    | 1:B:133:ASN:OD1  | 2.39                     | 0.55              |
| 1:B:1327:ASN:ND2 | 1:B:1544:ASP:OD1 | 2.39                     | 0.55              |
| 1:D:1057:LEU:O   | 1:D:1807:ASN:ND2 | 2.40                     | 0.55              |
| 1:D:2478:TYR:O   | 1:E:2343:ARG:NH2 | 2.39                     | 0.55              |
| 1:B:1057:LEU:O   | 1:B:1807:ASN:ND2 | 2.40                     | 0.55              |
| 1:B:1607:ARG:NH2 | 1:B:1638:PRO:O   | 2.40                     | 0.55              |
| 1:B:2390:ASN:ND2 | 1:B:2392:GLU:OE2 | 2.39                     | 0.55              |
| 1:C:879:THR:HG23 | 1:C:882:GLY:H    | 1.72                     | 0.55              |
| 1:D:735:ILE:O    | 1:D:739:ASN:ND2  | 2.39                     | 0.55              |
| 1:D:879:THR:HG23 | 1:D:882:GLY:H    | 1.72                     | 0.55              |
| 1:A:1607:ARG:NH2 | 1:A:1638:PRO:O   | 2.40                     | 0.55              |
| 1:B:566:THR:HG21 | 1:C:842:VAL:HG23 | 1.88                     | 0.55              |
| 1:C:1607:ARG:NH2 | 1:C:1638:PRO:O   | 2.40                     | 0.55              |
| 1:D:608:ASN:OD1  | 1:D:608:ASN:N    | 2.39                     | 0.55              |
| 1:E:22:LEU:HD23  | 1:E:25:ILE:HD12  | 1.87                     | 0.55              |
| 1:B:703:ALA:HB2  | 1:C:2272:GLY:HA3 | 1.88                     | 0.55              |
| 1:C:608:ASN:N    | 1:C:608:ASN:OD1  | 2.39                     | 0.55              |
| 1:E:2390:ASN:ND2 | 1:E:2392:GLU:OE2 | 2.39                     | 0.55              |
| 1:C:133:ASN:OD1  | 1:C:133:ASN:N    | 2.39                     | 0.55              |
| 1:D:496:SER:OG   | 1:D:497:VAL:N    | 2.39                     | 0.55              |
| 1:D:1607:ARG:NH2 | 1:D:1638:PRO:O   | 2.40                     | 0.55              |
| 1:D:2390:ASN:ND2 | 1:D:2392:GLU:OE2 | 2.39                     | 0.55              |
| 1:E:133:ASN:N    | 1:E:133:ASN:OD1  | 2.39                     | 0.55              |
| 1:A:508:ILE:HG23 | 1:A:519:HIS:HD2  | 1.72                     | 0.55              |
| 1:B:726:GLN:OE1  | 1:B:749:ASN:ND2  | 2.37                     | 0.55              |
| 1:E:496:SER:OG   | 1:E:497:VAL:N    | 2.39                     | 0.55              |
| 1:A:1725:SER:OG  | 1:A:1726:ALA:N   | 2.38                     | 0.55              |
| 1:A:2408:ALA:O   | 1:A:2419:ARG:NH1 | 2.40                     | 0.55              |
| 1:B:879:THR:HG23 | 1:B:882:GLY:H    | 1.72                     | 0.55              |
| 1:B:2408:ALA:O   | 1:B:2419:ARG:NH1 | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1057:LEU:O    | 1:C:1807:ASN:ND2  | 2.40                     | 0.54              |
| 1:E:1607:ARG:NH2  | 1:E:1638:PRO:O    | 2.40                     | 0.54              |
| 1:E:2095:ASP:OD1  | 1:E:2233:ARG:NH1  | 2.41                     | 0.54              |
| 1:A:726:GLN:OE1   | 1:A:749:ASN:ND2   | 2.37                     | 0.54              |
| 1:A:1312:ASN:ND2  | 1:A:1335:GLU:OE2  | 2.39                     | 0.54              |
| 1:A:2095:ASP:OD1  | 1:A:2233:ARG:NH1  | 2.41                     | 0.54              |
| 1:C:496:SER:OG    | 1:C:497:VAL:N     | 2.39                     | 0.54              |
| 1:D:2408:ALA:O    | 1:D:2419:ARG:NH1  | 2.40                     | 0.54              |
| 1:C:2408:ALA:O    | 1:C:2419:ARG:NH1  | 2.40                     | 0.54              |
| 1:D:59:GLN:OE1    | 1:D:1946:ARG:NH2  | 2.38                     | 0.54              |
| 1:D:2400:LEU:HD11 | 1:D:2405:LEU:HD21 | 1.90                     | 0.54              |
| 1:E:1327:ASN:ND2  | 1:E:1544:ASP:OD1  | 2.39                     | 0.54              |
| 1:E:1813:ARG:NH2  | 1:E:1817:TYR:OH   | 2.41                     | 0.54              |
| 1:B:496:SER:OG    | 1:B:497:VAL:N     | 2.39                     | 0.54              |
| 1:E:879:THR:HG23  | 1:E:882:GLY:H     | 1.72                     | 0.54              |
| 1:A:608:ASN:OD1   | 1:A:608:ASN:N     | 2.39                     | 0.54              |
| 1:A:879:THR:HG23  | 1:A:882:GLY:H     | 1.72                     | 0.54              |
| 1:D:1813:ARG:NH2  | 1:D:1817:TYR:OH   | 2.41                     | 0.54              |
| 1:D:2095:ASP:OD1  | 1:D:2233:ARG:NH1  | 2.41                     | 0.54              |
| 1:E:508:ILE:HG23  | 1:E:519:HIS:HD2   | 1.73                     | 0.54              |
| 1:A:1607:ARG:NH1  | 1:A:1637:GLU:OE1  | 2.41                     | 0.54              |
| 1:A:2034:ARG:NH1  | 1:A:2475:ASP:O    | 2.41                     | 0.54              |
| 1:B:1607:ARG:NH1  | 1:B:1637:GLU:OE1  | 2.41                     | 0.54              |
| 1:D:1607:ARG:NH1  | 1:D:1637:GLU:OE1  | 2.41                     | 0.54              |
| 1:E:1057:LEU:O    | 1:E:1807:ASN:ND2  | 2.40                     | 0.54              |
| 1:A:1327:ASN:ND2  | 1:A:1544:ASP:OD1  | 2.39                     | 0.54              |
| 1:A:1813:ARG:NH2  | 1:A:1817:TYR:OH   | 2.41                     | 0.54              |
| 1:B:1725:SER:OG   | 1:B:1726:ALA:N    | 2.38                     | 0.54              |
| 1:C:270:ASP:N     | 1:C:270:ASP:OD1   | 2.41                     | 0.54              |
| 1:C:2400:LEU:HD11 | 1:C:2405:LEU:HD21 | 1.90                     | 0.54              |
| 1:E:270:ASP:N     | 1:E:270:ASP:OD1   | 2.41                     | 0.54              |
| 1:E:706:GLN:O     | 1:E:765:ARG:NH2   | 2.41                     | 0.54              |
| 1:E:735:ILE:O     | 1:E:739:ASN:ND2   | 2.39                     | 0.54              |
| 1:E:2400:LEU:HD11 | 1:E:2405:LEU:HD21 | 1.90                     | 0.54              |
| 1:C:2452:ARG:NH1  | 1:D:2339:GLU:O    | 2.32                     | 0.54              |
| 1:D:572:TRP:O     | 1:D:576:ASN:ND2   | 2.41                     | 0.54              |
| 1:E:2408:ALA:O    | 1:E:2419:ARG:NH1  | 2.40                     | 0.54              |
| 1:B:706:GLN:O     | 1:B:765:ARG:NH2   | 2.41                     | 0.54              |
| 1:C:1081:VAL:O    | 1:C:1597:GLN:NE2  | 2.41                     | 0.54              |
| 1:C:2095:ASP:OD1  | 1:C:2233:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:687:SER:OG    | 1:D:688:LEU:N     | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:706:GLN:O     | 1:D:765:ARG:NH2   | 2.41                     | 0.54              |
| 1:E:726:GLN:OE1   | 1:E:749:ASN:ND2   | 2.37                     | 0.54              |
| 1:A:488:TYR:O     | 1:A:492:HIS:HB2   | 2.09                     | 0.53              |
| 1:A:1239:SER:HG   | 1:A:1242:SER:HG   | 1.55                     | 0.53              |
| 1:A:2400:LEU:HD11 | 1:A:2405:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:2478:TYR:O    | 1:B:2343:ARG:NH2  | 2.41                     | 0.53              |
| 1:B:508:ILE:HG23  | 1:B:519:HIS:HD2   | 1.72                     | 0.53              |
| 1:B:2095:ASP:OD1  | 1:B:2233:ARG:NH1  | 2.41                     | 0.53              |
| 1:D:488:TYR:O     | 1:D:492:HIS:HB2   | 2.09                     | 0.53              |
| 1:E:572:TRP:O     | 1:E:576:ASN:ND2   | 2.41                     | 0.53              |
| 1:A:496:SER:OG    | 1:A:497:VAL:N     | 2.39                     | 0.53              |
| 1:A:735:ILE:O     | 1:A:739:ASN:ND2   | 2.39                     | 0.53              |
| 1:C:1607:ARG:NH1  | 1:C:1637:GLU:OE1  | 2.41                     | 0.53              |
| 1:D:2427:THR:HG22 | 1:D:2429:PRO:HD3  | 1.91                     | 0.53              |
| 1:E:59:GLN:OE1    | 1:E:1946:ARG:NH2  | 2.38                     | 0.53              |
| 1:E:2034:ARG:NH1  | 1:E:2475:ASP:O    | 2.41                     | 0.53              |
| 1:E:2427:THR:HG22 | 1:E:2429:PRO:HD3  | 1.91                     | 0.53              |
| 1:A:1081:VAL:O    | 1:A:1597:GLN:NE2  | 2.41                     | 0.53              |
| 1:C:508:ILE:HG23  | 1:C:519:HIS:HD2   | 1.72                     | 0.53              |
| 1:C:1813:ARG:NH2  | 1:C:1817:TYR:OH   | 2.41                     | 0.53              |
| 1:C:2251:GLN:NE2  | 1:D:2013:SER:OG   | 2.33                     | 0.53              |
| 1:D:508:ILE:HG23  | 1:D:519:HIS:HD2   | 1.73                     | 0.53              |
| 1:D:2034:ARG:NH1  | 1:D:2475:ASP:O    | 2.41                     | 0.53              |
| 1:E:1607:ARG:NH1  | 1:E:1637:GLU:OE1  | 2.41                     | 0.53              |
| 1:A:1639:GLN:NE2  | 1:A:1642:GLU:O    | 2.42                     | 0.53              |
| 1:B:2034:ARG:NH1  | 1:B:2475:ASP:O    | 2.41                     | 0.53              |
| 1:B:2400:LEU:HD11 | 1:B:2405:LEU:HD21 | 1.90                     | 0.53              |
| 1:C:2034:ARG:NH1  | 1:C:2475:ASP:O    | 2.41                     | 0.53              |
| 1:A:687:SER:OG    | 1:A:688:LEU:N     | 2.41                     | 0.53              |
| 1:C:488:TYR:O     | 1:C:492:HIS:HB2   | 2.09                     | 0.53              |
| 1:C:1725:SER:O    | 1:C:1741:ASN:ND2  | 2.42                     | 0.53              |
| 1:B:1508:LYS:HG2  | 1:B:1513:ILE:HA   | 1.91                     | 0.53              |
| 1:C:572:TRP:O     | 1:C:576:ASN:ND2   | 2.41                     | 0.53              |
| 1:C:1639:GLN:NE2  | 1:C:1642:GLU:O    | 2.42                     | 0.53              |
| 1:C:1725:SER:OG   | 1:C:1726:ALA:N    | 2.38                     | 0.53              |
| 1:E:687:SER:OG    | 1:E:688:LEU:N     | 2.41                     | 0.53              |
| 1:A:572:TRP:O     | 1:A:576:ASN:ND2   | 2.41                     | 0.53              |
| 1:B:488:TYR:O     | 1:B:492:HIS:HB2   | 2.09                     | 0.53              |
| 1:B:524:PHE:O     | 1:B:559:ARG:NH2   | 2.41                     | 0.53              |
| 1:D:1725:SER:O    | 1:D:1741:ASN:ND2  | 2.42                     | 0.53              |
| 1:C:687:SER:OG    | 1:C:688:LEU:N     | 2.41                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:524:PHE:O     | 1:E:559:ARG:NH2  | 2.42                     | 0.53              |
| 1:E:1725:SER:O    | 1:E:1741:ASN:ND2 | 2.42                     | 0.53              |
| 1:A:482:LYS:NZ    | 1:A:504:CYS:O    | 2.40                     | 0.53              |
| 1:A:1725:SER:O    | 1:A:1741:ASN:ND2 | 2.42                     | 0.53              |
| 1:B:1639:GLN:NE2  | 1:B:1642:GLU:O   | 2.42                     | 0.53              |
| 1:B:1813:ARG:NH2  | 1:B:1817:TYR:OH  | 2.41                     | 0.53              |
| 1:C:1327:ASN:ND2  | 1:C:1544:ASP:OD1 | 2.39                     | 0.53              |
| 1:D:1327:ASN:ND2  | 1:D:1544:ASP:OD1 | 2.39                     | 0.53              |
| 1:E:1639:GLN:NE2  | 1:E:1642:GLU:O   | 2.42                     | 0.53              |
| 1:A:293:SER:O     | 1:A:311:ASN:ND2  | 2.43                     | 0.52              |
| 1:A:524:PHE:O     | 1:A:559:ARG:NH2  | 2.41                     | 0.52              |
| 1:B:580:ASN:OD1   | 1:B:580:ASN:N    | 2.42                     | 0.52              |
| 1:B:2427:THR:HG22 | 1:B:2429:PRO:HD3 | 1.91                     | 0.52              |
| 1:C:342:LEU:HA    | 1:C:362:LYS:H    | 1.75                     | 0.52              |
| 1:D:270:ASP:OD1   | 1:D:270:ASP:N    | 2.41                     | 0.52              |
| 1:D:524:PHE:O     | 1:D:559:ARG:NH2  | 2.41                     | 0.52              |
| 1:D:1639:GLN:NE2  | 1:D:1642:GLU:O   | 2.42                     | 0.52              |
| 1:D:1801:ARG:NH1  | 1:D:1804:GLN:OE1 | 2.42                     | 0.52              |
| 1:E:488:TYR:O     | 1:E:492:HIS:HB2  | 2.09                     | 0.52              |
| 1:A:270:ASP:OD1   | 1:A:270:ASP:N    | 2.41                     | 0.52              |
| 1:A:342:LEU:HA    | 1:A:362:LYS:H    | 1.74                     | 0.52              |
| 1:A:1508:LYS:HG2  | 1:A:1513:ILE:HA  | 1.91                     | 0.52              |
| 1:C:524:PHE:O     | 1:C:559:ARG:NH2  | 2.41                     | 0.52              |
| 1:C:1508:LYS:HG2  | 1:C:1513:ILE:HA  | 1.91                     | 0.52              |
| 1:E:1801:ARG:NH1  | 1:E:1804:GLN:OE1 | 2.42                     | 0.52              |
| 1:A:2427:THR:HG22 | 1:A:2429:PRO:HD3 | 1.91                     | 0.52              |
| 1:C:2453:GLY:H    | 1:D:2342:GLU:HB2 | 1.74                     | 0.52              |
| 1:B:293:SER:O     | 1:B:311:ASN:ND2  | 2.43                     | 0.52              |
| 1:C:706:GLN:O     | 1:C:765:ARG:NH2  | 2.41                     | 0.52              |
| 1:D:580:ASN:OD1   | 1:D:580:ASN:N    | 2.43                     | 0.52              |
| 1:D:1508:LYS:HG2  | 1:D:1513:ILE:HA  | 1.91                     | 0.52              |
| 1:E:1312:ASN:ND2  | 1:E:1335:GLU:OE2 | 2.39                     | 0.52              |
| 1:B:572:TRP:O     | 1:B:576:ASN:ND2  | 2.41                     | 0.52              |
| 1:B:1801:ARG:NH1  | 1:B:1804:GLN:OE1 | 2.42                     | 0.52              |
| 1:C:293:SER:O     | 1:C:311:ASN:ND2  | 2.43                     | 0.52              |
| 1:E:2500:SER:HA   | 1:E:2504:LYS:HD2 | 1.92                     | 0.52              |
| 1:A:372:ARG:HB2   | 1:A:415:TRP:HB2  | 1.92                     | 0.52              |
| 1:A:780:LYS:NZ    | 1:A:823:GLU:OE1  | 2.43                     | 0.52              |
| 1:A:1605:ARG:NH1  | 1:A:1640:LEU:O   | 2.43                     | 0.52              |
| 1:B:707:MET:O     | 1:C:2268:ASN:ND2 | 2.42                     | 0.52              |
| 1:C:792:GLN:HB2   | 1:C:797:THR:HG21 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:792:GLN:HB2   | 1:D:797:THR:HG21  | 1.92                     | 0.52              |
| 1:E:179:THR:OG1   | 1:E:180:ASP:N     | 2.43                     | 0.52              |
| 1:A:580:ASN:OD1   | 1:A:580:ASN:N     | 2.42                     | 0.52              |
| 1:B:1605:ARG:NH1  | 1:B:1640:LEU:O    | 2.43                     | 0.52              |
| 1:E:482:LYS:NZ    | 1:E:504:CYS:O     | 2.40                     | 0.52              |
| 1:E:1508:LYS:HG2  | 1:E:1513:ILE:HA   | 1.91                     | 0.52              |
| 1:B:1725:SER:O    | 1:B:1741:ASN:ND2  | 2.42                     | 0.52              |
| 1:C:1592:MET:HB2  | 1:C:1596:THR:HG23 | 1.92                     | 0.52              |
| 1:C:1801:ARG:NH1  | 1:C:1804:GLN:OE1  | 2.42                     | 0.52              |
| 1:A:250:LEU:HD23  | 1:A:447:LYS:HB2   | 1.92                     | 0.52              |
| 1:A:1801:ARG:NH1  | 1:A:1804:GLN:OE1  | 2.42                     | 0.52              |
| 1:B:735:ILE:O     | 1:B:739:ASN:ND2   | 2.39                     | 0.52              |
| 1:D:1278:THR:OG1  | 1:D:1279:ARG:N    | 2.43                     | 0.52              |
| 1:E:293:SER:O     | 1:E:311:ASN:ND2   | 2.43                     | 0.52              |
| 1:E:1605:ARG:NH1  | 1:E:1640:LEU:O    | 2.43                     | 0.52              |
| 1:A:1167:ASN:ND2  | 1:A:1169:SER:OG   | 2.43                     | 0.52              |
| 1:A:1670:ASN:ND2  | 1:A:1675:SER:OG   | 2.43                     | 0.52              |
| 1:B:792:GLN:HB2   | 1:B:797:THR:HG21  | 1.92                     | 0.52              |
| 1:C:580:ASN:N     | 1:C:580:ASN:OD1   | 2.42                     | 0.52              |
| 1:C:2427:THR:HG22 | 1:C:2429:PRO:HD3  | 1.91                     | 0.52              |
| 1:E:250:LEU:HD23  | 1:E:447:LYS:HB2   | 1.92                     | 0.52              |
| 1:E:527:PRO:O     | 1:E:559:ARG:NH1   | 2.43                     | 0.52              |
| 1:E:1780:ASN:ND2  | 1:E:1845:SER:O    | 2.43                     | 0.52              |
| 1:B:179:THR:OG1   | 1:B:180:ASP:N     | 2.43                     | 0.51              |
| 1:C:1780:ASN:ND2  | 1:C:1845:SER:O    | 2.43                     | 0.51              |
| 1:D:293:SER:O     | 1:D:311:ASN:ND2   | 2.43                     | 0.51              |
| 1:D:690:ASP:OD1   | 1:D:721:ASN:ND2   | 2.44                     | 0.51              |
| 1:D:780:LYS:NZ    | 1:D:823:GLU:OE1   | 2.43                     | 0.51              |
| 1:E:580:ASN:N     | 1:E:580:ASN:OD1   | 2.43                     | 0.51              |
| 1:A:690:ASP:OD1   | 1:A:721:ASN:ND2   | 2.44                     | 0.51              |
| 1:A:2020:GLN:H    | 1:A:2316:THR:HG22 | 1.76                     | 0.51              |
| 1:B:1278:THR:OG1  | 1:B:1279:ARG:N    | 2.43                     | 0.51              |
| 1:C:1167:ASN:ND2  | 1:C:1169:SER:OG   | 2.43                     | 0.51              |
| 1:D:179:THR:OG1   | 1:D:180:ASP:N     | 2.43                     | 0.51              |
| 1:D:1670:ASN:ND2  | 1:D:1675:SER:OG   | 2.43                     | 0.51              |
| 1:D:2500:SER:HA   | 1:D:2504:LYS:HD2  | 1.92                     | 0.51              |
| 1:E:792:GLN:HB2   | 1:E:797:THR:HG21  | 1.92                     | 0.51              |
| 1:B:1670:ASN:ND2  | 1:B:1675:SER:OG   | 2.43                     | 0.51              |
| 1:C:2468:GLN:NE2  | 1:D:2346:GLU:OE1  | 2.43                     | 0.51              |
| 1:D:1592:MET:HB2  | 1:D:1596:THR:HG23 | 1.92                     | 0.51              |
| 1:D:1605:ARG:NH1  | 1:D:1640:LEU:O    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1846:TRP:HE3  | 1:D:1847:ASN:HB2  | 1.75                     | 0.51              |
| 1:B:160:SER:HA    | 1:B:970:LYS:HA    | 1.92                     | 0.51              |
| 1:C:1670:ASN:ND2  | 1:C:1675:SER:OG   | 2.43                     | 0.51              |
| 1:D:1167:ASN:ND2  | 1:D:1169:SER:OG   | 2.43                     | 0.51              |
| 1:B:342:LEU:HA    | 1:B:362:LYS:H     | 1.74                     | 0.51              |
| 1:B:372:ARG:HB2   | 1:B:415:TRP:HB2   | 1.92                     | 0.51              |
| 1:B:780:LYS:NZ    | 1:B:823:GLU:OE1   | 2.43                     | 0.51              |
| 1:B:1167:ASN:ND2  | 1:B:1169:SER:OG   | 2.43                     | 0.51              |
| 1:C:1628:LEU:O    | 1:C:1836:ASN:ND2  | 2.44                     | 0.51              |
| 1:D:1081:VAL:O    | 1:D:1597:GLN:NE2  | 2.41                     | 0.51              |
| 1:E:372:ARG:HB2   | 1:E:415:TRP:HB2   | 1.92                     | 0.51              |
| 1:E:1151:TYR:OH   | 1:E:1225:ASP:O    | 2.26                     | 0.51              |
| 1:E:1278:THR:OG1  | 1:E:1279:ARG:N    | 2.43                     | 0.51              |
| 1:A:2048:GLN:HG2  | 1:B:2327:MET:HE2  | 1.92                     | 0.51              |
| 1:B:250:LEU:HD23  | 1:B:447:LYS:HB2   | 1.92                     | 0.51              |
| 1:B:1081:VAL:O    | 1:B:1597:GLN:NE2  | 2.41                     | 0.51              |
| 1:E:1628:LEU:O    | 1:E:1836:ASN:ND2  | 2.44                     | 0.51              |
| 1:E:1670:ASN:ND2  | 1:E:1675:SER:OG   | 2.43                     | 0.51              |
| 1:A:527:PRO:O     | 1:A:559:ARG:NH1   | 2.43                     | 0.51              |
| 1:A:792:GLN:HB2   | 1:A:797:THR:HG21  | 1.92                     | 0.51              |
| 1:A:1628:LEU:O    | 1:A:1836:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:2155:ASP:OD2  | 1:A:2169:ARG:NH2  | 2.44                     | 0.51              |
| 1:B:1592:MET:HB2  | 1:B:1596:THR:HG23 | 1.92                     | 0.51              |
| 1:C:179:THR:OG1   | 1:C:180:ASP:N     | 2.43                     | 0.51              |
| 1:C:250:LEU:HD23  | 1:C:447:LYS:HB2   | 1.92                     | 0.51              |
| 1:C:1605:ARG:NH1  | 1:C:1640:LEU:O    | 2.43                     | 0.51              |
| 1:C:1800:GLN:HE21 | 1:C:1804:GLN:HE21 | 1.59                     | 0.51              |
| 1:D:342:LEU:HA    | 1:D:362:LYS:H     | 1.74                     | 0.51              |
| 1:D:372:ARG:HB2   | 1:D:415:TRP:HB2   | 1.92                     | 0.51              |
| 1:D:1780:ASN:ND2  | 1:D:1845:SER:O    | 2.43                     | 0.51              |
| 1:E:160:SER:HA    | 1:E:970:LYS:HA    | 1.92                     | 0.51              |
| 1:E:342:LEU:HA    | 1:E:362:LYS:H     | 1.74                     | 0.51              |
| 1:E:2020:GLN:H    | 1:E:2316:THR:HG22 | 1.76                     | 0.51              |
| 1:A:179:THR:OG1   | 1:A:180:ASP:N     | 2.43                     | 0.51              |
| 1:B:270:ASP:OD1   | 1:B:270:ASP:N     | 2.41                     | 0.51              |
| 1:B:1628:LEU:O    | 1:B:1836:ASN:ND2  | 2.44                     | 0.51              |
| 1:B:1846:TRP:HE3  | 1:B:1847:ASN:HB2  | 1.75                     | 0.51              |
| 1:C:735:ILE:O     | 1:C:739:ASN:ND2   | 2.39                     | 0.51              |
| 1:C:1278:THR:OG1  | 1:C:1279:ARG:N    | 2.43                     | 0.51              |
| 1:D:160:SER:HA    | 1:D:970:LYS:HA    | 1.92                     | 0.51              |
| 1:B:1780:ASN:ND2  | 1:B:1845:SER:O    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:527:PRO:O     | 1:C:559:ARG:NH1   | 2.43                     | 0.51              |
| 1:D:2020:GLN:H    | 1:D:2316:THR:HG22 | 1.75                     | 0.51              |
| 1:E:2155:ASP:OD2  | 1:E:2169:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:160:SER:HA    | 1:A:970:LYS:HA    | 1.92                     | 0.51              |
| 1:A:706:GLN:O     | 1:A:765:ARG:NH2   | 2.41                     | 0.51              |
| 1:A:1780:ASN:ND2  | 1:A:1845:SER:O    | 2.43                     | 0.51              |
| 1:B:690:ASP:OD1   | 1:B:721:ASN:ND2   | 2.44                     | 0.51              |
| 1:B:1086:HIS:NE2  | 1:B:1091:VAL:O    | 2.44                     | 0.51              |
| 1:C:372:ARG:HB2   | 1:C:415:TRP:HB2   | 1.92                     | 0.51              |
| 1:D:1800:GLN:HE21 | 1:D:1804:GLN:HE21 | 1.59                     | 0.51              |
| 1:A:2500:SER:HA   | 1:A:2504:LYS:HD2  | 1.92                     | 0.50              |
| 1:B:527:PRO:O     | 1:B:559:ARG:NH1   | 2.43                     | 0.50              |
| 1:B:2020:GLN:H    | 1:B:2316:THR:HG22 | 1.75                     | 0.50              |
| 1:C:1846:TRP:HE3  | 1:C:1847:ASN:HB2  | 1.75                     | 0.50              |
| 1:E:1167:ASN:ND2  | 1:E:1169:SER:OG   | 2.43                     | 0.50              |
| 1:A:1088:SER:OG   | 1:A:1089:ILE:N    | 2.45                     | 0.50              |
| 1:A:1766:HIS:NE2  | 1:E:1531:SER:OG   | 2.40                     | 0.50              |
| 1:B:1800:GLN:HE21 | 1:B:1804:GLN:HE21 | 1.59                     | 0.50              |
| 1:B:2155:ASP:OD2  | 1:B:2169:ARG:NH2  | 2.44                     | 0.50              |
| 1:C:690:ASP:OD1   | 1:C:721:ASN:ND2   | 2.44                     | 0.50              |
| 1:C:2020:GLN:H    | 1:C:2316:THR:HG22 | 1.76                     | 0.50              |
| 1:D:250:LEU:HD23  | 1:D:447:LYS:HB2   | 1.92                     | 0.50              |
| 1:D:527:PRO:O     | 1:D:559:ARG:NH1   | 2.43                     | 0.50              |
| 1:D:1086:HIS:NE2  | 1:D:1091:VAL:O    | 2.44                     | 0.50              |
| 1:E:1592:MET:HB2  | 1:E:1596:THR:HG23 | 1.92                     | 0.50              |
| 1:A:1086:HIS:NE2  | 1:A:1091:VAL:O    | 2.44                     | 0.50              |
| 1:B:687:SER:OG    | 1:B:688:LEU:N     | 2.41                     | 0.50              |
| 1:B:2500:SER:HA   | 1:B:2504:LYS:HD2  | 1.92                     | 0.50              |
| 1:C:160:SER:HA    | 1:C:970:LYS:HA    | 1.92                     | 0.50              |
| 1:C:619:TYR:OH    | 1:C:634:GLN:NE2   | 2.45                     | 0.50              |
| 1:C:2500:SER:HA   | 1:C:2504:LYS:HD2  | 1.92                     | 0.50              |
| 1:D:2389:LEU:HD23 | 1:D:2396:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:1592:MET:HB2  | 1:A:1596:THR:HG23 | 1.92                     | 0.50              |
| 1:E:690:ASP:OD1   | 1:E:721:ASN:ND2   | 2.44                     | 0.50              |
| 1:A:1846:TRP:HE3  | 1:A:1847:ASN:HB2  | 1.75                     | 0.50              |
| 1:D:1628:LEU:O    | 1:D:1836:ASN:ND2  | 2.44                     | 0.50              |
| 1:C:1088:SER:OG   | 1:C:1089:ILE:N    | 2.45                     | 0.50              |
| 1:A:1278:THR:OG1  | 1:A:1279:ARG:N    | 2.43                     | 0.50              |
| 1:E:1086:HIS:NE2  | 1:E:1091:VAL:O    | 2.44                     | 0.50              |
| 1:E:1846:TRP:HE3  | 1:E:1847:ASN:HB2  | 1.75                     | 0.50              |
| 1:B:1088:SER:OG   | 1:B:1089:ILE:N    | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2422:LYS:H    | 1:B:2519:TYR:HA   | 1.77                     | 0.50              |
| 1:C:482:LYS:NZ    | 1:C:504:CYS:O     | 2.40                     | 0.50              |
| 1:C:1086:HIS:NE2  | 1:C:1091:VAL:O    | 2.44                     | 0.50              |
| 1:C:2422:LYS:H    | 1:C:2519:TYR:HA   | 1.77                     | 0.50              |
| 1:E:859:ASN:HB3   | 1:E:862:THR:HG22  | 1.94                     | 0.50              |
| 1:A:506:SER:O     | 1:A:595:ARG:NH1   | 2.45                     | 0.50              |
| 1:A:859:ASN:HB3   | 1:A:862:THR:HG22  | 1.94                     | 0.50              |
| 1:A:2032:MET:HG2  | 1:A:2452:ARG:HG3  | 1.94                     | 0.50              |
| 1:B:43:TRP:HA     | 1:B:46:THR:HB     | 1.94                     | 0.50              |
| 1:D:1088:SER:OG   | 1:D:1089:ILE:N    | 2.45                     | 0.50              |
| 1:E:2389:LEU:HD23 | 1:E:2396:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:2327:MET:HE2  | 1:E:2048:GLN:HG2  | 1.95                     | 0.49              |
| 1:A:2422:LYS:H    | 1:A:2519:TYR:HA   | 1.77                     | 0.49              |
| 1:D:2032:MET:HG2  | 1:D:2452:ARG:HG3  | 1.94                     | 0.49              |
| 1:E:1088:SER:OG   | 1:E:1089:ILE:N    | 2.45                     | 0.49              |
| 1:B:859:ASN:HB3   | 1:B:862:THR:HG22  | 1.94                     | 0.49              |
| 1:D:43:TRP:HA     | 1:D:46:THR:HB     | 1.95                     | 0.49              |
| 1:C:43:TRP:HA     | 1:C:46:THR:HB     | 1.94                     | 0.49              |
| 1:C:2149:MET:HB3  | 1:E:1106:PRO:HG2  | 1.95                     | 0.49              |
| 1:D:859:ASN:HB3   | 1:D:862:THR:HG22  | 1.94                     | 0.49              |
| 1:D:2155:ASP:OD2  | 1:D:2169:ARG:NH2  | 2.44                     | 0.49              |
| 1:E:43:TRP:HA     | 1:E:46:THR:HB     | 1.94                     | 0.49              |
| 1:A:43:TRP:HA     | 1:A:46:THR:HB     | 1.94                     | 0.49              |
| 1:A:1630:MET:O    | 1:A:1634:ASN:ND2  | 2.45                     | 0.49              |
| 1:B:21:LEU:H      | 1:B:24:ASN:HD22   | 1.61                     | 0.49              |
| 1:B:1151:TYR:OH   | 1:B:1225:ASP:O    | 2.26                     | 0.49              |
| 1:B:1630:MET:O    | 1:B:1634:ASN:ND2  | 2.45                     | 0.49              |
| 1:C:845:GLN:OE1   | 1:C:879:THR:OG1   | 2.31                     | 0.49              |
| 1:C:1167:ASN:ND2  | 1:C:1172:GLY:O    | 2.46                     | 0.49              |
| 1:C:1503:ILE:HG22 | 1:C:1558:ILE:HG12 | 1.95                     | 0.49              |
| 1:D:619:TYR:OH    | 1:D:634:GLN:NE2   | 2.45                     | 0.49              |
| 1:E:1800:GLN:HE21 | 1:E:1804:GLN:HE21 | 1.59                     | 0.49              |
| 1:B:1167:ASN:ND2  | 1:B:1172:GLY:O    | 2.46                     | 0.49              |
| 1:B:2349:ARG:NH1  | 1:B:2410:ASP:OD2  | 2.46                     | 0.49              |
| 1:D:2422:LYS:H    | 1:D:2519:TYR:HA   | 1.77                     | 0.49              |
| 1:E:1081:VAL:O    | 1:E:1597:GLN:NE2  | 2.41                     | 0.49              |
| 1:A:1800:GLN:HE21 | 1:A:1804:GLN:HE21 | 1.59                     | 0.49              |
| 1:A:2349:ARG:NH1  | 1:A:2410:ASP:OD2  | 2.46                     | 0.49              |
| 1:B:1503:ILE:HG22 | 1:B:1558:ILE:HG12 | 1.95                     | 0.49              |
| 1:D:482:LYS:NZ    | 1:D:504:CYS:O     | 2.40                     | 0.49              |
| 1:D:1503:ILE:HG22 | 1:D:1558:ILE:HG12 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2349:ARG:NH1  | 1:D:2410:ASP:OD2  | 2.46                     | 0.49              |
| 1:E:1503:ILE:HG22 | 1:E:1558:ILE:HG12 | 1.95                     | 0.49              |
| 1:A:21:LEU:H      | 1:A:24:ASN:HD22   | 1.61                     | 0.49              |
| 1:A:317:LEU:HA    | 1:A:327:ALA:HA    | 1.95                     | 0.49              |
| 1:B:459:PRO:HA    | 1:B:462:ILE:HG22  | 1.95                     | 0.49              |
| 1:B:2032:MET:HG2  | 1:B:2452:ARG:HG3  | 1.94                     | 0.49              |
| 1:C:1506:LEU:HB3  | 1:C:1555:GLU:HB2  | 1.95                     | 0.49              |
| 1:C:2155:ASP:OD2  | 1:C:2169:ARG:NH2  | 2.44                     | 0.49              |
| 1:D:1167:ASN:ND2  | 1:D:1172:GLY:O    | 2.46                     | 0.49              |
| 1:E:21:LEU:H      | 1:E:24:ASN:HD22   | 1.61                     | 0.49              |
| 1:E:72:ASN:ND2    | 1:E:74:GLN:OE1    | 2.43                     | 0.49              |
| 1:E:1167:ASN:ND2  | 1:E:1172:GLY:O    | 2.46                     | 0.49              |
| 1:E:2422:LYS:H    | 1:E:2519:TYR:HA   | 1.77                     | 0.49              |
| 1:A:459:PRO:HA    | 1:A:462:ILE:HG22  | 1.95                     | 0.49              |
| 1:C:506:SER:O     | 1:C:595:ARG:NH1   | 2.45                     | 0.49              |
| 1:C:709:SER:O     | 1:C:712:THR:OG1   | 2.31                     | 0.49              |
| 1:A:606:THR:OG1   | 1:A:609:GLU:OE2   | 2.31                     | 0.49              |
| 1:B:2469:PHE:CZ   | 1:C:2346:GLU:HB3  | 2.47                     | 0.49              |
| 1:C:780:LYS:NZ    | 1:C:823:GLU:OE1   | 2.43                     | 0.49              |
| 1:C:859:ASN:HB3   | 1:C:862:THR:HG22  | 1.94                     | 0.49              |
| 1:C:1312:ASN:ND2  | 1:C:1335:GLU:OE2  | 2.39                     | 0.49              |
| 1:C:2032:MET:HG2  | 1:C:2452:ARG:HG3  | 1.94                     | 0.49              |
| 1:E:506:SER:O     | 1:E:595:ARG:NH1   | 2.45                     | 0.49              |
| 1:B:845:GLN:OE1   | 1:B:879:THR:OG1   | 2.31                     | 0.48              |
| 1:B:2389:LEU:HD23 | 1:B:2396:LEU:HD11 | 1.94                     | 0.48              |
| 1:D:709:SER:O     | 1:D:712:THR:OG1   | 2.31                     | 0.48              |
| 1:D:2048:GLN:HG2  | 1:E:2327:MET:HE2  | 1.94                     | 0.48              |
| 1:D:2421:ILE:HD12 | 1:D:2484:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:1503:ILE:HG22 | 1:A:1558:ILE:HG12 | 1.95                     | 0.48              |
| 1:A:2421:ILE:HD12 | 1:A:2484:LEU:HB3  | 1.95                     | 0.48              |
| 1:B:1506:LEU:HB3  | 1:B:1555:GLU:HB2  | 1.95                     | 0.48              |
| 1:C:21:LEU:H      | 1:C:24:ASN:HD22   | 1.61                     | 0.48              |
| 1:D:506:SER:O     | 1:D:595:ARG:NH1   | 2.45                     | 0.48              |
| 1:E:619:TYR:OH    | 1:E:634:GLN:NE2   | 2.45                     | 0.48              |
| 1:E:1506:LEU:HB3  | 1:E:1555:GLU:HB2  | 1.95                     | 0.48              |
| 1:A:1167:ASN:ND2  | 1:A:1172:GLY:O    | 2.46                     | 0.48              |
| 1:B:2421:ILE:HD12 | 1:B:2484:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:1202:ASP:OD1  | 1:C:1202:ASP:N    | 2.37                     | 0.48              |
| 1:C:2389:LEU:HD23 | 1:C:2396:LEU:HD11 | 1.94                     | 0.48              |
| 1:D:375:ASN:OD1   | 1:D:375:ASN:N     | 2.47                     | 0.48              |
| 1:D:422:SER:OG    | 1:D:423:ASP:N     | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1147:ARG:NH1  | 1:E:1216:MET:O    | 2.46                     | 0.48              |
| 1:A:619:TYR:OH    | 1:A:634:GLN:NE2   | 2.45                     | 0.48              |
| 1:A:2389:LEU:HD23 | 1:A:2396:LEU:HD11 | 1.94                     | 0.48              |
| 1:B:709:SER:O     | 1:B:712:THR:OG1   | 2.31                     | 0.48              |
| 1:B:1206:ASN:O    | 1:B:1210:LYS:NZ   | 2.37                     | 0.48              |
| 1:D:21:LEU:H      | 1:D:24:ASN:HD22   | 1.61                     | 0.48              |
| 1:E:317:LEU:HA    | 1:E:327:ALA:HA    | 1.95                     | 0.48              |
| 1:B:506:SER:O     | 1:B:595:ARG:NH1   | 2.45                     | 0.48              |
| 1:D:506:SER:OG    | 1:D:507:ASP:N     | 2.47                     | 0.48              |
| 1:D:1147:ARG:NH1  | 1:D:1216:MET:O    | 2.46                     | 0.48              |
| 1:A:952:ARG:HH21  | 1:A:964:GLN:HG2   | 1.79                     | 0.48              |
| 1:A:1147:ARG:NH1  | 1:A:1216:MET:O    | 2.47                     | 0.48              |
| 1:A:2343:ARG:NH2  | 1:E:2478:TYR:O    | 2.46                     | 0.48              |
| 1:B:506:SER:OG    | 1:B:507:ASP:N     | 2.47                     | 0.48              |
| 1:B:952:ARG:HH21  | 1:B:964:GLN:HG2   | 1.79                     | 0.48              |
| 1:C:506:SER:OG    | 1:C:507:ASP:N     | 2.47                     | 0.48              |
| 1:E:2349:ARG:NH1  | 1:E:2410:ASP:OD2  | 2.46                     | 0.48              |
| 1:A:709:SER:O     | 1:A:712:THR:OG1   | 2.31                     | 0.48              |
| 1:A:950:LYS:N     | 1:A:954:GLU:OE1   | 2.42                     | 0.48              |
| 1:B:317:LEU:HA    | 1:B:327:ALA:HA    | 1.95                     | 0.48              |
| 1:B:482:LYS:NZ    | 1:B:504:CYS:O     | 2.40                     | 0.48              |
| 1:B:1147:ARG:NH1  | 1:B:1216:MET:O    | 2.47                     | 0.48              |
| 1:C:1272:THR:O    | 1:C:1272:THR:OG1  | 2.30                     | 0.48              |
| 1:A:1151:TYR:OH   | 1:A:1225:ASP:O    | 2.26                     | 0.48              |
| 1:C:459:PRO:HA    | 1:C:462:ILE:HG22  | 1.95                     | 0.48              |
| 1:C:1630:MET:O    | 1:C:1634:ASN:ND2  | 2.45                     | 0.48              |
| 1:E:780:LYS:NZ    | 1:E:823:GLU:OE1   | 2.43                     | 0.48              |
| 1:E:2032:MET:HG2  | 1:E:2452:ARG:HG3  | 1.94                     | 0.48              |
| 1:C:1147:ARG:NH1  | 1:C:1216:MET:O    | 2.47                     | 0.48              |
| 1:D:72:ASN:ND2    | 1:D:74:GLN:OE1    | 2.43                     | 0.48              |
| 1:E:2421:ILE:HD12 | 1:E:2484:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:375:ASN:OD1   | 1:A:375:ASN:N     | 2.47                     | 0.48              |
| 1:A:1167:ASN:HB3  | 1:A:1174:ILE:H    | 1.78                     | 0.48              |
| 1:B:72:ASN:ND2    | 1:B:74:GLN:OE1    | 2.43                     | 0.48              |
| 1:C:952:ARG:HH21  | 1:C:964:GLN:HG2   | 1.79                     | 0.48              |
| 1:D:459:PRO:HA    | 1:D:462:ILE:HG22  | 1.95                     | 0.48              |
| 1:D:845:GLN:OE1   | 1:D:879:THR:OG1   | 2.30                     | 0.48              |
| 1:E:1167:ASN:HB3  | 1:E:1174:ILE:H    | 1.78                     | 0.48              |
| 1:E:459:PRO:HA    | 1:E:462:ILE:HG22  | 1.95                     | 0.47              |
| 1:A:987:ARG:NH1   | 1:A:993:GLU:OE2   | 2.47                     | 0.47              |
| 1:B:1278:THR:HG23 | 1:B:1281:GLU:H    | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2421:ILE:HD12 | 1:C:2484:LEU:HB3  | 1.95                     | 0.47              |
| 1:E:2072:LEU:HA   | 1:E:2075:GLN:HE21 | 1.79                     | 0.47              |
| 1:A:1709:ARG:NE   | 1:A:1720:ASP:OD2  | 2.40                     | 0.47              |
| 1:B:987:ARG:NH1   | 1:B:993:GLU:OE2   | 2.48                     | 0.47              |
| 1:C:2202:ARG:NH2  | 1:E:1805:GLU:OE1  | 2.47                     | 0.47              |
| 1:C:2349:ARG:NH1  | 1:C:2410:ASP:OD2  | 2.46                     | 0.47              |
| 1:D:495:ILE:HB    | 1:D:499:ASP:HB3   | 1.97                     | 0.47              |
| 1:A:1278:THR:HG23 | 1:A:1281:GLU:H    | 1.80                     | 0.47              |
| 1:A:1506:LEU:HB3  | 1:A:1555:GLU:HB2  | 1.95                     | 0.47              |
| 1:C:1167:ASN:HB3  | 1:C:1174:ILE:H    | 1.78                     | 0.47              |
| 1:D:952:ARG:HH21  | 1:D:964:GLN:HG2   | 1.79                     | 0.47              |
| 1:E:987:ARG:NH1   | 1:E:993:GLU:OE2   | 2.47                     | 0.47              |
| 1:E:1206:ASN:O    | 1:E:1210:LYS:NZ   | 2.37                     | 0.47              |
| 1:B:495:ILE:HB    | 1:B:499:ASP:HB3   | 1.97                     | 0.47              |
| 1:C:495:ILE:HB    | 1:C:499:ASP:HB3   | 1.97                     | 0.47              |
| 1:C:606:THR:OG1   | 1:C:609:GLU:OE2   | 2.31                     | 0.47              |
| 1:C:1278:THR:HG23 | 1:C:1281:GLU:H    | 1.80                     | 0.47              |
| 1:D:317:LEU:HA    | 1:D:327:ALA:HA    | 1.95                     | 0.47              |
| 1:D:1312:ASN:ND2  | 1:D:1335:GLU:OE2  | 2.39                     | 0.47              |
| 1:E:952:ARG:HH21  | 1:E:964:GLN:HG2   | 1.79                     | 0.47              |
| 1:A:373:LEU:O     | 1:A:381:ILE:N     | 2.47                     | 0.47              |
| 1:B:422:SER:OG    | 1:B:423:ASP:N     | 2.47                     | 0.47              |
| 1:B:619:TYR:OH    | 1:B:634:GLN:NE2   | 2.45                     | 0.47              |
| 1:B:1727:PHE:H    | 1:B:1741:ASN:HD22 | 1.63                     | 0.47              |
| 1:C:2072:LEU:HA   | 1:C:2075:GLN:HE21 | 1.80                     | 0.47              |
| 1:D:987:ARG:NH1   | 1:D:993:GLU:OE2   | 2.47                     | 0.47              |
| 1:A:130:HIS:HD1   | 1:A:984:TYR:HH    | 1.60                     | 0.47              |
| 1:A:506:SER:OG    | 1:A:507:ASP:N     | 2.47                     | 0.47              |
| 1:B:42:THR:O      | 1:B:42:THR:OG1    | 2.33                     | 0.47              |
| 1:B:2072:LEU:HA   | 1:B:2075:GLN:HE21 | 1.79                     | 0.47              |
| 1:B:2127:GLU:OE1  | 1:B:2204:ARG:NH2  | 2.48                     | 0.47              |
| 1:C:317:LEU:HA    | 1:C:327:ALA:HA    | 1.95                     | 0.47              |
| 1:C:2127:GLU:OE1  | 1:C:2204:ARG:NH2  | 2.48                     | 0.47              |
| 1:C:2298:TYR:OH   | 1:C:2482:GLU:O    | 2.33                     | 0.47              |
| 1:D:1272:THR:O    | 1:D:1272:THR:OG1  | 2.30                     | 0.47              |
| 1:D:1506:LEU:HB3  | 1:D:1555:GLU:HB2  | 1.95                     | 0.47              |
| 1:E:495:ILE:HB    | 1:E:499:ASP:HB3   | 1.97                     | 0.47              |
| 1:E:562:ARG:NH1   | 1:E:601:ASP:OD2   | 2.48                     | 0.47              |
| 1:A:42:THR:O      | 1:A:42:THR:OG1    | 2.33                     | 0.47              |
| 1:C:375:ASN:OD1   | 1:C:375:ASN:N     | 2.47                     | 0.47              |
| 1:A:462:ILE:HA    | 1:A:465:VAL:HG22  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:495:ILE:HB    | 1:A:499:ASP:HB3   | 1.97                     | 0.47              |
| 1:A:1727:PHE:H    | 1:A:1741:ASN:HD22 | 1.63                     | 0.47              |
| 1:A:2127:GLU:OE1  | 1:A:2204:ARG:NH2  | 2.48                     | 0.47              |
| 1:B:373:LEU:O     | 1:B:381:ILE:N     | 2.47                     | 0.47              |
| 1:C:1151:TYR:OH   | 1:C:1225:ASP:O    | 2.26                     | 0.47              |
| 1:C:1727:PHE:H    | 1:C:1741:ASN:HD22 | 1.63                     | 0.47              |
| 1:E:1596:THR:OG1  | 1:E:1597:GLN:N    | 2.48                     | 0.47              |
| 1:A:99:ARG:NH1    | 1:A:1964:PHE:O    | 2.47                     | 0.47              |
| 1:A:562:ARG:NH1   | 1:A:601:ASP:OD2   | 2.48                     | 0.47              |
| 1:A:1596:THR:OG1  | 1:A:1597:GLN:N    | 2.48                     | 0.47              |
| 1:A:2049:LEU:HD11 | 1:A:2282:TYR:HA   | 1.97                     | 0.47              |
| 1:B:462:ILE:HA    | 1:B:465:VAL:HG22  | 1.97                     | 0.47              |
| 1:B:1956:THR:OG1  | 1:B:1957:ALA:N    | 2.48                     | 0.47              |
| 1:C:203:TYR:OH    | 1:C:237:ALA:O     | 2.30                     | 0.47              |
| 1:C:987:ARG:NH1   | 1:C:993:GLU:OE2   | 2.47                     | 0.47              |
| 1:C:2299:GLU:O    | 1:C:2420:ARG:NH1  | 2.48                     | 0.47              |
| 1:D:606:THR:OG1   | 1:D:609:GLU:OE2   | 2.31                     | 0.47              |
| 1:D:2072:LEU:HA   | 1:D:2075:GLN:HE21 | 1.79                     | 0.47              |
| 1:E:709:SER:O     | 1:E:712:THR:OG1   | 2.31                     | 0.47              |
| 1:B:1167:ASN:HB3  | 1:B:1174:ILE:H    | 1.78                     | 0.46              |
| 1:C:770:SER:HB3   | 1:D:2016:ILE:HG13 | 1.97                     | 0.46              |
| 1:D:1167:ASN:HB3  | 1:D:1174:ILE:H    | 1.79                     | 0.46              |
| 1:D:2049:LEU:HD11 | 1:D:2282:TYR:HA   | 1.97                     | 0.46              |
| 1:D:2299:GLU:O    | 1:D:2420:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:2072:LEU:HA   | 1:A:2075:GLN:HE21 | 1.79                     | 0.46              |
| 1:B:968:GLN:HB3   | 1:C:1989:ASN:HD22 | 1.80                     | 0.46              |
| 1:B:1312:ASN:ND2  | 1:B:1335:GLU:OE2  | 2.39                     | 0.46              |
| 1:C:562:ARG:NH1   | 1:C:601:ASP:OD2   | 2.48                     | 0.46              |
| 1:E:1278:THR:HG23 | 1:E:1281:GLU:H    | 1.80                     | 0.46              |
| 1:A:2251:GLN:NE2  | 1:B:2013:SER:OG   | 2.41                     | 0.46              |
| 1:C:373:LEU:O     | 1:C:381:ILE:N     | 2.47                     | 0.46              |
| 1:C:703:ALA:HB2   | 1:D:2272:GLY:HA3  | 1.97                     | 0.46              |
| 1:D:1038:ARG:NH2  | 1:D:1789:GLU:OE2  | 2.49                     | 0.46              |
| 1:D:2025:LEU:HD13 | 1:D:2310:PRO:HA   | 1.97                     | 0.46              |
| 1:E:296:VAL:HG13  | 1:E:315:ILE:HD11  | 1.98                     | 0.46              |
| 1:E:375:ASN:OD1   | 1:E:375:ASN:N     | 2.47                     | 0.46              |
| 1:E:1038:ARG:NH2  | 1:E:1789:GLU:OE2  | 2.49                     | 0.46              |
| 1:A:2025:LEU:HD13 | 1:A:2310:PRO:HA   | 1.97                     | 0.46              |
| 1:B:562:ARG:NH1   | 1:B:601:ASP:OD2   | 2.48                     | 0.46              |
| 1:D:950:LYS:N     | 1:D:954:GLU:OE1   | 2.42                     | 0.46              |
| 1:D:1956:THR:OG1  | 1:D:1957:ALA:N    | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1956:THR:OG1  | 1:E:1957:ALA:N    | 2.48                     | 0.46              |
| 1:B:1058:ASN:OD1  | 1:B:1058:ASN:N    | 2.49                     | 0.46              |
| 1:B:1789:GLU:HA   | 1:B:1793:TYR:HB2  | 1.98                     | 0.46              |
| 1:B:2049:LEU:HD11 | 1:B:2282:TYR:HA   | 1.97                     | 0.46              |
| 1:C:470:TYR:OH    | 1:C:478:ASN:ND2   | 2.49                     | 0.46              |
| 1:C:707:MET:HE2   | 1:C:761:SER:HB2   | 1.98                     | 0.46              |
| 1:C:1596:THR:OG1  | 1:C:1597:GLN:N    | 2.48                     | 0.46              |
| 1:E:845:GLN:OE1   | 1:E:879:THR:OG1   | 2.30                     | 0.46              |
| 1:E:2299:GLU:O    | 1:E:2420:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:296:VAL:HG13  | 1:A:315:ILE:HD11  | 1.98                     | 0.46              |
| 1:B:296:VAL:HG13  | 1:B:315:ILE:HD11  | 1.98                     | 0.46              |
| 1:D:1630:MET:O    | 1:D:1634:ASN:ND2  | 2.45                     | 0.46              |
| 1:A:470:TYR:OH    | 1:A:478:ASN:ND2   | 2.49                     | 0.46              |
| 1:B:1142:TRP:HH2  | 1:B:1214:ILE:HD12 | 1.81                     | 0.46              |
| 1:B:2025:LEU:HD13 | 1:B:2310:PRO:HA   | 1.97                     | 0.46              |
| 1:D:296:VAL:HG13  | 1:D:315:ILE:HD11  | 1.98                     | 0.46              |
| 1:D:1278:THR:HG23 | 1:D:1281:GLU:H    | 1.79                     | 0.46              |
| 1:E:1554:SER:OG   | 1:E:1572:SER:O    | 2.32                     | 0.46              |
| 1:B:707:MET:HE2   | 1:B:761:SER:HB2   | 1.98                     | 0.46              |
| 1:B:950:LYS:N     | 1:B:954:GLU:OE1   | 2.42                     | 0.46              |
| 1:B:1554:SER:OG   | 1:B:1572:SER:O    | 2.32                     | 0.46              |
| 1:C:841:GLN:HA    | 1:C:844:THR:HG22  | 1.98                     | 0.46              |
| 1:D:562:ARG:NH1   | 1:D:601:ASP:OD2   | 2.48                     | 0.46              |
| 1:D:2086:MET:HE3  | 1:D:2086:MET:HB2  | 1.74                     | 0.46              |
| 1:D:2127:GLU:OE1  | 1:D:2204:ARG:NH2  | 2.48                     | 0.46              |
| 1:D:2298:TYR:OH   | 1:D:2482:GLU:O    | 2.33                     | 0.46              |
| 1:A:2299:GLU:O    | 1:A:2420:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:462:ILE:HA    | 1:C:465:VAL:HG22  | 1.97                     | 0.46              |
| 1:D:42:THR:O      | 1:D:42:THR:OG1    | 2.33                     | 0.46              |
| 1:E:462:ILE:HA    | 1:E:465:VAL:HG22  | 1.97                     | 0.46              |
| 1:E:950:LYS:N     | 1:E:954:GLU:OE1   | 2.42                     | 0.46              |
| 1:A:1789:GLU:HA   | 1:A:1793:TYR:HB2  | 1.97                     | 0.46              |
| 1:B:841:GLN:HA    | 1:B:844:THR:HG22  | 1.98                     | 0.46              |
| 1:B:1596:THR:OG1  | 1:B:1597:GLN:N    | 2.48                     | 0.46              |
| 1:B:2299:GLU:O    | 1:B:2420:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:487:GLN:HE21  | 1:C:487:GLN:HB3   | 1.55                     | 0.46              |
| 1:C:1038:ARG:NH2  | 1:C:1789:GLU:OE2  | 2.49                     | 0.46              |
| 1:C:1789:GLU:HA   | 1:C:1793:TYR:HB2  | 1.97                     | 0.46              |
| 1:D:462:ILE:HA    | 1:D:465:VAL:HG22  | 1.97                     | 0.46              |
| 1:D:470:TYR:OH    | 1:D:478:ASN:ND2   | 2.49                     | 0.46              |
| 1:D:841:GLN:HA    | 1:D:844:THR:HG22  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1142:TRP:HH2  | 1:D:1214:ILE:HD12 | 1.81                     | 0.46              |
| 1:D:1596:THR:OG1  | 1:D:1597:GLN:N    | 2.48                     | 0.46              |
| 1:A:1142:TRP:HH2  | 1:A:1214:ILE:HD12 | 1.81                     | 0.45              |
| 1:B:2086:MET:HE3  | 1:B:2086:MET:HB2  | 1.74                     | 0.45              |
| 1:B:2298:TYR:OH   | 1:B:2482:GLU:O    | 2.33                     | 0.45              |
| 1:E:113:PHE:O     | 1:E:1016:TYR:OH   | 2.34                     | 0.45              |
| 1:A:1956:THR:OG1  | 1:A:1957:ALA:N    | 2.48                     | 0.45              |
| 1:B:375:ASN:OD1   | 1:B:375:ASN:N     | 2.47                     | 0.45              |
| 1:B:2174:PHE:HB2  | 1:C:2151:ALA:HB2  | 1.97                     | 0.45              |
| 1:C:788:THR:HG22  | 1:C:790:ALA:H     | 1.81                     | 0.45              |
| 1:C:2049:LEU:HD11 | 1:C:2282:TYR:HA   | 1.97                     | 0.45              |
| 1:C:2052:PHE:CE1  | 1:D:2324:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:1080:GLN:NE2  | 1:D:1101:TYR:OH   | 2.50                     | 0.45              |
| 1:E:506:SER:OG    | 1:E:507:ASP:N     | 2.47                     | 0.45              |
| 1:A:788:THR:HG22  | 1:A:790:ALA:H     | 1.82                     | 0.45              |
| 1:B:568:LEU:HD11  | 1:B:593:LEU:HD21  | 1.98                     | 0.45              |
| 1:C:1956:THR:OG1  | 1:C:1957:ALA:N    | 2.48                     | 0.45              |
| 1:A:29:SER:HB3    | 1:A:1003:ARG:HG2  | 1.99                     | 0.45              |
| 1:A:568:LEU:HD11  | 1:A:593:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:707:MET:HE2   | 1:A:761:SER:HB2   | 1.98                     | 0.45              |
| 1:A:1812:THR:OG1  | 1:E:1010:GLU:OE2  | 2.32                     | 0.45              |
| 1:B:29:SER:HB3    | 1:B:1003:ARG:HG2  | 1.99                     | 0.45              |
| 1:B:1080:GLN:NE2  | 1:B:1101:TYR:OH   | 2.50                     | 0.45              |
| 1:B:1118:LYS:HB2  | 1:B:1128:ALA:HB2  | 1.98                     | 0.45              |
| 1:D:1058:ASN:OD1  | 1:D:1058:ASN:N    | 2.49                     | 0.45              |
| 1:E:470:TYR:OH    | 1:E:478:ASN:ND2   | 2.49                     | 0.45              |
| 1:E:841:GLN:HA    | 1:E:844:THR:HG22  | 1.98                     | 0.45              |
| 1:E:1991:THR:OG1  | 1:E:1995:GLN:O    | 2.34                     | 0.45              |
| 1:A:418:LYS:HE2   | 1:A:420:ASN:HB3   | 1.98                     | 0.45              |
| 1:A:2298:TYR:OH   | 1:A:2482:GLU:O    | 2.33                     | 0.45              |
| 1:A:2397:GLN:HA   | 1:A:2495:SER:HA   | 1.99                     | 0.45              |
| 1:C:418:LYS:HE2   | 1:C:420:ASN:HB3   | 1.98                     | 0.45              |
| 1:C:1142:TRP:HH2  | 1:C:1214:ILE:HD12 | 1.81                     | 0.45              |
| 1:C:2025:LEU:HD13 | 1:C:2310:PRO:HA   | 1.97                     | 0.45              |
| 1:E:29:SER:HB3    | 1:E:1003:ARG:HG2  | 1.99                     | 0.45              |
| 1:E:1239:SER:HG   | 1:E:1242:SER:HG   | 1.62                     | 0.45              |
| 1:A:841:GLN:HA    | 1:A:844:THR:HG22  | 1.98                     | 0.45              |
| 1:A:1038:ARG:NH2  | 1:A:1789:GLU:OE2  | 2.49                     | 0.45              |
| 1:B:1232:HIS:ND1  | 1:B:1233:GLU:O    | 2.41                     | 0.45              |
| 1:C:296:VAL:HG13  | 1:C:315:ILE:HD11  | 1.98                     | 0.45              |
| 1:D:2369:ASP:OD1  | 1:D:2369:ASP:N    | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2437:ASP:OD2  | 1:E:2350:THR:N    | 2.45                     | 0.45              |
| 1:E:513:THR:OG1   | 1:E:516:GLN:NE2   | 2.50                     | 0.45              |
| 1:E:1727:PHE:H    | 1:E:1741:ASN:HD22 | 1.63                     | 0.45              |
| 1:A:513:THR:OG1   | 1:A:516:GLN:NE2   | 2.50                     | 0.45              |
| 1:A:2034:ARG:NH1  | 1:A:2477:LYS:O    | 2.50                     | 0.45              |
| 1:B:788:THR:HG22  | 1:B:790:ALA:H     | 1.81                     | 0.45              |
| 1:C:568:LEU:HD11  | 1:C:593:LEU:HD21  | 1.98                     | 0.45              |
| 1:C:1801:ARG:HD2  | 1:C:1801:ARG:HA   | 1.73                     | 0.45              |
| 1:D:418:LYS:HE2   | 1:D:420:ASN:HB3   | 1.98                     | 0.45              |
| 1:D:788:THR:HG22  | 1:D:790:ALA:H     | 1.81                     | 0.45              |
| 1:D:1118:LYS:HB2  | 1:D:1128:ALA:HB2  | 1.98                     | 0.45              |
| 1:D:2034:ARG:NH1  | 1:D:2477:LYS:O    | 2.50                     | 0.45              |
| 1:E:1657:GLU:OE2  | 1:E:1719:TYR:OH   | 2.35                     | 0.45              |
| 1:E:2049:LEU:HD11 | 1:E:2282:TYR:HA   | 1.97                     | 0.45              |
| 1:E:2127:GLU:OE1  | 1:E:2204:ARG:NH2  | 2.48                     | 0.45              |
| 1:E:2397:GLN:HA   | 1:E:2495:SER:HA   | 1.99                     | 0.45              |
| 1:B:99:ARG:NH1    | 1:B:1964:PHE:O    | 2.48                     | 0.45              |
| 1:B:470:TYR:OH    | 1:B:478:ASN:ND2   | 2.49                     | 0.45              |
| 1:B:513:THR:OG1   | 1:B:516:GLN:NE2   | 2.50                     | 0.45              |
| 1:B:1038:ARG:NH2  | 1:B:1789:GLU:OE2  | 2.49                     | 0.45              |
| 1:B:1657:GLU:OE2  | 1:B:1719:TYR:OH   | 2.35                     | 0.45              |
| 1:C:42:THR:O      | 1:C:42:THR:OG1    | 2.33                     | 0.45              |
| 1:D:263:MET:HA    | 1:D:443:LEU:HD21  | 1.99                     | 0.45              |
| 1:D:513:THR:OG1   | 1:D:516:GLN:NE2   | 2.50                     | 0.45              |
| 1:D:707:MET:HE2   | 1:D:761:SER:HB2   | 1.98                     | 0.45              |
| 1:D:1727:PHE:H    | 1:D:1741:ASN:HD22 | 1.63                     | 0.45              |
| 1:E:1058:ASN:OD1  | 1:E:1058:ASN:N    | 2.49                     | 0.45              |
| 1:E:1142:TRP:HH2  | 1:E:1214:ILE:HD12 | 1.81                     | 0.45              |
| 1:E:1893:ASP:OD1  | 1:E:1893:ASP:N    | 2.50                     | 0.45              |
| 1:E:2025:LEU:HD13 | 1:E:2310:PRO:HA   | 1.97                     | 0.45              |
| 1:E:2298:TYR:OH   | 1:E:2482:GLU:O    | 2.33                     | 0.45              |
| 1:E:2369:ASP:OD1  | 1:E:2369:ASP:N    | 2.50                     | 0.45              |
| 1:A:498:SER:HA    | 1:A:501:LEU:HD12  | 1.99                     | 0.45              |
| 1:A:1054:GLN:HE21 | 1:D:2194:LYS:HD2  | 1.82                     | 0.45              |
| 1:B:1700:LYS:HE3  | 1:B:1700:LYS:HB3  | 1.90                     | 0.45              |
| 1:B:2034:ARG:NH1  | 1:B:2477:LYS:O    | 2.50                     | 0.45              |
| 1:B:2397:GLN:HA   | 1:B:2495:SER:HA   | 1.99                     | 0.45              |
| 1:C:29:SER:HB3    | 1:C:1003:ARG:HG2  | 1.99                     | 0.45              |
| 1:C:498:SER:HA    | 1:C:501:LEU:HD12  | 1.99                     | 0.45              |
| 1:C:2086:MET:HE3  | 1:C:2086:MET:HB2  | 1.74                     | 0.45              |
| 1:D:568:LEU:HD11  | 1:D:593:LEU:HD21  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:42:THR:O      | 1:E:42:THR:OG1   | 2.33                     | 0.45              |
| 1:C:513:THR:OG1   | 1:C:516:GLN:NE2  | 2.50                     | 0.45              |
| 1:C:1118:LYS:HB2  | 1:C:1128:ALA:HB2 | 1.98                     | 0.45              |
| 1:D:1010:GLU:OE2  | 1:E:1812:THR:OG1 | 2.30                     | 0.45              |
| 1:D:1789:GLU:HA   | 1:D:1793:TYR:HB2 | 1.98                     | 0.45              |
| 1:E:263:MET:HA    | 1:E:443:LEU:HD21 | 1.99                     | 0.45              |
| 1:E:1118:LYS:HB2  | 1:E:1128:ALA:HB2 | 1.98                     | 0.45              |
| 1:A:413:ARG:HG3   | 1:A:428:ASN:HB3  | 1.99                     | 0.44              |
| 1:B:606:THR:OG1   | 1:B:609:GLU:OE2  | 2.31                     | 0.44              |
| 1:B:772:ASN:ND2   | 1:C:2017:THR:O   | 2.50                     | 0.44              |
| 1:B:1529:HIS:HA   | 1:B:1534:MET:HE2 | 2.00                     | 0.44              |
| 1:C:1080:GLN:NE2  | 1:C:1101:TYR:OH  | 2.50                     | 0.44              |
| 1:D:373:LEU:O     | 1:D:381:ILE:N    | 2.47                     | 0.44              |
| 1:E:568:LEU:HD11  | 1:E:593:LEU:HD21 | 1.98                     | 0.44              |
| 1:E:707:MET:HE2   | 1:E:761:SER:HB2  | 1.98                     | 0.44              |
| 1:E:1080:GLN:NE2  | 1:E:1101:TYR:OH  | 2.50                     | 0.44              |
| 1:E:1630:MET:O    | 1:E:1634:ASN:ND2 | 2.45                     | 0.44              |
| 1:A:1202:ASP:OD1  | 1:A:1202:ASP:N   | 2.37                     | 0.44              |
| 1:C:1893:ASP:OD1  | 1:C:1893:ASP:N   | 2.50                     | 0.44              |
| 1:D:29:SER:HB3    | 1:D:1003:ARG:HG2 | 1.99                     | 0.44              |
| 1:D:1893:ASP:N    | 1:D:1893:ASP:OD1 | 2.50                     | 0.44              |
| 1:E:78:ILE:HD13   | 1:E:81:LEU:HD22  | 2.00                     | 0.44              |
| 1:E:418:LYS:HE2   | 1:E:420:ASN:HB3  | 1.98                     | 0.44              |
| 1:E:422:SER:OG    | 1:E:423:ASP:N    | 2.46                     | 0.44              |
| 1:E:2134:TYR:HB3  | 1:E:2194:LYS:HB2 | 1.99                     | 0.44              |
| 1:A:845:GLN:OE1   | 1:A:879:THR:OG1  | 2.31                     | 0.44              |
| 1:A:1529:HIS:HA   | 1:A:1534:MET:HE2 | 2.00                     | 0.44              |
| 1:A:1554:SER:OG   | 1:A:1572:SER:O   | 2.32                     | 0.44              |
| 1:B:413:ARG:HG3   | 1:B:428:ASN:HB3  | 1.99                     | 0.44              |
| 1:D:413:ARG:HG3   | 1:D:428:ASN:HB3  | 1.99                     | 0.44              |
| 1:D:2397:GLN:HA   | 1:D:2495:SER:HA  | 1.99                     | 0.44              |
| 1:E:413:ARG:HG3   | 1:E:428:ASN:HB3  | 2.00                     | 0.44              |
| 1:E:788:THR:HG22  | 1:E:790:ALA:H    | 1.82                     | 0.44              |
| 1:E:1789:GLU:HA   | 1:E:1793:TYR:HB2 | 1.97                     | 0.44              |
| 1:A:1080:GLN:NE2  | 1:A:1101:TYR:OH  | 2.50                     | 0.44              |
| 1:A:1625:ASP:OD1  | 1:A:1817:TYR:OH  | 2.33                     | 0.44              |
| 1:A:1893:ASP:OD1  | 1:A:1893:ASP:N   | 2.50                     | 0.44              |
| 1:B:418:LYS:HE2   | 1:B:420:ASN:HB3  | 1.98                     | 0.44              |
| 1:B:2171:GLY:N    | 1:C:2155:ASP:OD1 | 2.43                     | 0.44              |
| 1:C:2059:ILE:HD13 | 1:C:2059:ILE:HA  | 1.84                     | 0.44              |
| 1:D:498:SER:HA    | 1:D:501:LEU:HD12 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1529:HIS:HA   | 1:E:1534:MET:HE2  | 2.00                     | 0.44              |
| 1:E:1709:ARG:NE   | 1:E:1720:ASP:OD2  | 2.40                     | 0.44              |
| 1:E:2034:ARG:NH1  | 1:E:2477:LYS:O    | 2.50                     | 0.44              |
| 1:A:78:ILE:HD13   | 1:A:81:LEU:HD22   | 2.00                     | 0.44              |
| 1:A:1118:LYS:HB2  | 1:A:1128:ALA:HB2  | 1.98                     | 0.44              |
| 1:A:2369:ASP:N    | 1:A:2369:ASP:OD1  | 2.50                     | 0.44              |
| 1:C:78:ILE:HD13   | 1:C:81:LEU:HD22   | 2.00                     | 0.44              |
| 1:C:1529:HIS:HA   | 1:C:1534:MET:HE2  | 2.00                     | 0.44              |
| 1:D:1801:ARG:HD2  | 1:D:1801:ARG:HA   | 1.73                     | 0.44              |
| 1:E:2086:MET:HE3  | 1:E:2086:MET:HB2  | 1.74                     | 0.44              |
| 1:A:200:HIS:HB3   | 1:A:203:TYR:HB3   | 1.99                     | 0.44              |
| 1:A:1799:PHE:HE2  | 1:A:1874:LYS:HB3  | 1.83                     | 0.44              |
| 1:C:2369:ASP:N    | 1:C:2369:ASP:OD1  | 2.50                     | 0.44              |
| 1:D:1529:HIS:HA   | 1:D:1534:MET:HE2  | 1.99                     | 0.44              |
| 1:E:1336:ILE:HD11 | 1:E:1503:ILE:HG21 | 2.00                     | 0.44              |
| 1:E:1799:PHE:HE2  | 1:E:1874:LYS:HB3  | 1.83                     | 0.44              |
| 1:A:451:LEU:HD22  | 1:A:462:ILE:HD12  | 2.00                     | 0.44              |
| 1:B:1002:THR:O    | 1:B:1002:THR:OG1  | 2.31                     | 0.44              |
| 1:C:72:ASN:ND2    | 1:C:74:GLN:OE1    | 2.43                     | 0.44              |
| 1:C:263:MET:HA    | 1:C:443:LEU:HD21  | 1.99                     | 0.44              |
| 1:A:1906:LEU:HD23 | 1:A:1906:LEU:HA   | 1.86                     | 0.44              |
| 1:C:1058:ASN:OD1  | 1:C:1058:ASN:N    | 2.49                     | 0.44              |
| 1:C:1293:LEU:HD23 | 1:C:1293:LEU:HA   | 1.88                     | 0.44              |
| 1:C:2397:GLN:HA   | 1:C:2495:SER:HA   | 1.99                     | 0.44              |
| 1:D:1799:PHE:HE2  | 1:D:1874:LYS:HB3  | 1.83                     | 0.44              |
| 1:E:1293:LEU:HD23 | 1:E:1293:LEU:HA   | 1.87                     | 0.44              |
| 1:A:263:MET:HA    | 1:A:443:LEU:HD21  | 1.99                     | 0.44              |
| 1:A:1002:THR:O    | 1:A:1002:THR:OG1  | 2.31                     | 0.44              |
| 1:A:1531:SER:OG   | 1:B:1766:HIS:NE2  | 2.40                     | 0.44              |
| 1:B:78:ILE:HD13   | 1:B:81:LEU:HD22   | 2.00                     | 0.44              |
| 1:B:200:HIS:HB3   | 1:B:203:TYR:HB3   | 2.00                     | 0.44              |
| 1:C:950:LYS:N     | 1:C:954:GLU:OE1   | 2.42                     | 0.44              |
| 1:D:200:HIS:HB3   | 1:D:203:TYR:HB3   | 1.99                     | 0.44              |
| 1:A:422:SER:OG    | 1:A:423:ASP:N     | 2.46                     | 0.43              |
| 1:A:1657:GLU:OE2  | 1:A:1719:TYR:OH   | 2.35                     | 0.43              |
| 1:B:2134:TYR:HB3  | 1:B:2194:LYS:HB2  | 1.99                     | 0.43              |
| 1:B:2194:LYS:HD2  | 1:D:1054:GLN:HE21 | 1.83                     | 0.43              |
| 1:C:2034:ARG:NH1  | 1:C:2477:LYS:O    | 2.50                     | 0.43              |
| 1:A:113:PHE:O     | 1:A:1016:TYR:OH   | 2.34                     | 0.43              |
| 1:A:597:ARG:NE    | 1:A:601:ASP:OD2   | 2.51                     | 0.43              |
| 1:B:263:MET:HA    | 1:B:443:LEU:HD21  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:141:ARG:NH1   | 1:C:958:TYR:O     | 2.51                     | 0.43              |
| 1:C:2478:TYR:O    | 1:D:2343:ARG:NH2  | 2.50                     | 0.43              |
| 1:D:597:ARG:NE    | 1:D:601:ASP:OD2   | 2.51                     | 0.43              |
| 1:D:1240:PHE:O    | 1:D:1270:LYS:NZ   | 2.43                     | 0.43              |
| 1:E:729:THR:OG1   | 1:E:731:ASP:O     | 2.35                     | 0.43              |
| 1:A:401:LEU:HD23  | 1:A:401:LEU:HA    | 1.84                     | 0.43              |
| 1:B:498:SER:HA    | 1:B:501:LEU:HD12  | 1.99                     | 0.43              |
| 1:C:413:ARG:HG3   | 1:C:428:ASN:HB3   | 1.99                     | 0.43              |
| 1:C:1709:ARG:NE   | 1:C:1720:ASP:OD2  | 2.40                     | 0.43              |
| 1:C:2348:THR:HA   | 1:C:2518:ARG:HA   | 2.01                     | 0.43              |
| 1:D:1709:ARG:NE   | 1:D:1720:ASP:OD2  | 2.40                     | 0.43              |
| 1:D:2059:ILE:HD13 | 1:D:2059:ILE:HA   | 1.84                     | 0.43              |
| 1:D:2345:LEU:HD23 | 1:D:2345:LEU:HA   | 1.84                     | 0.43              |
| 1:E:141:ARG:NH1   | 1:E:958:TYR:O     | 2.51                     | 0.43              |
| 1:E:498:SER:HA    | 1:E:501:LEU:HD12  | 1.99                     | 0.43              |
| 1:A:2013:SER:OG   | 1:E:2251:GLN:NE2  | 2.43                     | 0.43              |
| 1:B:1336:ILE:HD11 | 1:B:1503:ILE:HG21 | 2.00                     | 0.43              |
| 1:B:1893:ASP:OD1  | 1:B:1893:ASP:N    | 2.50                     | 0.43              |
| 1:D:1336:ILE:HD11 | 1:D:1503:ILE:HG21 | 2.00                     | 0.43              |
| 1:D:2251:GLN:NE2  | 1:E:2013:SER:OG   | 2.40                     | 0.43              |
| 1:E:451:LEU:HD22  | 1:E:462:ILE:HD12  | 2.00                     | 0.43              |
| 1:A:1010:GLU:OE2  | 1:B:1812:THR:OG1  | 2.32                     | 0.43              |
| 1:A:2134:TYR:HB3  | 1:A:2194:LYS:HB2  | 1.99                     | 0.43              |
| 1:B:1799:PHE:HE2  | 1:B:1874:LYS:HB3  | 1.83                     | 0.43              |
| 1:C:200:HIS:HB3   | 1:C:203:TYR:HB3   | 2.00                     | 0.43              |
| 1:C:597:ARG:NE    | 1:C:601:ASP:OD2   | 2.51                     | 0.43              |
| 1:C:1336:ILE:HD11 | 1:C:1503:ILE:HG21 | 2.00                     | 0.43              |
| 1:C:1531:SER:OG   | 1:D:1766:HIS:NE2  | 2.48                     | 0.43              |
| 1:C:2134:TYR:HB3  | 1:C:2194:LYS:HB2  | 1.99                     | 0.43              |
| 1:E:99:ARG:NH1    | 1:E:1964:PHE:O    | 2.48                     | 0.43              |
| 1:E:285:TYR:OH    | 1:E:446:ASN:OD1   | 2.37                     | 0.43              |
| 1:A:1058:ASN:N    | 1:A:1058:ASN:OD1  | 2.49                     | 0.43              |
| 1:A:1336:ILE:HD11 | 1:A:1503:ILE:HG21 | 2.00                     | 0.43              |
| 1:A:1863:ASP:HA   | 1:A:1864:PRO:HD3  | 1.83                     | 0.43              |
| 1:B:141:ARG:NH1   | 1:B:958:TYR:O     | 2.51                     | 0.43              |
| 1:B:597:ARG:NE    | 1:B:601:ASP:OD2   | 2.51                     | 0.43              |
| 1:B:2348:THR:HA   | 1:B:2518:ARG:HA   | 2.01                     | 0.43              |
| 1:C:138:LEU:HD23  | 1:C:138:LEU:HA    | 1.90                     | 0.43              |
| 1:D:78:ILE:HD13   | 1:D:81:LEU:HD22   | 2.00                     | 0.43              |
| 1:D:113:PHE:O     | 1:D:1016:TYR:OH   | 2.34                     | 0.43              |
| 1:D:141:ARG:NH1   | 1:D:958:TYR:O     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:203:TYR:OH    | 1:E:237:ALA:O    | 2.30                     | 0.43              |
| 1:E:1002:THR:O    | 1:E:1002:THR:OG1 | 2.31                     | 0.43              |
| 1:E:1923:GLU:H    | 1:E:1923:GLU:HG3 | 1.65                     | 0.43              |
| 1:E:2059:ILE:HD13 | 1:E:2059:ILE:HA  | 1.84                     | 0.43              |
| 1:E:2348:THR:HA   | 1:E:2518:ARG:HA  | 2.01                     | 0.43              |
| 1:B:1056:GLN:HB3  | 1:E:2128:LYS:HE3 | 2.00                     | 0.43              |
| 1:B:2128:LYS:HE3  | 1:D:1056:GLN:HB3 | 2.01                     | 0.43              |
| 1:B:2345:LEU:HD23 | 1:B:2345:LEU:HA  | 1.84                     | 0.43              |
| 1:B:2369:ASP:OD1  | 1:B:2369:ASP:N   | 2.50                     | 0.43              |
| 1:C:433:MET:HE3   | 1:C:433:MET:HB2  | 1.90                     | 0.43              |
| 1:C:1799:PHE:HE2  | 1:C:1874:LYS:HB3 | 1.83                     | 0.43              |
| 1:D:1151:TYR:OH   | 1:D:1225:ASP:O   | 2.26                     | 0.43              |
| 1:D:1657:GLU:OE2  | 1:D:1719:TYR:OH  | 2.35                     | 0.43              |
| 1:E:597:ARG:NE    | 1:E:601:ASP:OD2  | 2.51                     | 0.43              |
| 1:A:72:ASN:ND2    | 1:A:74:GLN:OE1   | 2.43                     | 0.43              |
| 1:A:1991:THR:OG1  | 1:A:1995:GLN:O   | 2.34                     | 0.43              |
| 1:B:1801:ARG:HD2  | 1:B:1801:ARG:HA  | 1.73                     | 0.43              |
| 1:C:272:VAL:HG12  | 1:C:442:LEU:HD12 | 2.01                     | 0.43              |
| 1:C:1326:ILE:HD12 | 1:C:1326:ILE:HA  | 1.88                     | 0.43              |
| 1:D:723:ILE:HD13  | 1:D:723:ILE:HA   | 1.87                     | 0.43              |
| 1:D:2134:TYR:HB3  | 1:D:2194:LYS:HB2 | 1.99                     | 0.43              |
| 1:E:1654:ASN:H    | 1:E:1658:HIS:CD2 | 2.37                     | 0.43              |
| 1:A:335:LYS:HB3   | 1:A:336:ASP:H    | 1.74                     | 0.43              |
| 1:A:1056:GLN:HB3  | 1:D:2128:LYS:HE3 | 2.00                     | 0.43              |
| 1:A:2034:ARG:NH2  | 1:A:2482:GLU:OE2 | 2.52                     | 0.43              |
| 1:A:2258:GLN:HB3  | 1:B:2015:ALA:HB2 | 2.00                     | 0.43              |
| 1:B:982:GLN:NE2   | 1:B:1014:ARG:O   | 2.52                     | 0.43              |
| 1:B:1204:ILE:O    | 1:B:1208:ILE:HB  | 2.19                     | 0.43              |
| 1:C:99:ARG:NH1    | 1:C:1964:PHE:O   | 2.47                     | 0.43              |
| 1:E:2101:LEU:HD12 | 1:E:2101:LEU:HA  | 1.92                     | 0.43              |
| 1:A:1884:ASP:OD1  | 1:A:1902:TYR:OH  | 2.37                     | 0.43              |
| 1:B:691:ASP:OD1   | 1:B:691:ASP:N    | 2.52                     | 0.43              |
| 1:B:2101:LEU:HD21 | 1:B:2225:GLN:HB3 | 2.01                     | 0.43              |
| 1:C:401:LEU:HD23  | 1:C:401:LEU:HA   | 1.84                     | 0.43              |
| 1:C:1044:MET:HE2  | 1:C:1044:MET:HB3 | 1.90                     | 0.43              |
| 1:C:2101:LEU:HD21 | 1:C:2225:GLN:HB3 | 2.01                     | 0.43              |
| 1:C:2270:LEU:HD12 | 1:C:2270:LEU:HA  | 1.90                     | 0.43              |
| 1:D:203:TYR:OH    | 1:D:237:ALA:O    | 2.30                     | 0.43              |
| 1:D:982:GLN:NE2   | 1:D:1014:ARG:O   | 2.52                     | 0.43              |
| 1:E:200:HIS:HB3   | 1:E:203:TYR:HB3  | 2.00                     | 0.43              |
| 1:E:1204:ILE:O    | 1:E:1208:ILE:HB  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1232:HIS:ND1  | 1:E:1233:GLU:O    | 2.41                     | 0.43              |
| 1:A:141:ARG:NH1   | 1:A:958:TYR:O     | 2.51                     | 0.42              |
| 1:B:451:LEU:HD22  | 1:B:462:ILE:HD12  | 2.00                     | 0.42              |
| 1:B:1054:GLN:HE21 | 1:E:2194:LYS:HD2  | 1.84                     | 0.42              |
| 1:C:982:GLN:NE2   | 1:C:1014:ARG:O    | 2.52                     | 0.42              |
| 1:C:1204:ILE:O    | 1:C:1208:ILE:HB   | 2.19                     | 0.42              |
| 1:E:606:THR:OG1   | 1:E:609:GLU:OE2   | 2.31                     | 0.42              |
| 1:E:2034:ARG:NH2  | 1:E:2482:GLU:OE2  | 2.52                     | 0.42              |
| 1:B:266:ASN:HD22  | 1:B:443:LEU:HD22  | 1.84                     | 0.42              |
| 1:B:656:VAL:O     | 1:B:660:THR:OG1   | 2.33                     | 0.42              |
| 1:C:266:ASN:HD22  | 1:C:443:LEU:HD22  | 1.84                     | 0.42              |
| 1:D:451:LEU:HD22  | 1:D:462:ILE:HD12  | 2.00                     | 0.42              |
| 1:E:250:LEU:HD22  | 1:E:451:LEU:HD12  | 2.02                     | 0.42              |
| 1:A:761:SER:OG    | 1:A:765:ARG:NH2   | 2.52                     | 0.42              |
| 1:A:1654:ASN:H    | 1:A:1658:HIS:CD2  | 2.37                     | 0.42              |
| 1:A:1934:MET:HE3  | 1:A:1960:LEU:HA   | 2.02                     | 0.42              |
| 1:A:2101:LEU:HD21 | 1:A:2225:GLN:HB3  | 2.01                     | 0.42              |
| 1:A:2178:ALA:HB2  | 1:B:2147:LEU:HB3  | 2.02                     | 0.42              |
| 1:B:761:SER:OG    | 1:B:765:ARG:NH2   | 2.52                     | 0.42              |
| 1:B:1272:THR:O    | 1:B:1272:THR:OG1  | 2.30                     | 0.42              |
| 1:B:2034:ARG:NH2  | 1:B:2482:GLU:OE2  | 2.52                     | 0.42              |
| 1:B:2059:ILE:HD13 | 1:B:2059:ILE:HA   | 1.84                     | 0.42              |
| 1:C:2034:ARG:NH2  | 1:C:2482:GLU:OE2  | 2.52                     | 0.42              |
| 1:D:1507:LEU:HD11 | 1:D:1552:LEU:HD13 | 2.01                     | 0.42              |
| 1:D:2034:ARG:NH2  | 1:D:2482:GLU:OE2  | 2.52                     | 0.42              |
| 1:E:263:MET:HE1   | 1:E:272:VAL:HA    | 2.01                     | 0.42              |
| 1:A:34:ARG:HA     | 1:A:34:ARG:HD2    | 1.85                     | 0.42              |
| 1:A:982:GLN:NE2   | 1:A:1014:ARG:O    | 2.52                     | 0.42              |
| 1:A:2348:THR:HA   | 1:A:2518:ARG:HA   | 2.01                     | 0.42              |
| 1:B:344:TYR:HD2   | 1:B:346:GLU:HG3   | 1.85                     | 0.42              |
| 1:B:1884:ASP:OD1  | 1:B:1902:TYR:OH   | 2.37                     | 0.42              |
| 1:D:1654:ASN:H    | 1:D:1658:HIS:CD2  | 2.37                     | 0.42              |
| 1:E:373:LEU:O     | 1:E:381:ILE:N     | 2.47                     | 0.42              |
| 1:E:982:GLN:NE2   | 1:E:1014:ARG:O    | 2.52                     | 0.42              |
| 1:E:1635:LEU:HD23 | 1:E:1635:LEU:HA   | 1.93                     | 0.42              |
| 1:A:169:LEU:HD23  | 1:A:169:LEU:HA    | 1.91                     | 0.42              |
| 1:A:263:MET:HE1   | 1:A:272:VAL:HA    | 2.01                     | 0.42              |
| 1:A:2306:HIS:NE2  | 1:A:2308:ILE:O    | 2.53                     | 0.42              |
| 1:B:272:VAL:HG12  | 1:B:442:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:356:LYS:HE2   | 1:B:396:SER:HB2   | 2.01                     | 0.42              |
| 1:B:2188:THR:HG23 | 1:C:2137:SER:HB2  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:335:LYS:HB3   | 1:C:336:ASP:H     | 1.74                     | 0.42              |
| 1:C:1096:THR:HG1  | 1:C:1116:HIS:HE2  | 1.61                     | 0.42              |
| 1:D:2178:ALA:HB2  | 1:E:2147:LEU:HB3  | 2.02                     | 0.42              |
| 1:E:272:VAL:HG12  | 1:E:442:LEU:HD12  | 2.01                     | 0.42              |
| 1:E:2306:HIS:NE2  | 1:E:2308:ILE:O    | 2.53                     | 0.42              |
| 1:A:1309:PHE:HD1  | 1:A:1336:ILE:HG12 | 1.85                     | 0.42              |
| 1:C:1273:LEU:HD23 | 1:C:1273:LEU:HA   | 1.90                     | 0.42              |
| 1:C:1884:ASP:OD1  | 1:C:1902:TYR:OH   | 2.37                     | 0.42              |
| 1:C:1970:LYS:HB3  | 1:C:1970:LYS:HE3  | 1.86                     | 0.42              |
| 1:D:250:LEU:HD22  | 1:D:451:LEU:HD12  | 2.02                     | 0.42              |
| 1:D:266:ASN:HD22  | 1:D:443:LEU:HD22  | 1.84                     | 0.42              |
| 1:D:487:GLN:HE21  | 1:D:487:GLN:HB3   | 1.55                     | 0.42              |
| 1:D:729:THR:OG1   | 1:D:731:ASP:O     | 2.35                     | 0.42              |
| 1:D:761:SER:OG    | 1:D:765:ARG:NH2   | 2.52                     | 0.42              |
| 1:D:1206:ASN:O    | 1:D:1210:LYS:NZ   | 2.37                     | 0.42              |
| 1:D:1934:MET:HE3  | 1:D:1960:LEU:HA   | 2.02                     | 0.42              |
| 1:E:401:LEU:HD23  | 1:E:401:LEU:HA    | 1.84                     | 0.42              |
| 1:B:666:THR:O     | 1:B:666:THR:OG1   | 2.36                     | 0.42              |
| 1:B:2270:LEU:HD12 | 1:B:2270:LEU:HA   | 1.91                     | 0.42              |
| 1:C:2469:PHE:CZ   | 1:D:2518:ARG:HB3  | 2.55                     | 0.42              |
| 1:D:263:MET:HE1   | 1:D:272:VAL:HA    | 2.01                     | 0.42              |
| 1:D:1193:SER:OG   | 1:D:1194:SER:N    | 2.53                     | 0.42              |
| 1:D:2306:HIS:NE2  | 1:D:2308:ILE:O    | 2.53                     | 0.42              |
| 1:D:2348:THR:HA   | 1:D:2518:ARG:HA   | 2.01                     | 0.42              |
| 1:E:1625:ASP:OD1  | 1:E:1817:TYR:OH   | 2.33                     | 0.42              |
| 1:A:162:LEU:HD11  | 1:A:933:THR:HG21  | 2.02                     | 0.42              |
| 1:B:1507:LEU:HD11 | 1:B:1552:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:1654:ASN:H    | 1:B:1658:HIS:CD2  | 2.37                     | 0.42              |
| 1:D:490:MET:HE2   | 1:D:490:MET:HB3   | 1.90                     | 0.42              |
| 1:D:544:THR:HA    | 1:D:545:PRO:HD3   | 1.91                     | 0.42              |
| 1:D:1204:ILE:O    | 1:D:1208:ILE:HB   | 2.19                     | 0.42              |
| 1:E:356:LYS:HE2   | 1:E:396:SER:HB2   | 2.01                     | 0.42              |
| 1:E:1309:PHE:HD1  | 1:E:1336:ILE:HG12 | 1.85                     | 0.42              |
| 1:A:691:ASP:OD1   | 1:A:691:ASP:N     | 2.52                     | 0.42              |
| 1:A:1983:LEU:HD23 | 1:A:1983:LEU:HA   | 1.87                     | 0.42              |
| 1:B:548:SER:OG    | 1:B:549:LYS:N     | 2.53                     | 0.42              |
| 1:B:1934:MET:HE3  | 1:B:1960:LEU:HA   | 2.02                     | 0.42              |
| 1:B:2409:THR:O    | 1:B:2409:THR:OG1  | 2.33                     | 0.42              |
| 1:C:344:TYR:HD2   | 1:C:346:GLU:HG3   | 1.85                     | 0.42              |
| 1:C:451:LEU:HD22  | 1:C:462:ILE:HD12  | 2.00                     | 0.42              |
| 1:C:1934:MET:HE3  | 1:C:1960:LEU:HA   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1983:LEU:HD23 | 1:C:1983:LEU:HA   | 1.87                     | 0.42              |
| 1:D:2452:ARG:NH1  | 1:E:2339:GLU:O    | 2.49                     | 0.42              |
| 1:E:240:THR:OG1   | 1:E:454:ALA:O     | 2.38                     | 0.42              |
| 1:A:356:LYS:HE2   | 1:A:396:SER:HB2   | 2.01                     | 0.42              |
| 1:A:723:ILE:HD13  | 1:A:723:ILE:HA    | 1.87                     | 0.42              |
| 1:A:1204:ILE:O    | 1:A:1208:ILE:HB   | 2.19                     | 0.42              |
| 1:B:393:THR:OG1   | 1:C:1925:ARG:NH2  | 2.52                     | 0.42              |
| 1:C:1309:PHE:HD1  | 1:C:1336:ILE:HG12 | 1.85                     | 0.42              |
| 1:C:1657:GLU:OE2  | 1:C:1719:TYR:OH   | 2.35                     | 0.42              |
| 1:D:785:GLN:HG2   | 1:D:861:ARG:HB2   | 2.02                     | 0.42              |
| 1:D:1015:ARG:HH22 | 1:E:1882:ARG:HH21 | 1.67                     | 0.42              |
| 1:E:162:LEU:HD11  | 1:E:933:THR:HG21  | 2.02                     | 0.42              |
| 1:A:240:THR:OG1   | 1:A:454:ALA:O     | 2.38                     | 0.41              |
| 1:A:344:TYR:HD2   | 1:A:346:GLU:HG3   | 1.85                     | 0.41              |
| 1:B:490:MET:HE2   | 1:B:490:MET:HB3   | 1.90                     | 0.41              |
| 1:C:548:SER:OG    | 1:C:549:LYS:N     | 2.53                     | 0.41              |
| 1:C:691:ASP:OD1   | 1:C:691:ASP:N     | 2.52                     | 0.41              |
| 1:C:1654:ASN:H    | 1:C:1658:HIS:CD2  | 2.37                     | 0.41              |
| 1:C:1863:ASP:HA   | 1:C:1864:PRO:HD3  | 1.83                     | 0.41              |
| 1:E:266:ASN:HD22  | 1:E:443:LEU:HD22  | 1.84                     | 0.41              |
| 1:E:1507:LEU:HD11 | 1:E:1552:LEU:HD13 | 2.01                     | 0.41              |
| 1:A:138:LEU:HD23  | 1:A:138:LEU:HA    | 1.90                     | 0.41              |
| 1:A:266:ASN:HD22  | 1:A:443:LEU:HD22  | 1.84                     | 0.41              |
| 1:B:285:TYR:OH    | 1:B:446:ASN:OD1   | 2.37                     | 0.41              |
| 1:B:433:MET:HE3   | 1:B:433:MET:HB2   | 1.90                     | 0.41              |
| 1:B:1044:MET:HE2  | 1:B:1044:MET:HB3  | 1.90                     | 0.41              |
| 1:B:2440:ALA:HB3  | 1:B:2459:ILE:HB   | 2.03                     | 0.41              |
| 1:C:109:ILE:HD13  | 1:C:155:MET:HB2   | 2.02                     | 0.41              |
| 1:C:785:GLN:HG2   | 1:C:861:ARG:HB2   | 2.02                     | 0.41              |
| 1:C:1507:LEU:HD11 | 1:C:1552:LEU:HD13 | 2.01                     | 0.41              |
| 1:D:1060:ASP:OD1  | 1:D:1060:ASP:N    | 2.53                     | 0.41              |
| 1:D:1232:HIS:ND1  | 1:D:1233:GLU:O    | 2.41                     | 0.41              |
| 1:D:1523:VAL:HG22 | 1:D:1538:PHE:HA   | 2.02                     | 0.41              |
| 1:D:1884:ASP:OD1  | 1:D:1902:TYR:OH   | 2.37                     | 0.41              |
| 1:D:2457:ILE:HG23 | 1:D:2481:PHE:HE2  | 1.85                     | 0.41              |
| 1:E:344:TYR:HD2   | 1:E:346:GLU:HG3   | 1.85                     | 0.41              |
| 1:E:652:SER:N     | 1:E:655:ASP:OD2   | 2.50                     | 0.41              |
| 1:A:203:TYR:OH    | 1:A:237:ALA:O     | 2.30                     | 0.41              |
| 1:A:2452:ARG:NH1  | 1:B:2339:GLU:O    | 2.47                     | 0.41              |
| 1:B:250:LEU:HD22  | 1:B:451:LEU:HD12  | 2.02                     | 0.41              |
| 1:B:1309:PHE:HD1  | 1:B:1336:ILE:HG12 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2306:HIS:NE2  | 1:B:2308:ILE:O    | 2.53                     | 0.41              |
| 1:B:2459:ILE:HD13 | 1:B:2459:ILE:HA   | 1.90                     | 0.41              |
| 1:C:130:HIS:HD1   | 1:C:984:TYR:HH    | 1.64                     | 0.41              |
| 1:C:356:LYS:HE2   | 1:C:396:SER:HB2   | 2.01                     | 0.41              |
| 1:C:656:VAL:O     | 1:C:660:THR:OG1   | 2.33                     | 0.41              |
| 1:C:2345:LEU:HD23 | 1:C:2345:LEU:HA   | 1.84                     | 0.41              |
| 1:D:272:VAL:HG12  | 1:D:442:LEU:HD12  | 2.01                     | 0.41              |
| 1:D:599:LEU:HD23  | 1:D:599:LEU:HA    | 1.91                     | 0.41              |
| 1:D:652:SER:N     | 1:D:655:ASP:OD2   | 2.50                     | 0.41              |
| 1:D:1239:SER:OG   | 1:D:1242:SER:OG   | 2.33                     | 0.41              |
| 1:D:2101:LEU:HD21 | 1:D:2225:GLN:HB3  | 2.01                     | 0.41              |
| 1:E:691:ASP:OD1   | 1:E:691:ASP:N     | 2.52                     | 0.41              |
| 1:E:1884:ASP:OD1  | 1:E:1902:TYR:OH   | 2.37                     | 0.41              |
| 1:E:2101:LEU:HD21 | 1:E:2225:GLN:HB3  | 2.01                     | 0.41              |
| 1:E:2330:LEU:HD23 | 1:E:2330:LEU:HA   | 1.92                     | 0.41              |
| 1:E:2457:ILE:HG23 | 1:E:2481:PHE:HE2  | 1.85                     | 0.41              |
| 1:A:1193:SER:OG   | 1:A:1194:SER:N    | 2.53                     | 0.41              |
| 1:A:2452:ARG:HB3  | 1:A:2453:GLY:H    | 1.69                     | 0.41              |
| 1:B:102:ARG:HH22  | 1:B:1965:LEU:HD11 | 1.86                     | 0.41              |
| 1:B:109:ILE:HD13  | 1:B:155:MET:HB2   | 2.02                     | 0.41              |
| 1:B:162:LEU:HD11  | 1:B:933:THR:HG21  | 2.02                     | 0.41              |
| 1:B:240:THR:OG1   | 1:B:454:ALA:O     | 2.38                     | 0.41              |
| 1:B:2419:ARG:HG2  | 1:B:2521:ILE:HG23 | 2.03                     | 0.41              |
| 1:C:761:SER:OG    | 1:C:765:ARG:NH2   | 2.52                     | 0.41              |
| 1:C:1060:ASP:OD1  | 1:C:1060:ASP:N    | 2.53                     | 0.41              |
| 1:C:2121:GLU:H    | 1:C:2121:GLU:HG3  | 1.74                     | 0.41              |
| 1:C:2306:HIS:NE2  | 1:C:2308:ILE:O    | 2.53                     | 0.41              |
| 1:C:2440:ALA:HB3  | 1:C:2459:ILE:HB   | 2.03                     | 0.41              |
| 1:D:356:LYS:HE2   | 1:D:396:SER:HB2   | 2.01                     | 0.41              |
| 1:D:707:MET:O     | 1:E:2268:ASN:ND2  | 2.53                     | 0.41              |
| 1:D:1700:LYS:HE3  | 1:D:1700:LYS:HB3  | 1.90                     | 0.41              |
| 1:D:1991:THR:OG1  | 1:D:1995:GLN:O    | 2.34                     | 0.41              |
| 1:E:1523:VAL:HG22 | 1:E:1538:PHE:HA   | 2.02                     | 0.41              |
| 1:A:592:LEU:HA    | 1:A:595:ARG:HB2   | 2.03                     | 0.41              |
| 1:A:2457:ILE:HG23 | 1:A:2481:PHE:HE2  | 1.85                     | 0.41              |
| 1:B:263:MET:HE1   | 1:B:272:VAL:HA    | 2.01                     | 0.41              |
| 1:B:703:ALA:HB1   | 1:C:2269:TRP:HA   | 2.02                     | 0.41              |
| 1:B:785:GLN:HG2   | 1:B:861:ARG:HB2   | 2.03                     | 0.41              |
| 1:B:2121:GLU:H    | 1:B:2121:GLU:HG3  | 1.74                     | 0.41              |
| 1:B:2238:LEU:HG   | 1:C:2086:MET:HE2  | 2.02                     | 0.41              |
| 1:C:250:LEU:HD22  | 1:C:451:LEU:HD12  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2419:ARG:HG2  | 1:C:2521:ILE:HG23 | 2.03                     | 0.41              |
| 1:D:548:SER:OG    | 1:D:549:LYS:N     | 2.53                     | 0.41              |
| 1:E:548:SER:OG    | 1:E:549:LYS:N     | 2.53                     | 0.41              |
| 1:E:2098:LYS:HE2  | 1:E:2102:GLN:HE21 | 1.86                     | 0.41              |
| 1:A:272:VAL:HG12  | 1:A:442:LEU:HD12  | 2.01                     | 0.41              |
| 1:A:508:ILE:HB    | 1:A:587:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:972:THR:OG1   | 1:A:973:ARG:N     | 2.54                     | 0.41              |
| 1:A:1507:LEU:HD11 | 1:A:1552:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:401:LEU:HD23  | 1:B:401:LEU:HA    | 1.84                     | 0.41              |
| 1:B:2457:ILE:HG23 | 1:B:2481:PHE:HE2  | 1.85                     | 0.41              |
| 1:C:544:THR:HA    | 1:C:545:PRO:HD3   | 1.91                     | 0.41              |
| 1:C:1070:LEU:HD23 | 1:C:1070:LEU:HA   | 1.92                     | 0.41              |
| 1:C:2098:LYS:HE2  | 1:C:2102:GLN:HE21 | 1.86                     | 0.41              |
| 1:D:691:ASP:OD1   | 1:D:691:ASP:N     | 2.52                     | 0.41              |
| 1:D:1165:LEU:HD23 | 1:D:1165:LEU:HA   | 1.92                     | 0.41              |
| 1:D:2098:LYS:HE2  | 1:D:2102:GLN:HE21 | 1.86                     | 0.41              |
| 1:D:2419:ARG:HG2  | 1:D:2521:ILE:HG23 | 2.03                     | 0.41              |
| 1:E:131:PRO:HG2   | 1:E:134:SER:HB2   | 2.03                     | 0.41              |
| 1:E:972:THR:OG1   | 1:E:973:ARG:N     | 2.54                     | 0.41              |
| 1:E:1272:THR:O    | 1:E:1272:THR:OG1  | 2.30                     | 0.41              |
| 1:A:2419:ARG:HG2  | 1:A:2521:ILE:HG23 | 2.03                     | 0.41              |
| 1:B:131:PRO:HG2   | 1:B:134:SER:HB2   | 2.03                     | 0.41              |
| 1:B:231:ASP:HB2   | 1:B:890:LYS:HE2   | 2.03                     | 0.41              |
| 1:B:819:LEU:HD12  | 1:C:2016:ILE:HG21 | 2.03                     | 0.41              |
| 1:B:1037:ILE:HA   | 1:B:1041:GLN:HE22 | 1.86                     | 0.41              |
| 1:B:1906:LEU:HD23 | 1:B:1906:LEU:HA   | 1.86                     | 0.41              |
| 1:B:2238:LEU:HD23 | 1:C:2086:MET:HA   | 2.02                     | 0.41              |
| 1:C:1523:VAL:HG22 | 1:C:1538:PHE:HA   | 2.02                     | 0.41              |
| 1:D:162:LEU:HD11  | 1:D:933:THR:HG21  | 2.02                     | 0.41              |
| 1:D:2258:GLN:HB3  | 1:E:2015:ALA:HB2  | 2.02                     | 0.41              |
| 1:E:472:ASP:OD1   | 1:E:472:ASP:N     | 2.54                     | 0.41              |
| 1:E:761:SER:OG    | 1:E:765:ARG:NH2   | 2.52                     | 0.41              |
| 1:A:231:ASP:HB2   | 1:A:890:LYS:HE2   | 2.03                     | 0.41              |
| 1:A:350:ILE:HB    | 1:A:354:GLU:HG2   | 2.03                     | 0.41              |
| 1:A:381:ILE:HG21  | 1:A:399:ILE:HG23  | 2.03                     | 0.41              |
| 1:A:472:ASP:OD1   | 1:A:472:ASP:N     | 2.54                     | 0.41              |
| 1:A:548:SER:OG    | 1:A:549:LYS:N     | 2.53                     | 0.41              |
| 1:A:785:GLN:HG2   | 1:A:861:ARG:HB2   | 2.02                     | 0.41              |
| 1:A:2015:ALA:HB2  | 1:E:2258:GLN:HB3  | 2.02                     | 0.41              |
| 1:A:2098:LYS:HE2  | 1:A:2102:GLN:HE21 | 1.86                     | 0.41              |
| 1:A:2440:ALA:HB3  | 1:A:2459:ILE:HB   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:972:THR:OG1   | 1:B:973:ARG:N     | 2.54                     | 0.41              |
| 1:C:231:ASP:HB2   | 1:C:890:LYS:HE2   | 2.03                     | 0.41              |
| 1:C:263:MET:HE1   | 1:C:272:VAL:HA    | 2.01                     | 0.41              |
| 1:D:344:TYR:HD2   | 1:D:346:GLU:HG3   | 1.85                     | 0.41              |
| 1:E:335:LYS:HB3   | 1:E:336:ASP:H     | 1.74                     | 0.41              |
| 1:E:785:GLN:HG2   | 1:E:861:ARG:HB2   | 2.03                     | 0.41              |
| 1:E:2419:ARG:HG2  | 1:E:2521:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:656:VAL:O     | 1:A:660:THR:OG1   | 2.33                     | 0.41              |
| 1:A:2268:ASN:ND2  | 1:E:707:MET:O     | 2.54                     | 0.41              |
| 1:A:2339:GLU:O    | 1:E:2452:ARG:NH1  | 2.51                     | 0.41              |
| 1:B:472:ASP:N     | 1:B:472:ASP:OD1   | 2.54                     | 0.41              |
| 1:B:599:LEU:HD23  | 1:B:599:LEU:HA    | 1.90                     | 0.41              |
| 1:B:1507:LEU:HB3  | 1:B:1515:VAL:HB   | 2.03                     | 0.41              |
| 1:C:169:LEU:HD23  | 1:C:169:LEU:HA    | 1.91                     | 0.41              |
| 1:C:212:LEU:HD23  | 1:C:212:LEU:HA    | 1.95                     | 0.41              |
| 1:C:783:LYS:HA    | 1:C:783:LYS:HD3   | 1.90                     | 0.41              |
| 1:C:2101:LEU:HD12 | 1:C:2101:LEU:HA   | 1.92                     | 0.41              |
| 1:C:2457:ILE:HG23 | 1:C:2481:PHE:HE2  | 1.85                     | 0.41              |
| 1:C:2459:ILE:HD13 | 1:C:2459:ILE:HA   | 1.90                     | 0.41              |
| 1:D:109:ILE:HD13  | 1:D:155:MET:HB2   | 2.02                     | 0.41              |
| 1:D:373:LEU:HD13  | 1:D:399:ILE:HD11  | 2.03                     | 0.41              |
| 1:D:1037:ILE:HA   | 1:D:1041:GLN:HE22 | 1.86                     | 0.41              |
| 1:D:1202:ASP:OD1  | 1:D:1202:ASP:N    | 2.37                     | 0.41              |
| 1:D:1309:PHE:HD1  | 1:D:1336:ILE:HG12 | 1.85                     | 0.41              |
| 1:D:1963:LEU:HD23 | 1:D:1963:LEU:HA   | 1.94                     | 0.41              |
| 1:E:508:ILE:HB    | 1:E:587:ILE:HD11  | 2.03                     | 0.41              |
| 1:E:1759:LYS:HA   | 1:E:1759:LYS:HD3  | 1.93                     | 0.41              |
| 1:E:1934:MET:HE3  | 1:E:1960:LEU:HA   | 2.02                     | 0.41              |
| 1:A:373:LEU:HD13  | 1:A:399:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:1273:LEU:HD23 | 1:A:1273:LEU:HA   | 1.90                     | 0.41              |
| 1:A:1700:LYS:HE3  | 1:A:1700:LYS:HB3  | 1.90                     | 0.41              |
| 1:A:2086:MET:HB2  | 1:A:2086:MET:HE3  | 1.74                     | 0.41              |
| 1:A:2147:LEU:HB3  | 1:E:2178:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:34:ARG:HA     | 1:B:34:ARG:HD2    | 1.85                     | 0.41              |
| 1:B:373:LEU:HD13  | 1:B:399:ILE:HD11  | 2.03                     | 0.41              |
| 1:B:785:GLN:HA    | 1:B:859:ASN:HD21  | 1.86                     | 0.41              |
| 1:C:102:ARG:HH22  | 1:C:1965:LEU:HD11 | 1.86                     | 0.41              |
| 1:C:131:PRO:HG2   | 1:C:134:SER:HB2   | 2.03                     | 0.41              |
| 1:C:1923:GLU:H    | 1:C:1923:GLU:HG3  | 1.65                     | 0.41              |
| 1:C:2118:LEU:HD23 | 1:C:2118:LEU:HA   | 1.90                     | 0.41              |
| 1:C:2194:LYS:HD2  | 1:E:1054:GLN:NE2  | 2.32                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:335:LYS:HB3   | 1:D:336:ASP:H     | 1.74                     | 0.41              |
| 1:D:381:ILE:HG21  | 1:D:399:ILE:HG23  | 2.03                     | 0.41              |
| 1:D:679:LEU:HD12  | 1:D:679:LEU:HA    | 1.90                     | 0.41              |
| 1:E:350:ILE:HB    | 1:E:354:GLU:HG2   | 2.03                     | 0.41              |
| 1:E:373:LEU:HD13  | 1:E:399:ILE:HD11  | 2.03                     | 0.41              |
| 1:E:592:LEU:HA    | 1:E:595:ARG:HB2   | 2.03                     | 0.41              |
| 1:E:1863:ASP:HA   | 1:E:1864:PRO:HD3  | 1.83                     | 0.41              |
| 1:A:433:MET:HE3   | 1:A:433:MET:HB2   | 1.90                     | 0.40              |
| 1:A:1863:ASP:N    | 1:A:1863:ASP:OD1  | 2.54                     | 0.40              |
| 1:A:2335:LYS:HE2  | 1:A:2335:LYS:HB3  | 1.98                     | 0.40              |
| 1:A:2442:LEU:HB3  | 1:A:2457:ILE:HG12 | 2.03                     | 0.40              |
| 1:B:705:ILE:H     | 1:B:705:ILE:HG12  | 1.69                     | 0.40              |
| 1:B:1523:VAL:HG22 | 1:B:1538:PHE:HA   | 2.02                     | 0.40              |
| 1:C:679:LEU:HD12  | 1:C:679:LEU:HA    | 1.91                     | 0.40              |
| 1:C:1193:SER:OG   | 1:C:1194:SER:N    | 2.53                     | 0.40              |
| 1:D:102:ARG:HH22  | 1:D:1965:LEU:HD11 | 1.86                     | 0.40              |
| 1:D:240:THR:OG1   | 1:D:454:ALA:O     | 2.38                     | 0.40              |
| 1:D:2440:ALA:HB3  | 1:D:2459:ILE:HB   | 2.02                     | 0.40              |
| 1:E:1240:PHE:O    | 1:E:1270:LYS:NZ   | 2.43                     | 0.40              |
| 1:E:1946:ARG:H    | 1:E:1946:ARG:HG2  | 1.75                     | 0.40              |
| 1:A:109:ILE:HD13  | 1:A:155:MET:HB2   | 2.02                     | 0.40              |
| 1:A:250:LEU:HD22  | 1:A:451:LEU:HD12  | 2.02                     | 0.40              |
| 1:A:285:TYR:OH    | 1:A:446:ASN:OD1   | 2.37                     | 0.40              |
| 1:A:1702:TYR:HB3  | 1:A:1703:TYR:HD1  | 1.87                     | 0.40              |
| 1:A:1970:LYS:HE3  | 1:A:1970:LYS:HB3  | 1.86                     | 0.40              |
| 1:B:164:LEU:HD23  | 1:B:164:LEU:HA    | 1.95                     | 0.40              |
| 1:B:592:LEU:HA    | 1:B:595:ARG:HB2   | 2.03                     | 0.40              |
| 1:B:2461:HIS:CE1  | 1:B:2463:MET:HB3  | 2.57                     | 0.40              |
| 1:C:42:THR:OG1    | 1:C:1571:GLU:OE2  | 2.38                     | 0.40              |
| 1:C:240:THR:OG1   | 1:C:454:ALA:O     | 2.38                     | 0.40              |
| 1:C:373:LEU:HD13  | 1:C:399:ILE:HD11  | 2.03                     | 0.40              |
| 1:C:972:THR:OG1   | 1:C:973:ARG:N     | 2.54                     | 0.40              |
| 1:D:1835:TRP:CZ2  | 1:D:1868:LYS:HG3  | 2.56                     | 0.40              |
| 1:D:2263:ASN:OD1  | 1:D:2263:ASN:N    | 2.54                     | 0.40              |
| 1:E:1702:TYR:HB3  | 1:E:1703:TYR:HD1  | 1.86                     | 0.40              |
| 1:A:1865:MET:HE2  | 1:A:1865:MET:HB3  | 1.99                     | 0.40              |
| 1:B:508:ILE:HB    | 1:B:587:ILE:HD11  | 2.03                     | 0.40              |
| 1:B:1060:ASP:OD1  | 1:B:1060:ASP:N    | 2.53                     | 0.40              |
| 1:B:2183:ILE:HD12 | 1:B:2183:ILE:HA   | 1.92                     | 0.40              |
| 1:C:162:LEU:HD11  | 1:C:933:THR:HG21  | 2.02                     | 0.40              |
| 1:C:785:GLN:HA    | 1:C:859:ASN:HD21  | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1139:ILE:HG23 | 1:C:1159:TRP:CE2  | 2.57                     | 0.40              |
| 1:C:2452:ARG:HB3  | 1:C:2453:GLY:H    | 1.69                     | 0.40              |
| 1:D:231:ASP:HB2   | 1:D:890:LYS:HE2   | 2.03                     | 0.40              |
| 1:D:1002:THR:O    | 1:D:1002:THR:OG1  | 2.31                     | 0.40              |
| 1:D:2454:CYS:HB3  | 1:D:2480:PRO:HA   | 2.04                     | 0.40              |
| 1:E:1193:SER:OG   | 1:E:1194:SER:N    | 2.53                     | 0.40              |
| 1:A:2461:HIS:CE1  | 1:A:2463:MET:HB3  | 2.57                     | 0.40              |
| 1:C:61:LYS:HE3    | 1:C:61:LYS:HB3    | 1.93                     | 0.40              |
| 1:C:113:PHE:O     | 1:C:1016:TYR:OH   | 2.34                     | 0.40              |
| 1:D:972:THR:OG1   | 1:D:973:ARG:N     | 2.54                     | 0.40              |
| 1:D:1507:LEU:HB3  | 1:D:1515:VAL:HB   | 2.03                     | 0.40              |
| 1:E:381:ILE:HG21  | 1:E:399:ILE:HG23  | 2.03                     | 0.40              |
| 1:E:2442:LEU:HB3  | 1:E:2457:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:236:LEU:HD13  | 1:A:484:PHE:HA    | 2.04                     | 0.40              |
| 1:A:785:GLN:HA    | 1:A:859:ASN:HD21  | 1.87                     | 0.40              |
| 1:A:1835:TRP:CZ2  | 1:A:1868:LYS:HG3  | 2.56                     | 0.40              |
| 1:A:1946:ARG:H    | 1:A:1946:ARG:HG2  | 1.74                     | 0.40              |
| 1:A:2453:GLY:H    | 1:B:2342:GLU:HB2  | 1.87                     | 0.40              |
| 1:B:1597:GLN:HB3  | 1:B:1609:ASN:HB2  | 2.04                     | 0.40              |
| 1:C:1635:LEU:HA   | 1:C:1636:PRO:HD3  | 1.93                     | 0.40              |
| 1:C:1863:ASP:OD1  | 1:C:1863:ASP:N    | 2.54                     | 0.40              |
| 1:D:1179:TYR:H    | 1:D:1201:THR:HB   | 1.87                     | 0.40              |
| 1:D:2461:HIS:CE1  | 1:D:2463:MET:HB3  | 2.57                     | 0.40              |
| 1:E:236:LEU:HD13  | 1:E:484:PHE:HA    | 2.04                     | 0.40              |
| 1:E:525:ASN:HD22  | 1:E:525:ASN:HA    | 1.72                     | 0.40              |
| 1:E:627:PHE:HD1   | 1:E:627:PHE:HA    | 1.77                     | 0.40              |
| 1:E:1979:LEU:HA   | 1:E:1979:LEU:HD23 | 1.90                     | 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     | 2331/2523 (92%)   | 2158 (93%)  | 170 (7%) | 3 (0%)   | 48          | 78 |
| 1   | B     | 2331/2523 (92%)   | 2158 (93%)  | 170 (7%) | 3 (0%)   | 48          | 78 |
| 1   | C     | 2331/2523 (92%)   | 2160 (93%)  | 168 (7%) | 3 (0%)   | 48          | 78 |
| 1   | D     | 2331/2523 (92%)   | 2159 (93%)  | 169 (7%) | 3 (0%)   | 48          | 78 |
| 1   | E     | 2331/2523 (92%)   | 2160 (93%)  | 168 (7%) | 3 (0%)   | 48          | 78 |
| All | All   | 11655/12615 (92%) | 10795 (93%) | 845 (7%) | 15 (0%)  | 49          | 78 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1949 | ALA  |
| 1   | C     | 1949 | ALA  |
| 1   | D     | 1949 | ALA  |
| 1   | A     | 2453 | GLY  |
| 1   | B     | 1949 | ALA  |
| 1   | B     | 2453 | GLY  |
| 1   | C     | 2453 | GLY  |
| 1   | D     | 2453 | GLY  |
| 1   | E     | 1949 | ALA  |
| 1   | E     | 2453 | GLY  |
| 1   | A     | 581  | PRO  |
| 1   | B     | 581  | PRO  |
| 1   | C     | 581  | PRO  |
| 1   | D     | 581  | PRO  |
| 1   | E     | 581  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 2049/2222 (92%) | 1883 (92%) | 166 (8%) | 11          | 36 |
| 1   | B     | 2049/2222 (92%) | 1883 (92%) | 166 (8%) | 11          | 36 |
| 1   | C     | 2049/2222 (92%) | 1882 (92%) | 167 (8%) | 10          | 36 |
| 1   | D     | 2049/2222 (92%) | 1883 (92%) | 166 (8%) | 11          | 36 |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|----------|-------------|----|
| 1   | E     | 2049/2222 (92%)   | 1883 (92%) | 166 (8%) | 11          | 36 |
| All | All   | 10245/11110 (92%) | 9414 (92%) | 831 (8%) | 13          | 36 |

All (831) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | THR  |
| 1   | A     | 42  | THR  |
| 1   | A     | 65  | LEU  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 104 | VAL  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 144 | ASP  |
| 1   | A     | 176 | LEU  |
| 1   | A     | 179 | THR  |
| 1   | A     | 187 | MET  |
| 1   | A     | 190 | THR  |
| 1   | A     | 226 | VAL  |
| 1   | A     | 251 | VAL  |
| 1   | A     | 260 | THR  |
| 1   | A     | 270 | ASP  |
| 1   | A     | 272 | VAL  |
| 1   | A     | 281 | LEU  |
| 1   | A     | 288 | SER  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 333 | THR  |
| 1   | A     | 342 | LEU  |
| 1   | A     | 369 | LEU  |
| 1   | A     | 373 | LEU  |
| 1   | A     | 379 | GLU  |
| 1   | A     | 394 | HIS  |
| 1   | A     | 411 | THR  |
| 1   | A     | 426 | ASN  |
| 1   | A     | 440 | ILE  |
| 1   | A     | 442 | LEU  |
| 1   | A     | 451 | LEU  |
| 1   | A     | 453 | LYS  |
| 1   | A     | 473 | LEU  |
| 1   | A     | 474 | THR  |
| 1   | A     | 478 | ASN  |
| 1   | A     | 483 | LEU  |
| 1   | A     | 487 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 513  | THR  |
| 1   | A     | 526  | THR  |
| 1   | A     | 529  | LEU  |
| 1   | A     | 537  | ASP  |
| 1   | A     | 539  | THR  |
| 1   | A     | 544  | THR  |
| 1   | A     | 554  | LEU  |
| 1   | A     | 563  | VAL  |
| 1   | A     | 566  | THR  |
| 1   | A     | 592  | LEU  |
| 1   | A     | 606  | THR  |
| 1   | A     | 608  | ASN  |
| 1   | A     | 613  | LEU  |
| 1   | A     | 630  | THR  |
| 1   | A     | 646  | LEU  |
| 1   | A     | 658  | LEU  |
| 1   | A     | 660  | THR  |
| 1   | A     | 691  | ASP  |
| 1   | A     | 694  | ILE  |
| 1   | A     | 701  | ILE  |
| 1   | A     | 705  | ILE  |
| 1   | A     | 706  | GLN  |
| 1   | A     | 732  | ASP  |
| 1   | A     | 763  | ILE  |
| 1   | A     | 767  | ILE  |
| 1   | A     | 771  | GLU  |
| 1   | A     | 775  | THR  |
| 1   | A     | 795  | LEU  |
| 1   | A     | 798  | LEU  |
| 1   | A     | 816  | THR  |
| 1   | A     | 819  | LEU  |
| 1   | A     | 879  | THR  |
| 1   | A     | 892  | VAL  |
| 1   | A     | 901  | THR  |
| 1   | A     | 992  | VAL  |
| 1   | A     | 1011 | THR  |
| 1   | A     | 1030 | GLU  |
| 1   | A     | 1031 | ASN  |
| 1   | A     | 1033 | ILE  |
| 1   | A     | 1047 | ASN  |
| 1   | A     | 1058 | ASN  |
| 1   | A     | 1059 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1060 | ASP  |
| 1   | A     | 1076 | VAL  |
| 1   | A     | 1092 | ASN  |
| 1   | A     | 1095 | LEU  |
| 1   | A     | 1096 | THR  |
| 1   | A     | 1104 | THR  |
| 1   | A     | 1114 | VAL  |
| 1   | A     | 1137 | ILE  |
| 1   | A     | 1141 | VAL  |
| 1   | A     | 1146 | ILE  |
| 1   | A     | 1149 | VAL  |
| 1   | A     | 1157 | LEU  |
| 1   | A     | 1180 | ILE  |
| 1   | A     | 1183 | LEU  |
| 1   | A     | 1202 | ASP  |
| 1   | A     | 1208 | ILE  |
| 1   | A     | 1227 | ILE  |
| 1   | A     | 1250 | THR  |
| 1   | A     | 1256 | THR  |
| 1   | A     | 1262 | GLU  |
| 1   | A     | 1272 | THR  |
| 1   | A     | 1277 | ASP  |
| 1   | A     | 1290 | THR  |
| 1   | A     | 1323 | ASN  |
| 1   | A     | 1334 | MET  |
| 1   | A     | 1500 | ASP  |
| 1   | A     | 1503 | ILE  |
| 1   | A     | 1545 | ILE  |
| 1   | A     | 1554 | SER  |
| 1   | A     | 1596 | THR  |
| 1   | A     | 1656 | GLU  |
| 1   | A     | 1690 | THR  |
| 1   | A     | 1692 | VAL  |
| 1   | A     | 1704 | ILE  |
| 1   | A     | 1712 | VAL  |
| 1   | A     | 1725 | SER  |
| 1   | A     | 1740 | ILE  |
| 1   | A     | 1796 | MET  |
| 1   | A     | 1803 | LEU  |
| 1   | A     | 1811 | SER  |
| 1   | A     | 1813 | ARG  |
| 1   | A     | 1818 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1842 | GLU  |
| 1   | A     | 1854 | VAL  |
| 1   | A     | 1875 | MET  |
| 1   | A     | 1893 | ASP  |
| 1   | A     | 1900 | MET  |
| 1   | A     | 1903 | VAL  |
| 1   | A     | 1911 | ASP  |
| 1   | A     | 1936 | HIS  |
| 1   | A     | 1951 | LEU  |
| 1   | A     | 1953 | THR  |
| 1   | A     | 1956 | THR  |
| 1   | A     | 1965 | LEU  |
| 1   | A     | 1991 | THR  |
| 1   | A     | 1999 | LEU  |
| 1   | A     | 2001 | LEU  |
| 1   | A     | 2017 | THR  |
| 1   | A     | 2025 | LEU  |
| 1   | A     | 2049 | LEU  |
| 1   | A     | 2057 | LEU  |
| 1   | A     | 2081 | LEU  |
| 1   | A     | 2105 | ARG  |
| 1   | A     | 2121 | GLU  |
| 1   | A     | 2131 | MET  |
| 1   | A     | 2135 | LEU  |
| 1   | A     | 2142 | THR  |
| 1   | A     | 2145 | THR  |
| 1   | A     | 2147 | LEU  |
| 1   | A     | 2160 | ILE  |
| 1   | A     | 2229 | LEU  |
| 1   | A     | 2243 | LEU  |
| 1   | A     | 2259 | SER  |
| 1   | A     | 2268 | ASN  |
| 1   | A     | 2270 | LEU  |
| 1   | A     | 2308 | ILE  |
| 1   | A     | 2316 | THR  |
| 1   | A     | 2348 | THR  |
| 1   | A     | 2360 | LEU  |
| 1   | A     | 2363 | ASN  |
| 1   | A     | 2366 | ILE  |
| 1   | A     | 2390 | ASN  |
| 1   | A     | 2409 | THR  |
| 1   | A     | 2448 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2450 | MET  |
| 1   | A     | 2486 | VAL  |
| 1   | A     | 2506 | LEU  |
| 1   | A     | 2510 | LEU  |
| 1   | B     | 40   | THR  |
| 1   | B     | 42   | THR  |
| 1   | B     | 65   | LEU  |
| 1   | B     | 81   | LEU  |
| 1   | B     | 104  | VAL  |
| 1   | B     | 133  | ASN  |
| 1   | B     | 144  | ASP  |
| 1   | B     | 176  | LEU  |
| 1   | B     | 179  | THR  |
| 1   | B     | 187  | MET  |
| 1   | B     | 190  | THR  |
| 1   | B     | 226  | VAL  |
| 1   | B     | 251  | VAL  |
| 1   | B     | 260  | THR  |
| 1   | B     | 270  | ASP  |
| 1   | B     | 272  | VAL  |
| 1   | B     | 281  | LEU  |
| 1   | B     | 288  | SER  |
| 1   | B     | 322  | ASN  |
| 1   | B     | 333  | THR  |
| 1   | B     | 342  | LEU  |
| 1   | B     | 369  | LEU  |
| 1   | B     | 373  | LEU  |
| 1   | B     | 379  | GLU  |
| 1   | B     | 394  | HIS  |
| 1   | B     | 411  | THR  |
| 1   | B     | 426  | ASN  |
| 1   | B     | 440  | ILE  |
| 1   | B     | 442  | LEU  |
| 1   | B     | 451  | LEU  |
| 1   | B     | 453  | LYS  |
| 1   | B     | 473  | LEU  |
| 1   | B     | 474  | THR  |
| 1   | B     | 478  | ASN  |
| 1   | B     | 483  | LEU  |
| 1   | B     | 487  | GLN  |
| 1   | B     | 513  | THR  |
| 1   | B     | 526  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 529  | LEU  |
| 1   | B     | 537  | ASP  |
| 1   | B     | 539  | THR  |
| 1   | B     | 544  | THR  |
| 1   | B     | 554  | LEU  |
| 1   | B     | 563  | VAL  |
| 1   | B     | 566  | THR  |
| 1   | B     | 592  | LEU  |
| 1   | B     | 606  | THR  |
| 1   | B     | 608  | ASN  |
| 1   | B     | 613  | LEU  |
| 1   | B     | 630  | THR  |
| 1   | B     | 646  | LEU  |
| 1   | B     | 658  | LEU  |
| 1   | B     | 660  | THR  |
| 1   | B     | 691  | ASP  |
| 1   | B     | 694  | ILE  |
| 1   | B     | 701  | ILE  |
| 1   | B     | 705  | ILE  |
| 1   | B     | 706  | GLN  |
| 1   | B     | 732  | ASP  |
| 1   | B     | 763  | ILE  |
| 1   | B     | 767  | ILE  |
| 1   | B     | 771  | GLU  |
| 1   | B     | 775  | THR  |
| 1   | B     | 795  | LEU  |
| 1   | B     | 798  | LEU  |
| 1   | B     | 816  | THR  |
| 1   | B     | 819  | LEU  |
| 1   | B     | 879  | THR  |
| 1   | B     | 892  | VAL  |
| 1   | B     | 901  | THR  |
| 1   | B     | 992  | VAL  |
| 1   | B     | 1011 | THR  |
| 1   | B     | 1030 | GLU  |
| 1   | B     | 1031 | ASN  |
| 1   | B     | 1033 | ILE  |
| 1   | B     | 1047 | ASN  |
| 1   | B     | 1058 | ASN  |
| 1   | B     | 1059 | ILE  |
| 1   | B     | 1060 | ASP  |
| 1   | B     | 1076 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1092 | ASN  |
| 1   | B     | 1095 | LEU  |
| 1   | B     | 1096 | THR  |
| 1   | B     | 1104 | THR  |
| 1   | B     | 1114 | VAL  |
| 1   | B     | 1137 | ILE  |
| 1   | B     | 1141 | VAL  |
| 1   | B     | 1146 | ILE  |
| 1   | B     | 1149 | VAL  |
| 1   | B     | 1157 | LEU  |
| 1   | B     | 1180 | ILE  |
| 1   | B     | 1183 | LEU  |
| 1   | B     | 1202 | ASP  |
| 1   | B     | 1208 | ILE  |
| 1   | B     | 1227 | ILE  |
| 1   | B     | 1250 | THR  |
| 1   | B     | 1256 | THR  |
| 1   | B     | 1262 | GLU  |
| 1   | B     | 1272 | THR  |
| 1   | B     | 1277 | ASP  |
| 1   | B     | 1290 | THR  |
| 1   | B     | 1323 | ASN  |
| 1   | B     | 1334 | MET  |
| 1   | B     | 1500 | ASP  |
| 1   | B     | 1503 | ILE  |
| 1   | B     | 1545 | ILE  |
| 1   | B     | 1554 | SER  |
| 1   | B     | 1596 | THR  |
| 1   | B     | 1656 | GLU  |
| 1   | B     | 1690 | THR  |
| 1   | B     | 1692 | VAL  |
| 1   | B     | 1704 | ILE  |
| 1   | B     | 1712 | VAL  |
| 1   | B     | 1725 | SER  |
| 1   | B     | 1740 | ILE  |
| 1   | B     | 1796 | MET  |
| 1   | B     | 1803 | LEU  |
| 1   | B     | 1811 | SER  |
| 1   | B     | 1813 | ARG  |
| 1   | B     | 1818 | ILE  |
| 1   | B     | 1842 | GLU  |
| 1   | B     | 1854 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1875 | MET  |
| 1   | B     | 1893 | ASP  |
| 1   | B     | 1900 | MET  |
| 1   | B     | 1903 | VAL  |
| 1   | B     | 1911 | ASP  |
| 1   | B     | 1936 | HIS  |
| 1   | B     | 1951 | LEU  |
| 1   | B     | 1953 | THR  |
| 1   | B     | 1956 | THR  |
| 1   | B     | 1965 | LEU  |
| 1   | B     | 1991 | THR  |
| 1   | B     | 1999 | LEU  |
| 1   | B     | 2001 | LEU  |
| 1   | B     | 2017 | THR  |
| 1   | B     | 2025 | LEU  |
| 1   | B     | 2049 | LEU  |
| 1   | B     | 2057 | LEU  |
| 1   | B     | 2081 | LEU  |
| 1   | B     | 2105 | ARG  |
| 1   | B     | 2121 | GLU  |
| 1   | B     | 2131 | MET  |
| 1   | B     | 2135 | LEU  |
| 1   | B     | 2142 | THR  |
| 1   | B     | 2145 | THR  |
| 1   | B     | 2147 | LEU  |
| 1   | B     | 2160 | ILE  |
| 1   | B     | 2229 | LEU  |
| 1   | B     | 2243 | LEU  |
| 1   | B     | 2259 | SER  |
| 1   | B     | 2268 | ASN  |
| 1   | B     | 2270 | LEU  |
| 1   | B     | 2308 | ILE  |
| 1   | B     | 2316 | THR  |
| 1   | B     | 2348 | THR  |
| 1   | B     | 2360 | LEU  |
| 1   | B     | 2363 | ASN  |
| 1   | B     | 2366 | ILE  |
| 1   | B     | 2390 | ASN  |
| 1   | B     | 2409 | THR  |
| 1   | B     | 2448 | THR  |
| 1   | B     | 2450 | MET  |
| 1   | B     | 2486 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2506 | LEU  |
| 1   | B     | 2510 | LEU  |
| 1   | C     | 40   | THR  |
| 1   | C     | 42   | THR  |
| 1   | C     | 65   | LEU  |
| 1   | C     | 81   | LEU  |
| 1   | C     | 104  | VAL  |
| 1   | C     | 133  | ASN  |
| 1   | C     | 144  | ASP  |
| 1   | C     | 176  | LEU  |
| 1   | C     | 179  | THR  |
| 1   | C     | 187  | MET  |
| 1   | C     | 190  | THR  |
| 1   | C     | 226  | VAL  |
| 1   | C     | 251  | VAL  |
| 1   | C     | 260  | THR  |
| 1   | C     | 270  | ASP  |
| 1   | C     | 272  | VAL  |
| 1   | C     | 281  | LEU  |
| 1   | C     | 288  | SER  |
| 1   | C     | 322  | ASN  |
| 1   | C     | 333  | THR  |
| 1   | C     | 342  | LEU  |
| 1   | C     | 369  | LEU  |
| 1   | C     | 373  | LEU  |
| 1   | C     | 379  | GLU  |
| 1   | C     | 394  | HIS  |
| 1   | C     | 411  | THR  |
| 1   | C     | 426  | ASN  |
| 1   | C     | 440  | ILE  |
| 1   | C     | 442  | LEU  |
| 1   | C     | 451  | LEU  |
| 1   | C     | 453  | LYS  |
| 1   | C     | 473  | LEU  |
| 1   | C     | 474  | THR  |
| 1   | C     | 478  | ASN  |
| 1   | C     | 483  | LEU  |
| 1   | C     | 487  | GLN  |
| 1   | C     | 513  | THR  |
| 1   | C     | 526  | THR  |
| 1   | C     | 529  | LEU  |
| 1   | C     | 537  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 539  | THR  |
| 1   | C     | 544  | THR  |
| 1   | C     | 554  | LEU  |
| 1   | C     | 563  | VAL  |
| 1   | C     | 566  | THR  |
| 1   | C     | 592  | LEU  |
| 1   | C     | 606  | THR  |
| 1   | C     | 608  | ASN  |
| 1   | C     | 613  | LEU  |
| 1   | C     | 630  | THR  |
| 1   | C     | 646  | LEU  |
| 1   | C     | 658  | LEU  |
| 1   | C     | 660  | THR  |
| 1   | C     | 691  | ASP  |
| 1   | C     | 694  | ILE  |
| 1   | C     | 701  | ILE  |
| 1   | C     | 705  | ILE  |
| 1   | C     | 706  | GLN  |
| 1   | C     | 732  | ASP  |
| 1   | C     | 763  | ILE  |
| 1   | C     | 767  | ILE  |
| 1   | C     | 771  | GLU  |
| 1   | C     | 775  | THR  |
| 1   | C     | 795  | LEU  |
| 1   | C     | 798  | LEU  |
| 1   | C     | 816  | THR  |
| 1   | C     | 819  | LEU  |
| 1   | C     | 879  | THR  |
| 1   | C     | 892  | VAL  |
| 1   | C     | 901  | THR  |
| 1   | C     | 992  | VAL  |
| 1   | C     | 1011 | THR  |
| 1   | C     | 1030 | GLU  |
| 1   | C     | 1031 | ASN  |
| 1   | C     | 1033 | ILE  |
| 1   | C     | 1047 | ASN  |
| 1   | C     | 1058 | ASN  |
| 1   | C     | 1059 | ILE  |
| 1   | C     | 1060 | ASP  |
| 1   | C     | 1076 | VAL  |
| 1   | C     | 1092 | ASN  |
| 1   | C     | 1095 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1096 | THR  |
| 1   | C     | 1104 | THR  |
| 1   | C     | 1114 | VAL  |
| 1   | C     | 1137 | ILE  |
| 1   | C     | 1141 | VAL  |
| 1   | C     | 1146 | ILE  |
| 1   | C     | 1149 | VAL  |
| 1   | C     | 1157 | LEU  |
| 1   | C     | 1180 | ILE  |
| 1   | C     | 1183 | LEU  |
| 1   | C     | 1202 | ASP  |
| 1   | C     | 1208 | ILE  |
| 1   | C     | 1227 | ILE  |
| 1   | C     | 1250 | THR  |
| 1   | C     | 1256 | THR  |
| 1   | C     | 1262 | GLU  |
| 1   | C     | 1272 | THR  |
| 1   | C     | 1277 | ASP  |
| 1   | C     | 1290 | THR  |
| 1   | C     | 1323 | ASN  |
| 1   | C     | 1334 | MET  |
| 1   | C     | 1500 | ASP  |
| 1   | C     | 1503 | ILE  |
| 1   | C     | 1545 | ILE  |
| 1   | C     | 1554 | SER  |
| 1   | C     | 1596 | THR  |
| 1   | C     | 1656 | GLU  |
| 1   | C     | 1690 | THR  |
| 1   | C     | 1692 | VAL  |
| 1   | C     | 1704 | ILE  |
| 1   | C     | 1712 | VAL  |
| 1   | C     | 1725 | SER  |
| 1   | C     | 1740 | ILE  |
| 1   | C     | 1796 | MET  |
| 1   | C     | 1803 | LEU  |
| 1   | C     | 1811 | SER  |
| 1   | C     | 1813 | ARG  |
| 1   | C     | 1818 | ILE  |
| 1   | C     | 1842 | GLU  |
| 1   | C     | 1854 | VAL  |
| 1   | C     | 1875 | MET  |
| 1   | C     | 1893 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1900 | MET  |
| 1   | C     | 1903 | VAL  |
| 1   | C     | 1911 | ASP  |
| 1   | C     | 1936 | HIS  |
| 1   | C     | 1951 | LEU  |
| 1   | C     | 1953 | THR  |
| 1   | C     | 1956 | THR  |
| 1   | C     | 1965 | LEU  |
| 1   | C     | 1991 | THR  |
| 1   | C     | 1999 | LEU  |
| 1   | C     | 2001 | LEU  |
| 1   | C     | 2017 | THR  |
| 1   | C     | 2025 | LEU  |
| 1   | C     | 2049 | LEU  |
| 1   | C     | 2057 | LEU  |
| 1   | C     | 2081 | LEU  |
| 1   | C     | 2105 | ARG  |
| 1   | C     | 2121 | GLU  |
| 1   | C     | 2131 | MET  |
| 1   | C     | 2135 | LEU  |
| 1   | C     | 2142 | THR  |
| 1   | C     | 2145 | THR  |
| 1   | C     | 2147 | LEU  |
| 1   | C     | 2160 | ILE  |
| 1   | C     | 2229 | LEU  |
| 1   | C     | 2243 | LEU  |
| 1   | C     | 2259 | SER  |
| 1   | C     | 2268 | ASN  |
| 1   | C     | 2270 | LEU  |
| 1   | C     | 2290 | LEU  |
| 1   | C     | 2308 | ILE  |
| 1   | C     | 2316 | THR  |
| 1   | C     | 2348 | THR  |
| 1   | C     | 2360 | LEU  |
| 1   | C     | 2363 | ASN  |
| 1   | C     | 2366 | ILE  |
| 1   | C     | 2390 | ASN  |
| 1   | C     | 2409 | THR  |
| 1   | C     | 2448 | THR  |
| 1   | C     | 2450 | MET  |
| 1   | C     | 2486 | VAL  |
| 1   | C     | 2506 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2510 | LEU  |
| 1   | D     | 40   | THR  |
| 1   | D     | 42   | THR  |
| 1   | D     | 65   | LEU  |
| 1   | D     | 81   | LEU  |
| 1   | D     | 104  | VAL  |
| 1   | D     | 133  | ASN  |
| 1   | D     | 144  | ASP  |
| 1   | D     | 176  | LEU  |
| 1   | D     | 179  | THR  |
| 1   | D     | 187  | MET  |
| 1   | D     | 190  | THR  |
| 1   | D     | 226  | VAL  |
| 1   | D     | 251  | VAL  |
| 1   | D     | 260  | THR  |
| 1   | D     | 270  | ASP  |
| 1   | D     | 272  | VAL  |
| 1   | D     | 281  | LEU  |
| 1   | D     | 288  | SER  |
| 1   | D     | 322  | ASN  |
| 1   | D     | 333  | THR  |
| 1   | D     | 342  | LEU  |
| 1   | D     | 369  | LEU  |
| 1   | D     | 373  | LEU  |
| 1   | D     | 379  | GLU  |
| 1   | D     | 394  | HIS  |
| 1   | D     | 411  | THR  |
| 1   | D     | 426  | ASN  |
| 1   | D     | 440  | ILE  |
| 1   | D     | 442  | LEU  |
| 1   | D     | 451  | LEU  |
| 1   | D     | 453  | LYS  |
| 1   | D     | 473  | LEU  |
| 1   | D     | 474  | THR  |
| 1   | D     | 478  | ASN  |
| 1   | D     | 483  | LEU  |
| 1   | D     | 487  | GLN  |
| 1   | D     | 513  | THR  |
| 1   | D     | 526  | THR  |
| 1   | D     | 529  | LEU  |
| 1   | D     | 537  | ASP  |
| 1   | D     | 539  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 544  | THR  |
| 1   | D     | 554  | LEU  |
| 1   | D     | 563  | VAL  |
| 1   | D     | 566  | THR  |
| 1   | D     | 592  | LEU  |
| 1   | D     | 606  | THR  |
| 1   | D     | 608  | ASN  |
| 1   | D     | 613  | LEU  |
| 1   | D     | 630  | THR  |
| 1   | D     | 646  | LEU  |
| 1   | D     | 658  | LEU  |
| 1   | D     | 660  | THR  |
| 1   | D     | 691  | ASP  |
| 1   | D     | 694  | ILE  |
| 1   | D     | 701  | ILE  |
| 1   | D     | 705  | ILE  |
| 1   | D     | 706  | GLN  |
| 1   | D     | 732  | ASP  |
| 1   | D     | 763  | ILE  |
| 1   | D     | 767  | ILE  |
| 1   | D     | 771  | GLU  |
| 1   | D     | 775  | THR  |
| 1   | D     | 795  | LEU  |
| 1   | D     | 798  | LEU  |
| 1   | D     | 816  | THR  |
| 1   | D     | 819  | LEU  |
| 1   | D     | 879  | THR  |
| 1   | D     | 892  | VAL  |
| 1   | D     | 901  | THR  |
| 1   | D     | 992  | VAL  |
| 1   | D     | 1011 | THR  |
| 1   | D     | 1030 | GLU  |
| 1   | D     | 1031 | ASN  |
| 1   | D     | 1033 | ILE  |
| 1   | D     | 1047 | ASN  |
| 1   | D     | 1058 | ASN  |
| 1   | D     | 1059 | ILE  |
| 1   | D     | 1060 | ASP  |
| 1   | D     | 1076 | VAL  |
| 1   | D     | 1092 | ASN  |
| 1   | D     | 1095 | LEU  |
| 1   | D     | 1096 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1104 | THR  |
| 1   | D     | 1114 | VAL  |
| 1   | D     | 1137 | ILE  |
| 1   | D     | 1141 | VAL  |
| 1   | D     | 1146 | ILE  |
| 1   | D     | 1149 | VAL  |
| 1   | D     | 1157 | LEU  |
| 1   | D     | 1180 | ILE  |
| 1   | D     | 1183 | LEU  |
| 1   | D     | 1202 | ASP  |
| 1   | D     | 1208 | ILE  |
| 1   | D     | 1227 | ILE  |
| 1   | D     | 1250 | THR  |
| 1   | D     | 1256 | THR  |
| 1   | D     | 1262 | GLU  |
| 1   | D     | 1272 | THR  |
| 1   | D     | 1277 | ASP  |
| 1   | D     | 1290 | THR  |
| 1   | D     | 1323 | ASN  |
| 1   | D     | 1334 | MET  |
| 1   | D     | 1500 | ASP  |
| 1   | D     | 1503 | ILE  |
| 1   | D     | 1545 | ILE  |
| 1   | D     | 1554 | SER  |
| 1   | D     | 1596 | THR  |
| 1   | D     | 1656 | GLU  |
| 1   | D     | 1690 | THR  |
| 1   | D     | 1692 | VAL  |
| 1   | D     | 1704 | ILE  |
| 1   | D     | 1712 | VAL  |
| 1   | D     | 1725 | SER  |
| 1   | D     | 1740 | ILE  |
| 1   | D     | 1796 | MET  |
| 1   | D     | 1803 | LEU  |
| 1   | D     | 1811 | SER  |
| 1   | D     | 1813 | ARG  |
| 1   | D     | 1818 | ILE  |
| 1   | D     | 1842 | GLU  |
| 1   | D     | 1854 | VAL  |
| 1   | D     | 1875 | MET  |
| 1   | D     | 1893 | ASP  |
| 1   | D     | 1900 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1903 | VAL  |
| 1   | D     | 1911 | ASP  |
| 1   | D     | 1936 | HIS  |
| 1   | D     | 1951 | LEU  |
| 1   | D     | 1953 | THR  |
| 1   | D     | 1956 | THR  |
| 1   | D     | 1965 | LEU  |
| 1   | D     | 1991 | THR  |
| 1   | D     | 1999 | LEU  |
| 1   | D     | 2001 | LEU  |
| 1   | D     | 2017 | THR  |
| 1   | D     | 2025 | LEU  |
| 1   | D     | 2049 | LEU  |
| 1   | D     | 2057 | LEU  |
| 1   | D     | 2081 | LEU  |
| 1   | D     | 2105 | ARG  |
| 1   | D     | 2121 | GLU  |
| 1   | D     | 2131 | MET  |
| 1   | D     | 2135 | LEU  |
| 1   | D     | 2142 | THR  |
| 1   | D     | 2145 | THR  |
| 1   | D     | 2147 | LEU  |
| 1   | D     | 2160 | ILE  |
| 1   | D     | 2229 | LEU  |
| 1   | D     | 2243 | LEU  |
| 1   | D     | 2259 | SER  |
| 1   | D     | 2268 | ASN  |
| 1   | D     | 2270 | LEU  |
| 1   | D     | 2308 | ILE  |
| 1   | D     | 2316 | THR  |
| 1   | D     | 2348 | THR  |
| 1   | D     | 2360 | LEU  |
| 1   | D     | 2363 | ASN  |
| 1   | D     | 2366 | ILE  |
| 1   | D     | 2390 | ASN  |
| 1   | D     | 2409 | THR  |
| 1   | D     | 2448 | THR  |
| 1   | D     | 2450 | MET  |
| 1   | D     | 2486 | VAL  |
| 1   | D     | 2506 | LEU  |
| 1   | D     | 2510 | LEU  |
| 1   | E     | 40   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 42  | THR  |
| 1   | E     | 65  | LEU  |
| 1   | E     | 81  | LEU  |
| 1   | E     | 104 | VAL  |
| 1   | E     | 133 | ASN  |
| 1   | E     | 144 | ASP  |
| 1   | E     | 176 | LEU  |
| 1   | E     | 179 | THR  |
| 1   | E     | 187 | MET  |
| 1   | E     | 190 | THR  |
| 1   | E     | 226 | VAL  |
| 1   | E     | 251 | VAL  |
| 1   | E     | 260 | THR  |
| 1   | E     | 270 | ASP  |
| 1   | E     | 272 | VAL  |
| 1   | E     | 281 | LEU  |
| 1   | E     | 288 | SER  |
| 1   | E     | 322 | ASN  |
| 1   | E     | 333 | THR  |
| 1   | E     | 342 | LEU  |
| 1   | E     | 369 | LEU  |
| 1   | E     | 373 | LEU  |
| 1   | E     | 379 | GLU  |
| 1   | E     | 394 | HIS  |
| 1   | E     | 411 | THR  |
| 1   | E     | 426 | ASN  |
| 1   | E     | 440 | ILE  |
| 1   | E     | 442 | LEU  |
| 1   | E     | 451 | LEU  |
| 1   | E     | 453 | LYS  |
| 1   | E     | 473 | LEU  |
| 1   | E     | 474 | THR  |
| 1   | E     | 478 | ASN  |
| 1   | E     | 483 | LEU  |
| 1   | E     | 487 | GLN  |
| 1   | E     | 513 | THR  |
| 1   | E     | 526 | THR  |
| 1   | E     | 529 | LEU  |
| 1   | E     | 537 | ASP  |
| 1   | E     | 539 | THR  |
| 1   | E     | 544 | THR  |
| 1   | E     | 554 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 563  | VAL  |
| 1   | E     | 566  | THR  |
| 1   | E     | 592  | LEU  |
| 1   | E     | 606  | THR  |
| 1   | E     | 608  | ASN  |
| 1   | E     | 613  | LEU  |
| 1   | E     | 630  | THR  |
| 1   | E     | 646  | LEU  |
| 1   | E     | 658  | LEU  |
| 1   | E     | 660  | THR  |
| 1   | E     | 691  | ASP  |
| 1   | E     | 694  | ILE  |
| 1   | E     | 701  | ILE  |
| 1   | E     | 705  | ILE  |
| 1   | E     | 706  | GLN  |
| 1   | E     | 732  | ASP  |
| 1   | E     | 763  | ILE  |
| 1   | E     | 767  | ILE  |
| 1   | E     | 771  | GLU  |
| 1   | E     | 775  | THR  |
| 1   | E     | 795  | LEU  |
| 1   | E     | 798  | LEU  |
| 1   | E     | 816  | THR  |
| 1   | E     | 819  | LEU  |
| 1   | E     | 879  | THR  |
| 1   | E     | 892  | VAL  |
| 1   | E     | 901  | THR  |
| 1   | E     | 992  | VAL  |
| 1   | E     | 1011 | THR  |
| 1   | E     | 1030 | GLU  |
| 1   | E     | 1031 | ASN  |
| 1   | E     | 1033 | ILE  |
| 1   | E     | 1047 | ASN  |
| 1   | E     | 1058 | ASN  |
| 1   | E     | 1059 | ILE  |
| 1   | E     | 1060 | ASP  |
| 1   | E     | 1076 | VAL  |
| 1   | E     | 1092 | ASN  |
| 1   | E     | 1095 | LEU  |
| 1   | E     | 1096 | THR  |
| 1   | E     | 1104 | THR  |
| 1   | E     | 1114 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1137 | ILE  |
| 1   | E     | 1141 | VAL  |
| 1   | E     | 1146 | ILE  |
| 1   | E     | 1149 | VAL  |
| 1   | E     | 1157 | LEU  |
| 1   | E     | 1180 | ILE  |
| 1   | E     | 1183 | LEU  |
| 1   | E     | 1202 | ASP  |
| 1   | E     | 1208 | ILE  |
| 1   | E     | 1227 | ILE  |
| 1   | E     | 1250 | THR  |
| 1   | E     | 1256 | THR  |
| 1   | E     | 1262 | GLU  |
| 1   | E     | 1272 | THR  |
| 1   | E     | 1277 | ASP  |
| 1   | E     | 1290 | THR  |
| 1   | E     | 1323 | ASN  |
| 1   | E     | 1334 | MET  |
| 1   | E     | 1500 | ASP  |
| 1   | E     | 1503 | ILE  |
| 1   | E     | 1545 | ILE  |
| 1   | E     | 1554 | SER  |
| 1   | E     | 1596 | THR  |
| 1   | E     | 1656 | GLU  |
| 1   | E     | 1690 | THR  |
| 1   | E     | 1692 | VAL  |
| 1   | E     | 1704 | ILE  |
| 1   | E     | 1712 | VAL  |
| 1   | E     | 1725 | SER  |
| 1   | E     | 1740 | ILE  |
| 1   | E     | 1796 | MET  |
| 1   | E     | 1803 | LEU  |
| 1   | E     | 1811 | SER  |
| 1   | E     | 1813 | ARG  |
| 1   | E     | 1818 | ILE  |
| 1   | E     | 1842 | GLU  |
| 1   | E     | 1854 | VAL  |
| 1   | E     | 1875 | MET  |
| 1   | E     | 1893 | ASP  |
| 1   | E     | 1900 | MET  |
| 1   | E     | 1903 | VAL  |
| 1   | E     | 1911 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1936 | HIS  |
| 1   | E     | 1951 | LEU  |
| 1   | E     | 1953 | THR  |
| 1   | E     | 1956 | THR  |
| 1   | E     | 1965 | LEU  |
| 1   | E     | 1991 | THR  |
| 1   | E     | 1999 | LEU  |
| 1   | E     | 2001 | LEU  |
| 1   | E     | 2017 | THR  |
| 1   | E     | 2025 | LEU  |
| 1   | E     | 2049 | LEU  |
| 1   | E     | 2057 | LEU  |
| 1   | E     | 2081 | LEU  |
| 1   | E     | 2105 | ARG  |
| 1   | E     | 2121 | GLU  |
| 1   | E     | 2131 | MET  |
| 1   | E     | 2135 | LEU  |
| 1   | E     | 2142 | THR  |
| 1   | E     | 2145 | THR  |
| 1   | E     | 2147 | LEU  |
| 1   | E     | 2160 | ILE  |
| 1   | E     | 2229 | LEU  |
| 1   | E     | 2243 | LEU  |
| 1   | E     | 2259 | SER  |
| 1   | E     | 2268 | ASN  |
| 1   | E     | 2270 | LEU  |
| 1   | E     | 2308 | ILE  |
| 1   | E     | 2316 | THR  |
| 1   | E     | 2348 | THR  |
| 1   | E     | 2360 | LEU  |
| 1   | E     | 2363 | ASN  |
| 1   | E     | 2366 | ILE  |
| 1   | E     | 2390 | ASN  |
| 1   | E     | 2409 | THR  |
| 1   | E     | 2448 | THR  |
| 1   | E     | 2450 | MET  |
| 1   | E     | 2486 | VAL  |
| 1   | E     | 2506 | LEU  |
| 1   | E     | 2510 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (269) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 80   | ASN  |
| 1   | A     | 139  | ASN  |
| 1   | A     | 152  | GLN  |
| 1   | A     | 171  | HIS  |
| 1   | A     | 172  | ASN  |
| 1   | A     | 200  | HIS  |
| 1   | A     | 216  | ASN  |
| 1   | A     | 266  | ASN  |
| 1   | A     | 311  | ASN  |
| 1   | A     | 341  | HIS  |
| 1   | A     | 374  | GLN  |
| 1   | A     | 408  | ASN  |
| 1   | A     | 478  | ASN  |
| 1   | A     | 491  | GLN  |
| 1   | A     | 516  | GLN  |
| 1   | A     | 519  | HIS  |
| 1   | A     | 551  | HIS  |
| 1   | A     | 634  | GLN  |
| 1   | A     | 681  | ASN  |
| 1   | A     | 706  | GLN  |
| 1   | A     | 722  | GLN  |
| 1   | A     | 766  | ASN  |
| 1   | A     | 793  | HIS  |
| 1   | A     | 849  | GLN  |
| 1   | A     | 855  | ASN  |
| 1   | A     | 919  | GLN  |
| 1   | A     | 1041 | GLN  |
| 1   | A     | 1054 | GLN  |
| 1   | A     | 1056 | GLN  |
| 1   | A     | 1080 | GLN  |
| 1   | A     | 1145 | ASN  |
| 1   | A     | 1167 | ASN  |
| 1   | A     | 1197 | ASN  |
| 1   | A     | 1206 | ASN  |
| 1   | A     | 1502 | ASN  |
| 1   | A     | 1518 | ASN  |
| 1   | A     | 1522 | HIS  |
| 1   | A     | 1621 | ASN  |
| 1   | A     | 1670 | ASN  |
| 1   | A     | 1741 | ASN  |
| 1   | A     | 1800 | GLN  |
| 1   | A     | 1939 | GLN  |
| 1   | A     | 2048 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2073 | GLN  |
| 1   | A     | 2075 | GLN  |
| 1   | A     | 2102 | GLN  |
| 1   | A     | 2109 | GLN  |
| 1   | A     | 2129 | GLN  |
| 1   | A     | 2159 | ASN  |
| 1   | A     | 2251 | GLN  |
| 1   | A     | 2314 | HIS  |
| 1   | A     | 2376 | ASN  |
| 1   | A     | 2390 | ASN  |
| 1   | A     | 2397 | GLN  |
| 1   | B     | 54   | HIS  |
| 1   | B     | 80   | ASN  |
| 1   | B     | 139  | ASN  |
| 1   | B     | 152  | GLN  |
| 1   | B     | 171  | HIS  |
| 1   | B     | 172  | ASN  |
| 1   | B     | 200  | HIS  |
| 1   | B     | 216  | ASN  |
| 1   | B     | 266  | ASN  |
| 1   | B     | 311  | ASN  |
| 1   | B     | 341  | HIS  |
| 1   | B     | 374  | GLN  |
| 1   | B     | 408  | ASN  |
| 1   | B     | 478  | ASN  |
| 1   | B     | 491  | GLN  |
| 1   | B     | 516  | GLN  |
| 1   | B     | 519  | HIS  |
| 1   | B     | 551  | HIS  |
| 1   | B     | 634  | GLN  |
| 1   | B     | 681  | ASN  |
| 1   | B     | 706  | GLN  |
| 1   | B     | 722  | GLN  |
| 1   | B     | 766  | ASN  |
| 1   | B     | 793  | HIS  |
| 1   | B     | 919  | GLN  |
| 1   | B     | 943  | ASN  |
| 1   | B     | 1041 | GLN  |
| 1   | B     | 1054 | GLN  |
| 1   | B     | 1056 | GLN  |
| 1   | B     | 1080 | GLN  |
| 1   | B     | 1145 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1167 | ASN  |
| 1   | B     | 1197 | ASN  |
| 1   | B     | 1206 | ASN  |
| 1   | B     | 1285 | ASN  |
| 1   | B     | 1502 | ASN  |
| 1   | B     | 1518 | ASN  |
| 1   | B     | 1522 | HIS  |
| 1   | B     | 1621 | ASN  |
| 1   | B     | 1670 | ASN  |
| 1   | B     | 1741 | ASN  |
| 1   | B     | 1800 | GLN  |
| 1   | B     | 1939 | GLN  |
| 1   | B     | 2073 | GLN  |
| 1   | B     | 2075 | GLN  |
| 1   | B     | 2102 | GLN  |
| 1   | B     | 2109 | GLN  |
| 1   | B     | 2129 | GLN  |
| 1   | B     | 2159 | ASN  |
| 1   | B     | 2314 | HIS  |
| 1   | B     | 2390 | ASN  |
| 1   | B     | 2397 | GLN  |
| 1   | C     | 54   | HIS  |
| 1   | C     | 55   | GLN  |
| 1   | C     | 139  | ASN  |
| 1   | C     | 152  | GLN  |
| 1   | C     | 171  | HIS  |
| 1   | C     | 172  | ASN  |
| 1   | C     | 200  | HIS  |
| 1   | C     | 213  | GLN  |
| 1   | C     | 216  | ASN  |
| 1   | C     | 266  | ASN  |
| 1   | C     | 311  | ASN  |
| 1   | C     | 341  | HIS  |
| 1   | C     | 374  | GLN  |
| 1   | C     | 408  | ASN  |
| 1   | C     | 478  | ASN  |
| 1   | C     | 491  | GLN  |
| 1   | C     | 516  | GLN  |
| 1   | C     | 519  | HIS  |
| 1   | C     | 551  | HIS  |
| 1   | C     | 634  | GLN  |
| 1   | C     | 681  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 706  | GLN  |
| 1   | C     | 722  | GLN  |
| 1   | C     | 766  | ASN  |
| 1   | C     | 793  | HIS  |
| 1   | C     | 849  | GLN  |
| 1   | C     | 943  | ASN  |
| 1   | C     | 1041 | GLN  |
| 1   | C     | 1054 | GLN  |
| 1   | C     | 1056 | GLN  |
| 1   | C     | 1080 | GLN  |
| 1   | C     | 1145 | ASN  |
| 1   | C     | 1167 | ASN  |
| 1   | C     | 1197 | ASN  |
| 1   | C     | 1206 | ASN  |
| 1   | C     | 1285 | ASN  |
| 1   | C     | 1502 | ASN  |
| 1   | C     | 1518 | ASN  |
| 1   | C     | 1522 | HIS  |
| 1   | C     | 1621 | ASN  |
| 1   | C     | 1670 | ASN  |
| 1   | C     | 1741 | ASN  |
| 1   | C     | 1800 | GLN  |
| 1   | C     | 1939 | GLN  |
| 1   | C     | 1989 | ASN  |
| 1   | C     | 2048 | GLN  |
| 1   | C     | 2073 | GLN  |
| 1   | C     | 2102 | GLN  |
| 1   | C     | 2109 | GLN  |
| 1   | C     | 2129 | GLN  |
| 1   | C     | 2148 | HIS  |
| 1   | C     | 2159 | ASN  |
| 1   | C     | 2251 | GLN  |
| 1   | C     | 2314 | HIS  |
| 1   | C     | 2390 | ASN  |
| 1   | C     | 2397 | GLN  |
| 1   | C     | 2468 | GLN  |
| 1   | D     | 55   | GLN  |
| 1   | D     | 139  | ASN  |
| 1   | D     | 152  | GLN  |
| 1   | D     | 172  | ASN  |
| 1   | D     | 200  | HIS  |
| 1   | D     | 216  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 266  | ASN  |
| 1   | D     | 311  | ASN  |
| 1   | D     | 341  | HIS  |
| 1   | D     | 374  | GLN  |
| 1   | D     | 408  | ASN  |
| 1   | D     | 478  | ASN  |
| 1   | D     | 491  | GLN  |
| 1   | D     | 516  | GLN  |
| 1   | D     | 519  | HIS  |
| 1   | D     | 551  | HIS  |
| 1   | D     | 634  | GLN  |
| 1   | D     | 681  | ASN  |
| 1   | D     | 706  | GLN  |
| 1   | D     | 722  | GLN  |
| 1   | D     | 766  | ASN  |
| 1   | D     | 793  | HIS  |
| 1   | D     | 849  | GLN  |
| 1   | D     | 919  | GLN  |
| 1   | D     | 1041 | GLN  |
| 1   | D     | 1054 | GLN  |
| 1   | D     | 1056 | GLN  |
| 1   | D     | 1080 | GLN  |
| 1   | D     | 1145 | ASN  |
| 1   | D     | 1167 | ASN  |
| 1   | D     | 1197 | ASN  |
| 1   | D     | 1206 | ASN  |
| 1   | D     | 1325 | HIS  |
| 1   | D     | 1502 | ASN  |
| 1   | D     | 1518 | ASN  |
| 1   | D     | 1522 | HIS  |
| 1   | D     | 1621 | ASN  |
| 1   | D     | 1670 | ASN  |
| 1   | D     | 1741 | ASN  |
| 1   | D     | 1800 | GLN  |
| 1   | D     | 1939 | GLN  |
| 1   | D     | 2048 | GLN  |
| 1   | D     | 2073 | GLN  |
| 1   | D     | 2075 | GLN  |
| 1   | D     | 2102 | GLN  |
| 1   | D     | 2109 | GLN  |
| 1   | D     | 2129 | GLN  |
| 1   | D     | 2159 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 2251 | GLN  |
| 1   | D     | 2390 | ASN  |
| 1   | D     | 2397 | GLN  |
| 1   | D     | 2461 | HIS  |
| 1   | E     | 55   | GLN  |
| 1   | E     | 80   | ASN  |
| 1   | E     | 139  | ASN  |
| 1   | E     | 152  | GLN  |
| 1   | E     | 171  | HIS  |
| 1   | E     | 172  | ASN  |
| 1   | E     | 200  | HIS  |
| 1   | E     | 216  | ASN  |
| 1   | E     | 266  | ASN  |
| 1   | E     | 311  | ASN  |
| 1   | E     | 341  | HIS  |
| 1   | E     | 374  | GLN  |
| 1   | E     | 408  | ASN  |
| 1   | E     | 478  | ASN  |
| 1   | E     | 491  | GLN  |
| 1   | E     | 516  | GLN  |
| 1   | E     | 519  | HIS  |
| 1   | E     | 551  | HIS  |
| 1   | E     | 634  | GLN  |
| 1   | E     | 681  | ASN  |
| 1   | E     | 706  | GLN  |
| 1   | E     | 722  | GLN  |
| 1   | E     | 766  | ASN  |
| 1   | E     | 793  | HIS  |
| 1   | E     | 849  | GLN  |
| 1   | E     | 919  | GLN  |
| 1   | E     | 1041 | GLN  |
| 1   | E     | 1054 | GLN  |
| 1   | E     | 1056 | GLN  |
| 1   | E     | 1080 | GLN  |
| 1   | E     | 1145 | ASN  |
| 1   | E     | 1167 | ASN  |
| 1   | E     | 1197 | ASN  |
| 1   | E     | 1206 | ASN  |
| 1   | E     | 1502 | ASN  |
| 1   | E     | 1518 | ASN  |
| 1   | E     | 1522 | HIS  |
| 1   | E     | 1621 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1639 | GLN  |
| 1   | E     | 1670 | ASN  |
| 1   | E     | 1741 | ASN  |
| 1   | E     | 1800 | GLN  |
| 1   | E     | 1939 | GLN  |
| 1   | E     | 2048 | GLN  |
| 1   | E     | 2073 | GLN  |
| 1   | E     | 2102 | GLN  |
| 1   | E     | 2109 | GLN  |
| 1   | E     | 2129 | GLN  |
| 1   | E     | 2159 | ASN  |
| 1   | E     | 2251 | GLN  |
| 1   | E     | 2314 | HIS  |
| 1   | E     | 2390 | ASN  |
| 1   | E     | 2397 | GLN  |
| 1   | E     | 2461 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

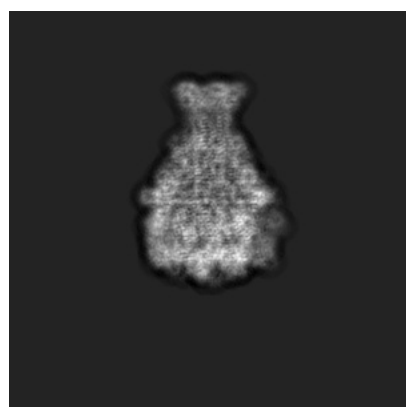
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10797. These allow visual inspection of the internal detail of the map and identification of artifacts.

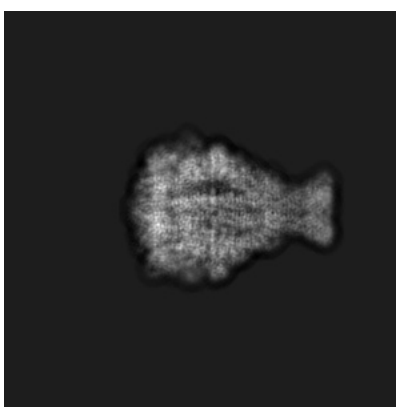
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

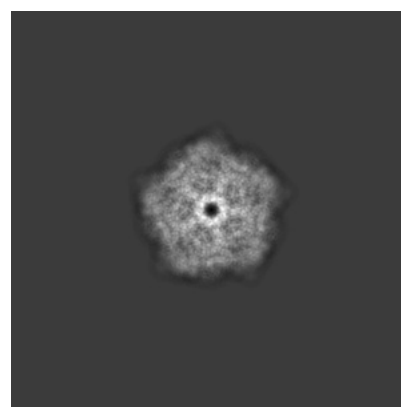
#### 6.1.1 Primary map



X



Y

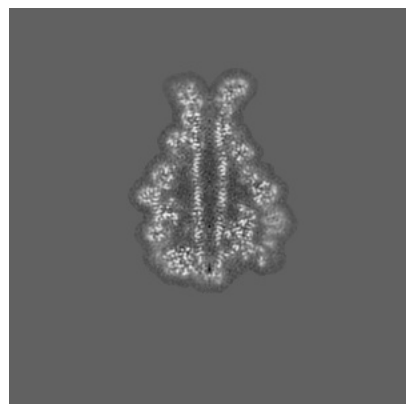


Z

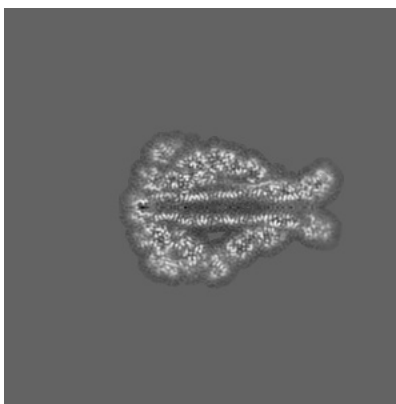
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

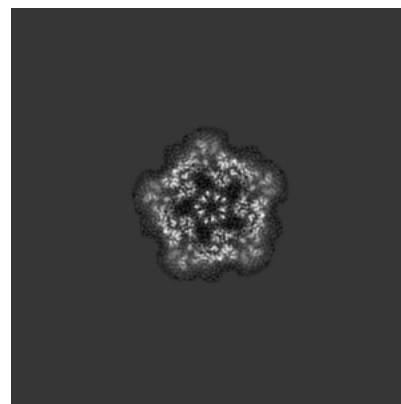
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

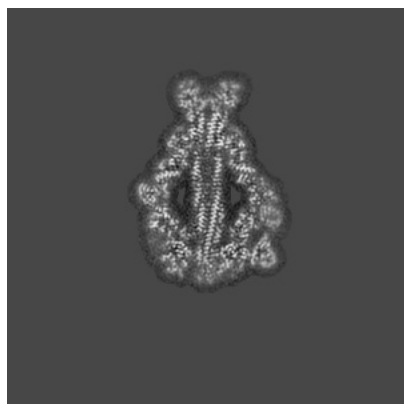


Z Index: 200

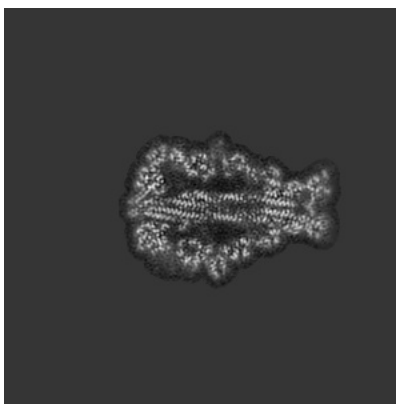
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

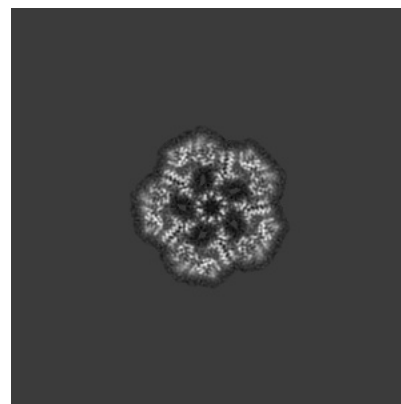
### 6.3.1 Primary map



X Index: 192



Y Index: 192

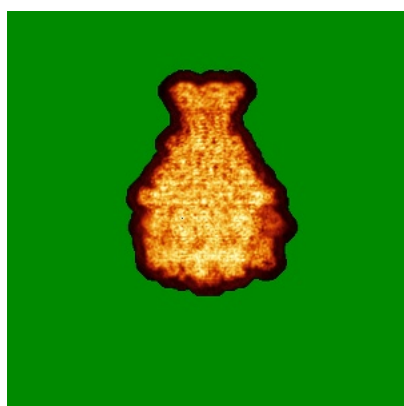


Z Index: 208

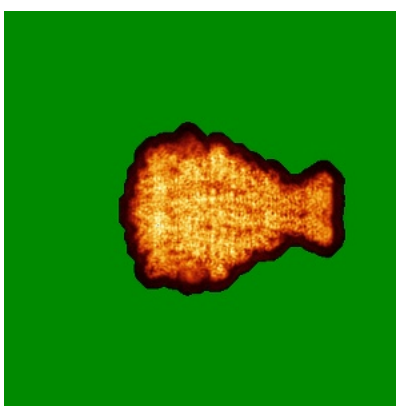
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

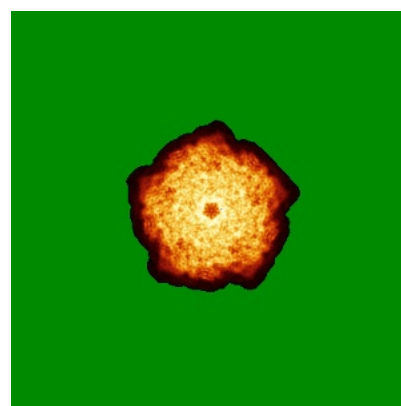
### 6.4.1 Primary map



X



Y

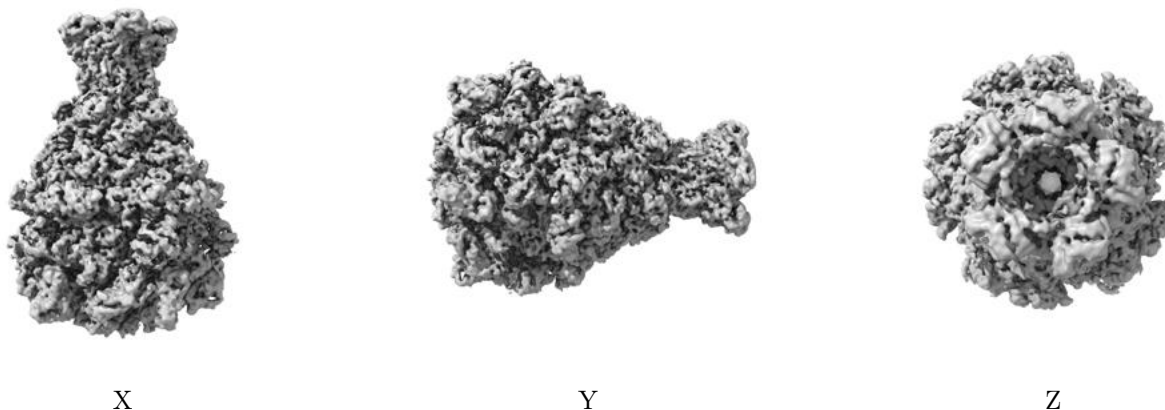


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

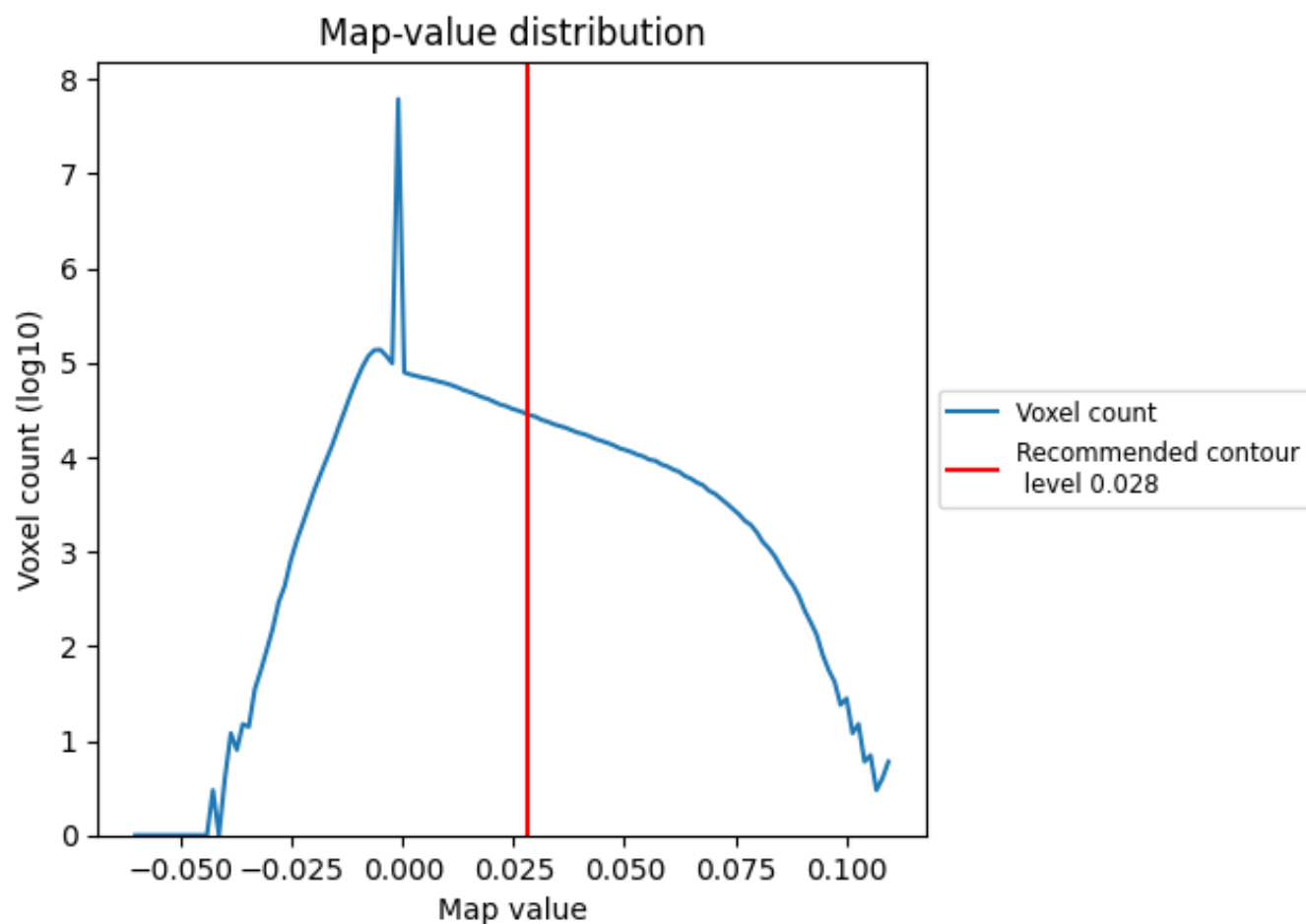
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

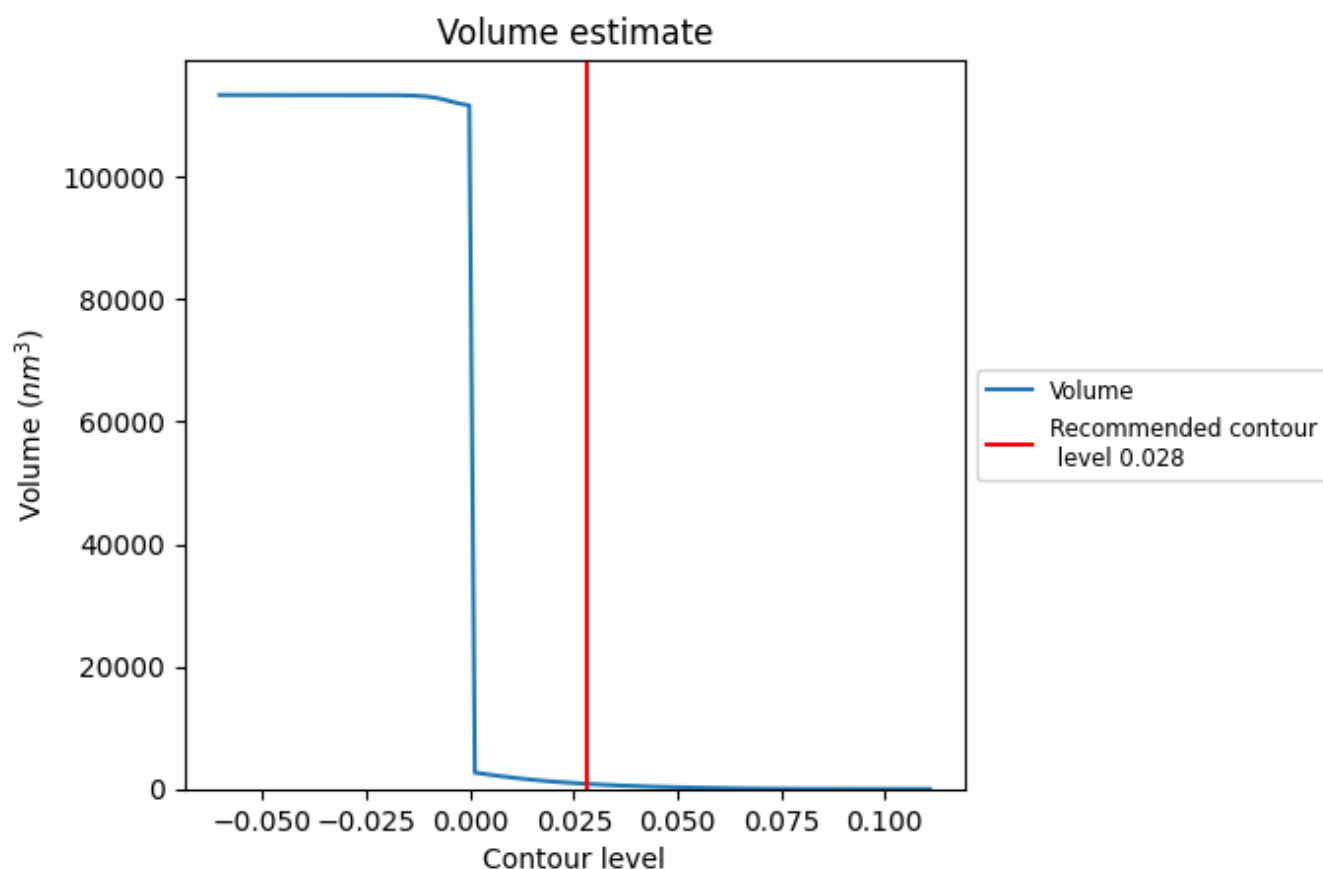
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

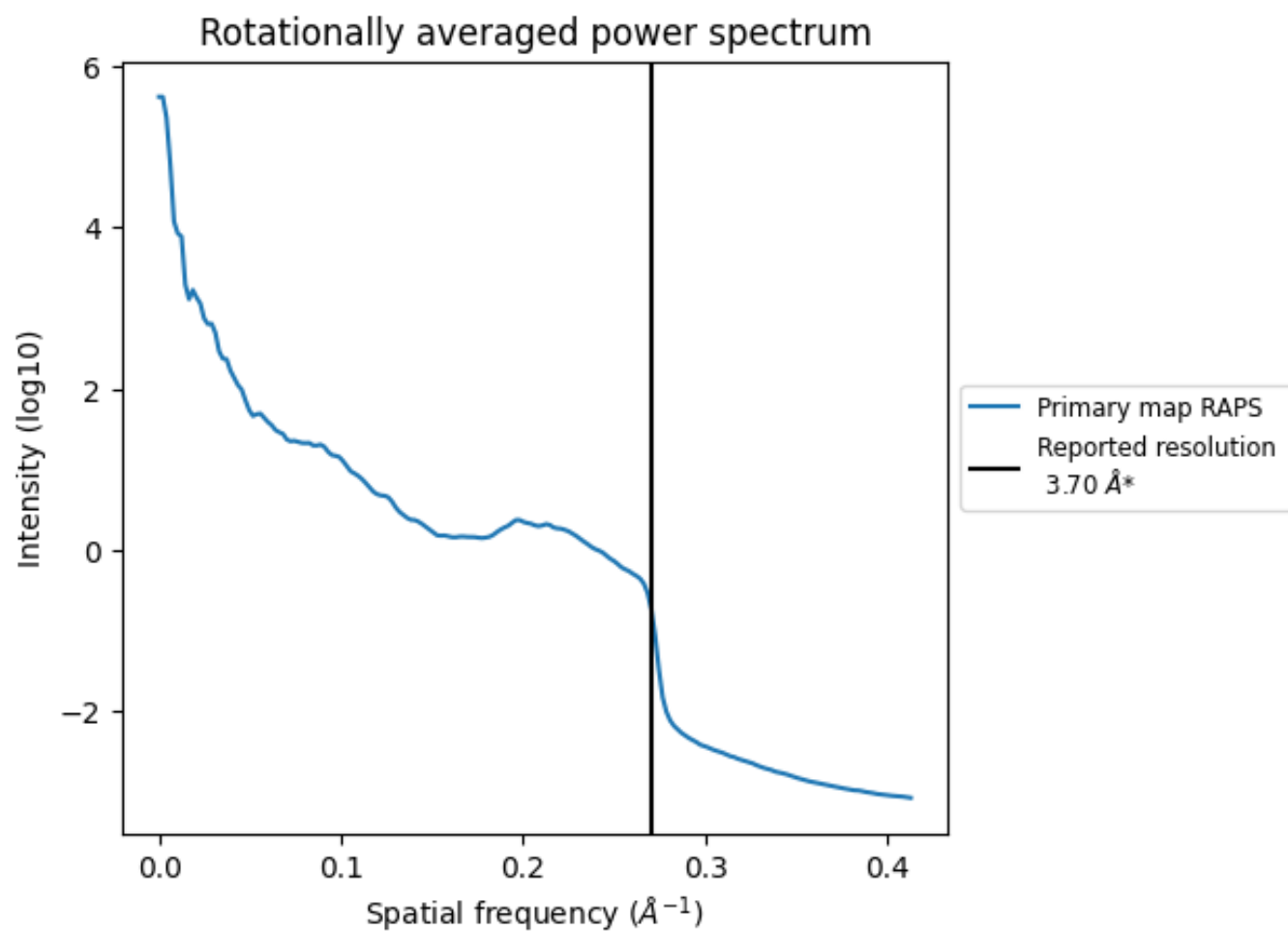
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm<sup>3</sup>; this corresponds to an approximate mass of 755 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

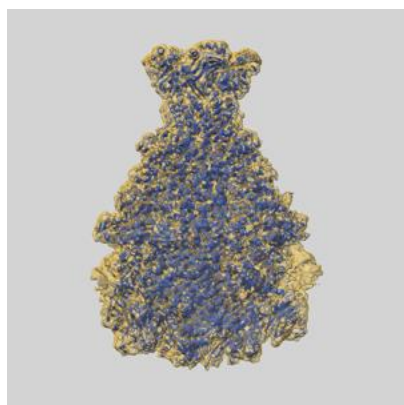
## 8 Fourier-Shell correlation ⓘ

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

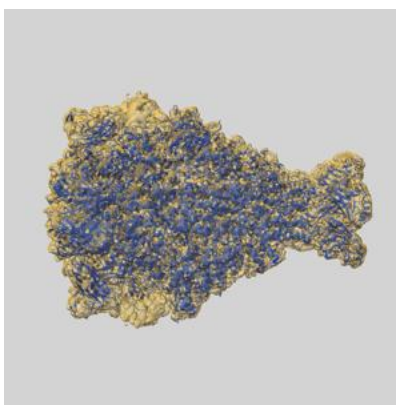
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10797 and PDB model 6YEEY. Per-residue inclusion information can be found in section [3](#) on page [5](#).

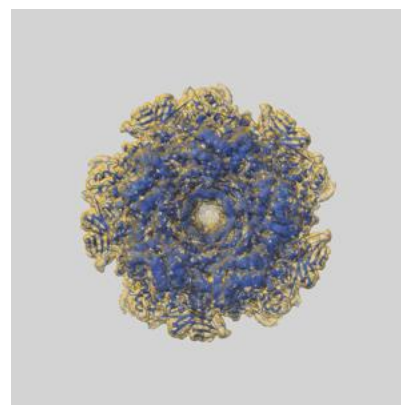
### 9.1 Map-model overlay [i](#)



X



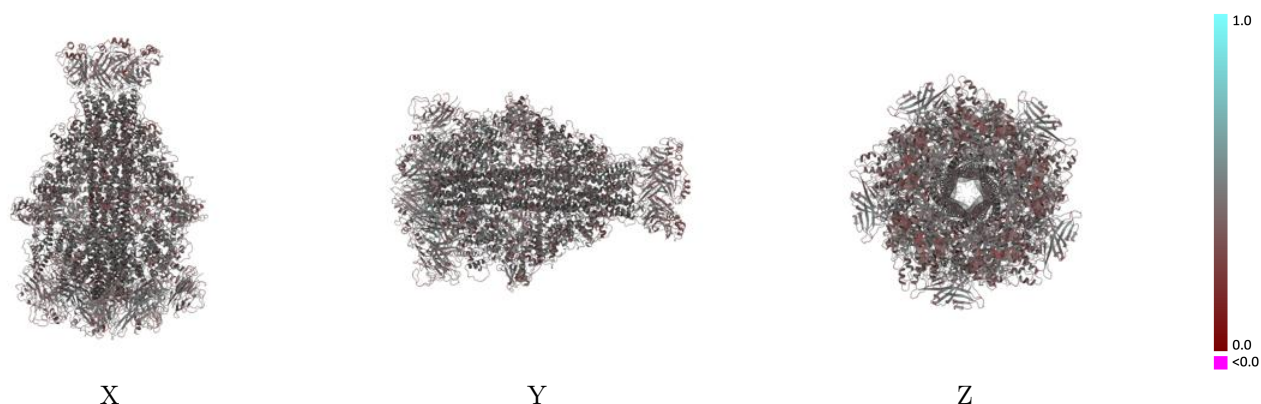
Y



Z

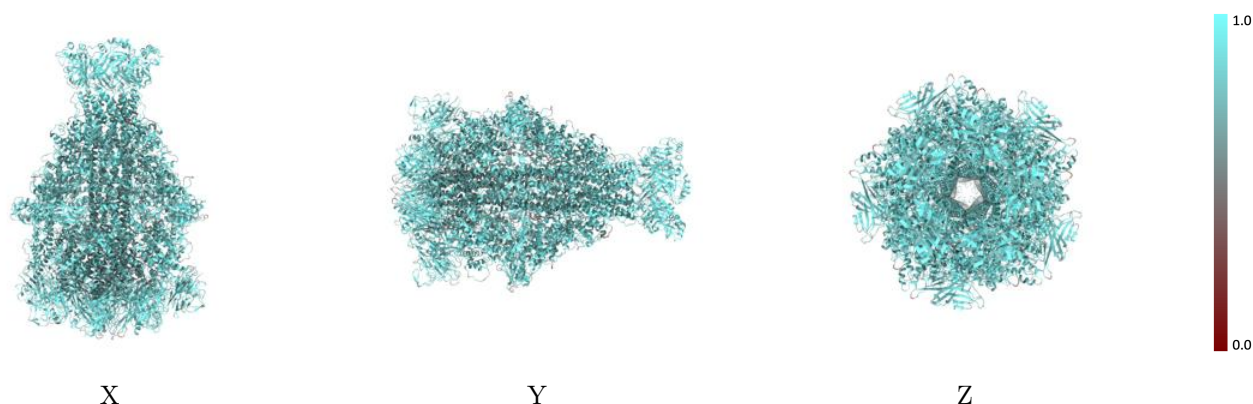
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



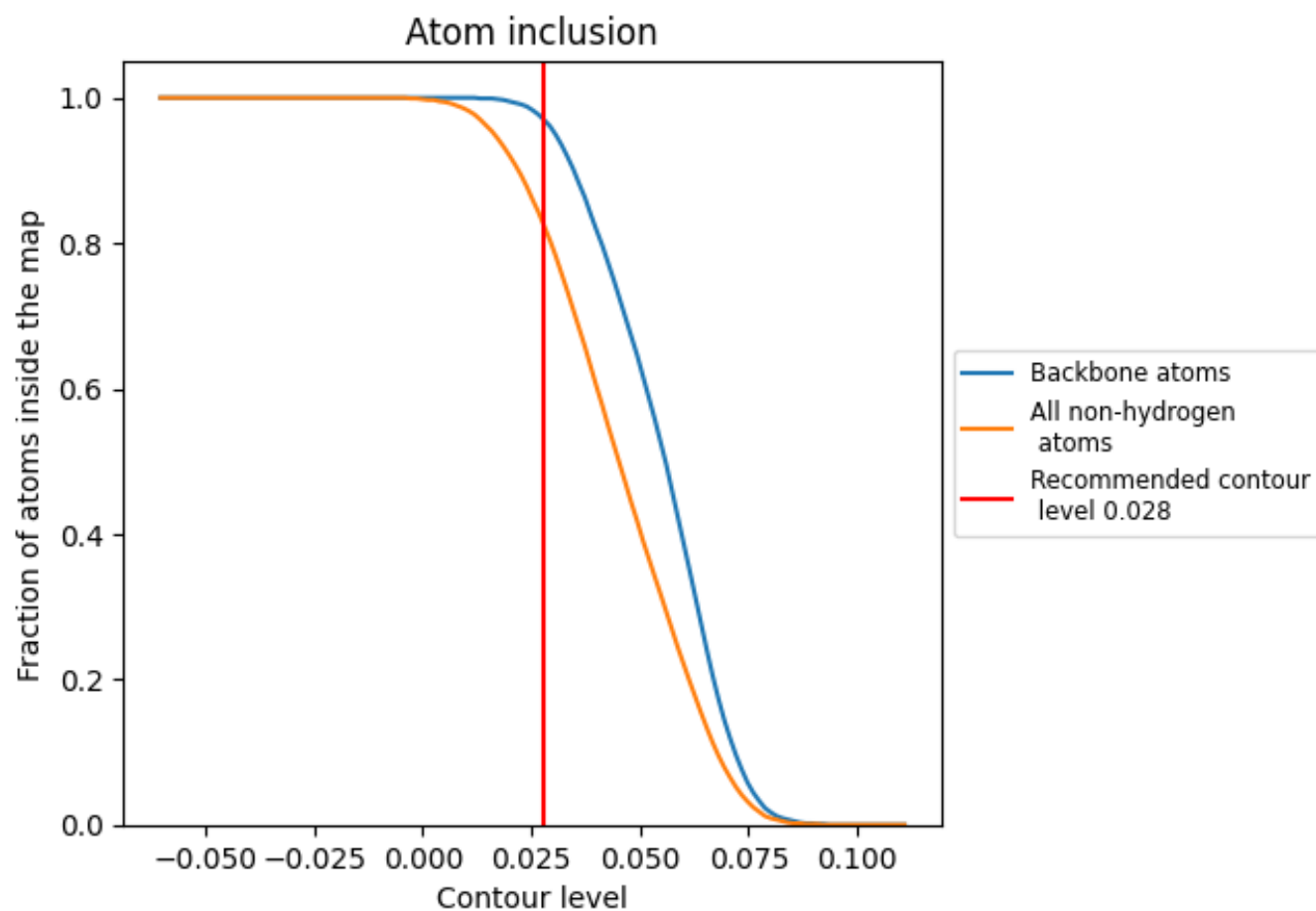
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.028) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8230 | <div></div> 0.4340 |
| A     | <div></div> 0.8250 | <div></div> 0.4360 |
| B     | <div></div> 0.8240 | <div></div> 0.4360 |
| C     | <div></div> 0.8150 | <div></div> 0.4230 |
| D     | <div></div> 0.8240 | <div></div> 0.4370 |
| E     | <div></div> 0.8260 | <div></div> 0.4360 |

