



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:57 PM JST

PDB ID : 5X9Z  
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain  
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.  
Deposited on : 2017-03-10  
Resolution : 7.31 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

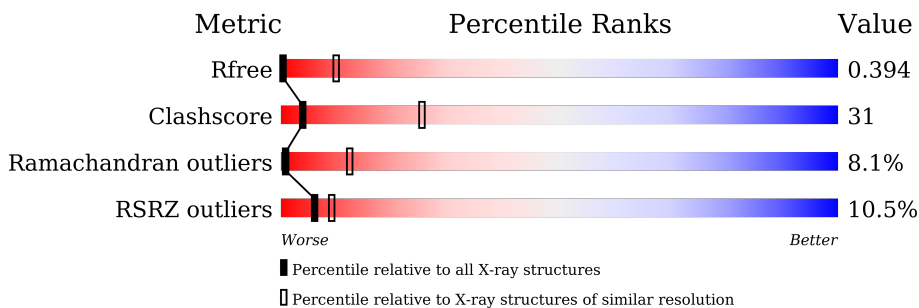
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 7.31 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1004 (10.00-3.90)                                     |
| Clashscore            | 141614                      | 1069 (10.00-3.90)                                     |
| Ramachandran outliers | 138981                      | 1002 (10.00-3.90)                                     |
| RSRZ outliers         | 127900                      | 1004 (9.50-3.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 2217   |  |
| 1   | B     | 2217   |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16948 atoms, of which 0 are hydrogens and 0 are deuteriums.

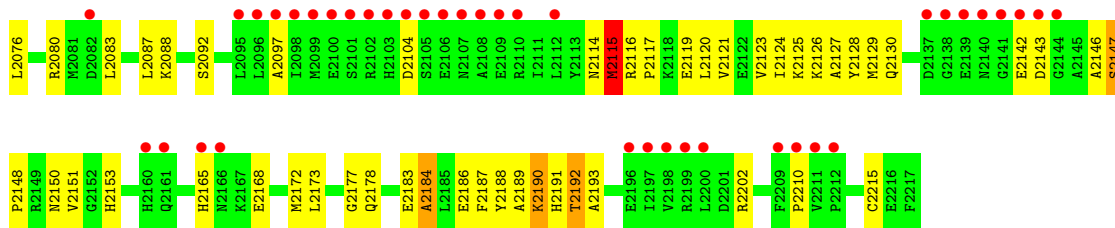
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

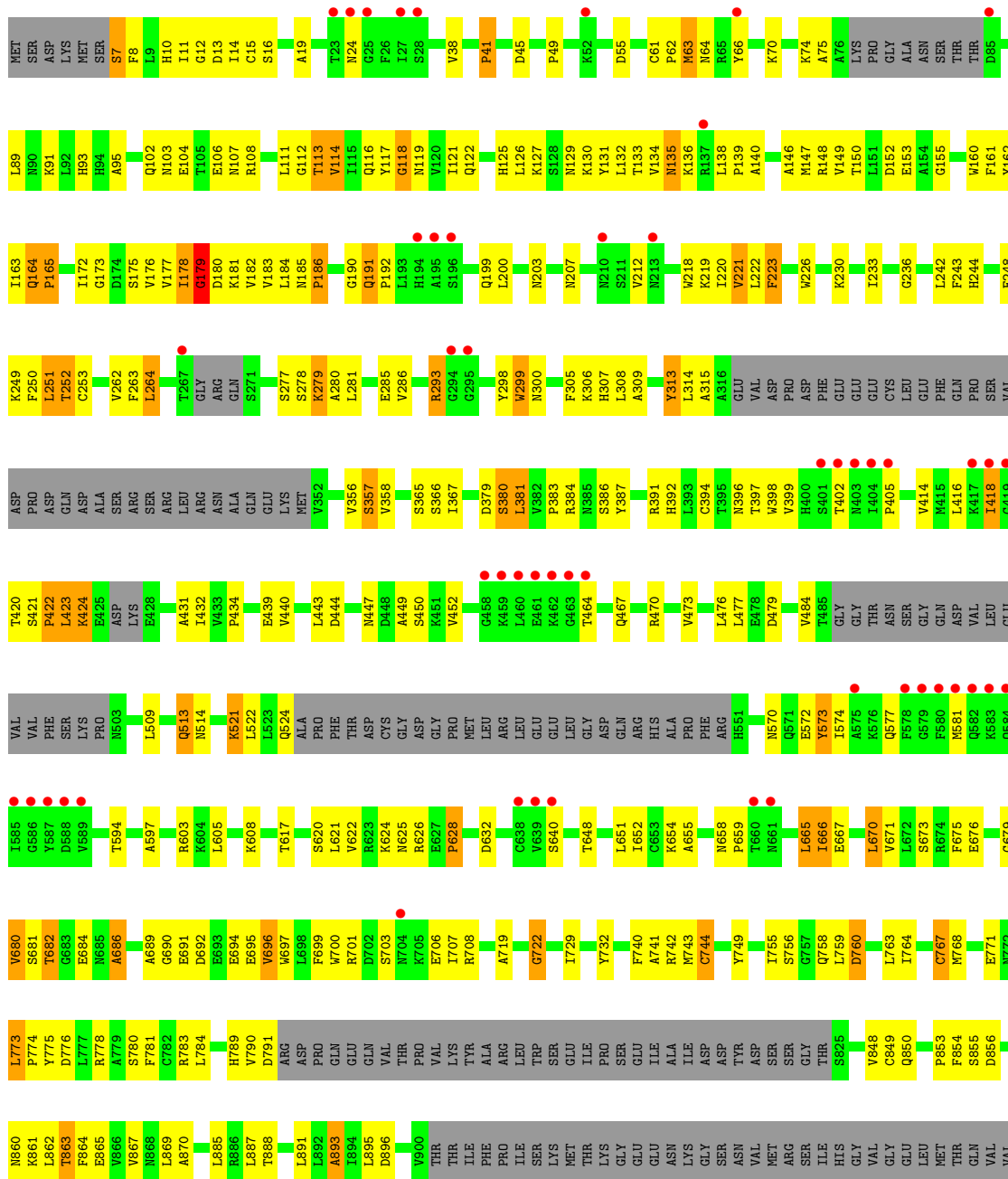
| Mol | Chain | Residues | Atoms |      |      |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|---------|-------|
|     |       |          | Total | C    | N    | O    |         |         |       |
| 1   | A     | 1710     | 8479  | 5059 | 1710 | 1710 | 0       | 0       | 0     |
| 1   | B     | 1708     | 8469  | 5053 | 1708 | 1708 | 0       | 0       | 0     |

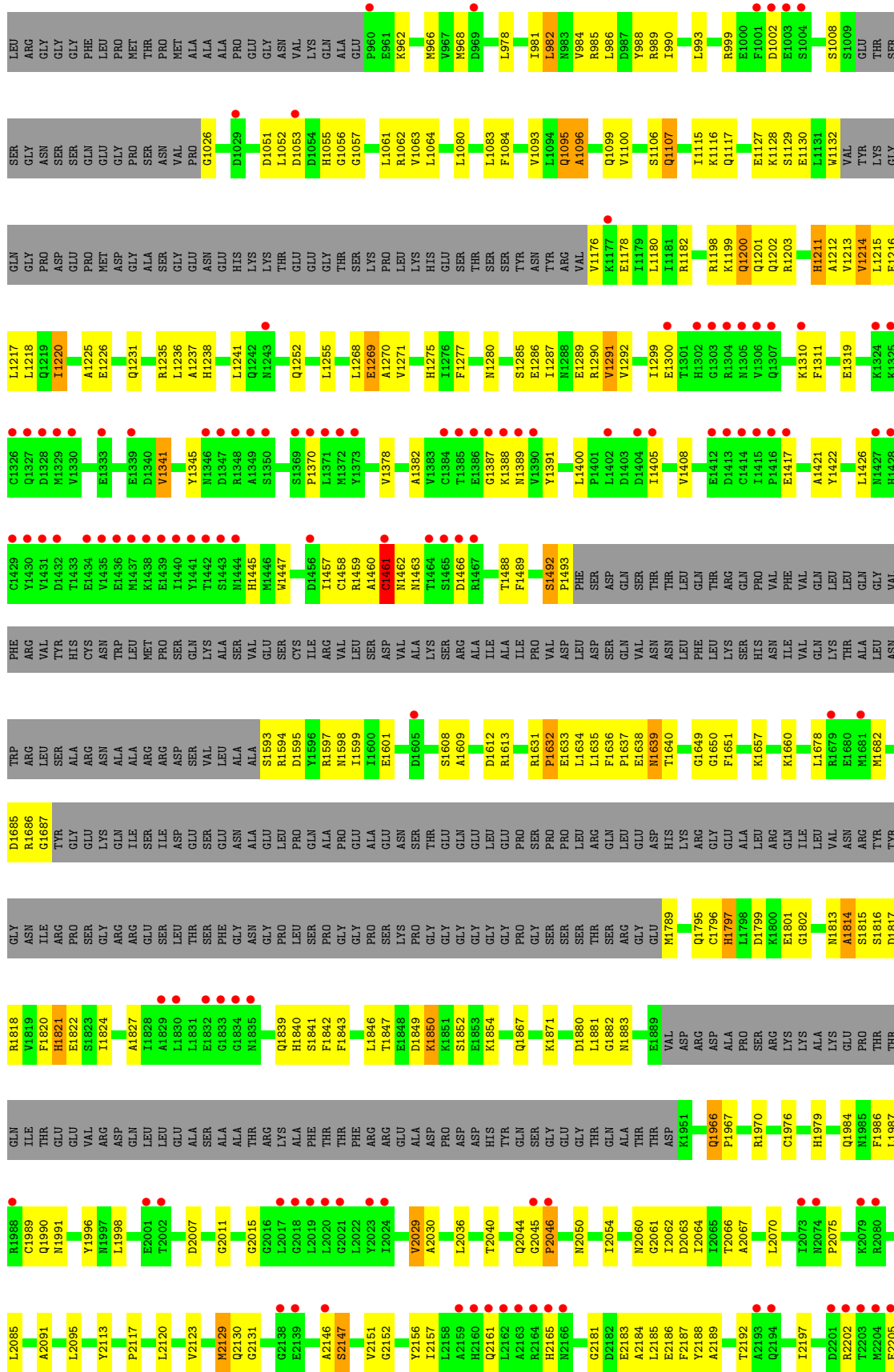


|      |     |       |       |       |       |       |       |     |     |       |     |     |       |
|------|-----|-------|-------|-------|-------|-------|-------|-----|-----|-------|-----|-----|-------|
| A893 | THR | GLY   | E1034 | GLY   | V1214 | K1310 | L1399 | GLN | GLN | R1886 | ASN | LEU | Q1990 |
| I894 | THR | ASN   | E1035 | ASN   | L1215 | K1317 | L1400 | VAL | VAL | G1887 | ILE | LEU | N1991 |
| L896 | THR | VAL   | Q1036 | VAL   | P1221 | A1318 | C1414 | ASN | ASN | TYR   | ARG | GLU | N1992 |
| C897 | THR | LYS   | I1040 | LYS   | P1224 | E1319 | L1415 | LEU | LEU | GLY   | PRO | ALA | K1993 |
| V898 | THR | ALA   | G1043 | ALA   | K1224 | P1416 | E1417 | PHE | PHE | LYS   | GLY | ALA | L2003 |
| H899 | THR | GLU   | T1048 | GLU   | M1230 | I1323 | V1418 | LEU | LEU | ILE   | ARG | THR | D2007 |
| Y900 | THR | P960  | T1049 | P960  | Q1231 | M1329 | K1419 | SER | SER | SER   | GLU | ARG | C2008 |
|      | THR | K973  | L1050 | K973  | R1235 | A1332 | I1420 | HIS | HIS | ILE   | LEU | LEU | I2009 |
|      | ILE | I974  | D1053 | I974  | H1238 | E1333 | A1421 | VAL | VAL | GLU   | THR | PHE | C2010 |
|      | PHE | I975  | D1054 | I975  | E1239 | L1334 | M1424 | ILE | ILE | GLU   | THR | THR | G2011 |
|      | PRO | E976  | H1055 | E976  | F1240 | V1335 | F1425 | VAL | VAL | SER   | PHE | THR | S2012 |
|      | ILE | I977  | L1061 | I977  | L1241 | V1341 | T1433 | GLN | GLN | ASN   | GLY | PHE | T2013 |
|      | SER | L978  | M1243 | L978  | Q1242 | F1344 | Y1435 | LEU | LEU | ASN   | ALA | ARG | G2016 |
|      | LYS | Q979  | L1062 | Q979  | F1244 | Y1345 | E1436 | GLY | GLY | ALA   | ALA | ARG | L2017 |
|      | LYS | I981  | H1066 | I981  | C1245 | M1346 | M1437 | ASN | ASN | PRO   | THR | LEU | G2018 |
|      | GLY | L982  | R1085 | L982  | M1251 | D1347 | K1438 | TRP | TRP | ALA   | GLY | LEU | L2019 |
|      | LYS | M983  | R985  | M983  | Q1252 | R1348 | I1439 | ARG | ARG | ALA   | PRO | ALA | L2020 |
|      | GLY | V984  | L986  | V984  | L1255 | A1349 | I1440 | LEU | LEU | ALA   | GLY | GLY | G2021 |
|      | GLU | R985  | F1087 | R985  | H1256 | Y1441 | Y1441 | VAL | VAL | ALA   | PRO | GLY | L2022 |
|      | GLU | L986  | S1088 | L986  | L1255 | Q1352 | E1451 | HIS | HIS | ALA   | ALA | ALA | Y2023 |
|      | ASN | D987  | Q1089 | D987  | H1256 | S1360 | L1452 | ASN | ASN | ASN   | LYS | THR | I2024 |
|      | LYS | Y988  | Q1090 | Y988  | M1264 | D1366 | F1453 | TRP | TRP | ASN   | PRO | LYS | N2025 |
|      | GLY | R989  | A1096 | R989  | M1267 | E1367 | F1454 | ALA | ALA | THR   | PRO | GLY | E2026 |
|      | SER | I990  | F1000 | I990  | I1267 | L1455 | L1455 | LEU | LEU | THR   | GLY | GLY | K2027 |
|      | ASN | Q1007 | F1001 | Q1007 | A1270 | M1368 | L1457 | ALA | ALA | GLU   | GLY | GLY | N1883 |
|      | VAL | S1008 | Q1101 | S1008 | V1271 | S1369 | C1458 | VAL | VAL | LEU   | LEU | GLY | K1884 |
|      | GLY | S1009 | D1108 | S1009 | T1272 | P1370 | R1459 | ALA | ALA | PRO   | PRO | GLY | K1885 |
|      | LEU | THR   | D1108 | THR   | H1275 | L1374 | A1460 | SER | SER | VAL   | VAL | GLY | K1886 |
|      | LEU | THR   | M1111 | THR   | I1276 | I1375 | C1461 | GLU | GLU | ALA   | ALA | GLY | L1872 |
|      | MET | THR   | Y1115 | THR   | F1277 | H1376 | M1463 | SER | SER | S1593 | ALA | GLY | T1873 |
|      | GLN | GLN   | K1116 | GLN   | M1278 | L1377 | T1464 | CYS | CYS | D1605 | ALA | GLY | G1887 |
|      | VAL | VAL   | Q1117 | VAL   | N1280 | V1378 | T1466 | ILE | ILE | A1609 | GLY | GLY | E1888 |
|      | VAL | GLY   | D1118 | VAL   | M1283 | E1379 | R1467 | ARG | ARG | H1630 | LEU | GLY | E1889 |
|      | LEU | ASN   | L1119 | LEU   | C1283 | L1380 | K1468 | VAL | VAL | R1631 | ASP | GLY | V1876 |
|      | ARG | SER   | D1120 | ARG   | S1285 | L1381 | E1472 | ASP | ASP | H1636 | LYS | GLY | L1881 |
|      | GLY | SER   | Q1121 | GLY   | M1288 | A1382 | S1472 | VAL | VAL | F1637 | ARG | GLY | G1882 |
|      | GLY | GLY   | L1122 | GLY   | E1288 | C1384 | K1476 | VAL | VAL | P1637 | GLY | THR | G1883 |
|      | PHE | GLY   | I1125 | PHE   | E1289 | T1385 | Y1477 | ALA | ALA | E1638 | ALA | THR | K1884 |
|      | LEU | PRO   | V1126 | LEU   | R1290 | E1386 | E1480 | SER | SER | M1639 | GLY | GLY | K1885 |
|      | PRO | SER   | Q1200 | PRO   | V1291 | G1387 | E1480 | ARG | ARG | T1640 | LEU | GLY | K1886 |
|      | MET | ASN   | Q1201 | MET   | H1294 | K1388 | T1488 | ALA | ALA | D1641 | ARG | THR | D1887 |
|      | THR | ASN   | Q1202 | THR   | F1295 | M1389 | F1489 | ILE | ILE | A1642 | GLN | THR | E1888 |
|      | PRO | VAL   | M1207 | PRO   | V1296 | T1392 | F1489 | ALA | ALA | S1648 | LEU | THR | E1889 |
|      | ALA | PRO   | M1208 | ALA   | H1297 | E1393 | S1491 | ILE | ILE | V1648 | LEU | THR | K1951 |
|      | ALA | ALA   | G1209 | ALA   | C1298 | I1394 | S1492 | VAL | VAL | E1680 | VAL | THR | K1952 |
|      | ALA | LYS   | A1210 | ALA   | I1299 | K1395 | F1493 | ASP | ASP | M1681 | GLY | VAL | K1953 |
|      | PRO | GLN   | H1211 | PRO   | T1301 | C1396 | PHE   | LEU | LEU | M1682 | ARG | ARG | D1954 |
|      | GLU | GLN   | V1213 | GLU   | S1398 | S1398 | ASP   | SER | SER | D1685 | TYR | GLY | D1955 |



● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1





|       |   |
|-------|---|
| Q2206 | • |
| L2207 | • |
| V2208 |   |
| F2209 |   |
| P2210 |   |
| V2211 |   |
| P2212 |   |
| C2215 | • |
| E2216 | • |
| F2217 | • |



## 4 Data and refinement statistics i

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 212.50Å 221.73Å 318.45Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.15 – 7.31<br>49.15 – 7.31                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (49.15-7.31)<br>88.5 (49.15-7.31)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.20  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.77 (at 7.37Å)   | Xtrriage         |
| Refinement program  | PHENIX (1.10.1_2155: ???)                                   | Depositor        |
| R, $R_{free}$   | 0.317 , 0.394<br>0.316 , 0.394                              | Depositor<br>DCC |
| $R_{free}$ test set   | 536 reflections (5.02%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 209.8   | Xtrriage         |
| Anisotropy  | 0.044   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 335.1  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.10$ | Xtrriage         |
| Estimated twinning fraction   | 0.219 for -k,-h,-l  | Xtrriage         |
| $F_o, F_c$ correlation  | 0.64  | EDS              |
| Total number of atoms   | 16948   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 170.0   | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.48         | 1/8465 (0.0%)  | 0.72        | 6/11786 (0.1%) |
| 1   | B     | 0.49         | 1/8455 (0.0%)  | 0.72        | 1/11772 (0.0%) |
| All | All   | 0.48         | 2/16920 (0.0%) | 0.72        | 7/23558 (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                   | 25                  |
| 1   | B     | 0                   | 22                  |
| All | All   | 0                   | 47                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | B     | 178  | ILE  | C-O   | 7.16 | 1.36        | 1.23     |
| 1   | A     | 1048 | THR  | C-N   | 5.11 | 1.44        | 1.34     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 999 | ARG  | N-CA-C | -7.07 | 91.92       | 111.00   |
| 1   | A     | 177 | VAL  | N-CA-C | 6.68  | 129.03      | 111.00   |
| 1   | B     | 743 | MET  | C-N-CA | 5.66  | 135.84      | 121.70   |
| 1   | A     | 176 | VAL  | C-N-CA | 5.44  | 135.31      | 121.70   |
| 1   | A     | 554 | ARG  | CA-C-O | -5.28 | 109.02      | 120.10   |
| 1   | A     | 553 | CYS  | C-N-CA | -5.22 | 108.65      | 121.70   |
| 1   | A     | 998 | LYS  | C-N-CA | 5.01  | 134.23      | 121.70   |

There are no chirality outliers.

All (47) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1054 | ASP  | Peptide |
| 1   | A     | 1055 | HIS  | Peptide |
| 1   | A     | 118  | GLY  | Peptide |
| 1   | A     | 1202 | GLN  | Peptide |
| 1   | A     | 1375 | ILE  | Peptide |
| 1   | A     | 1380 | LEU  | Peptide |
| 1   | A     | 1383 | VAL  | Peptide |
| 1   | A     | 1461 | CYS  | Peptide |
| 1   | A     | 15   | CYS  | Peptide |
| 1   | A     | 1639 | ASN  | Peptide |
| 1   | A     | 176  | VAL  | Peptide |
| 1   | A     | 1815 | SER  | Peptide |
| 1   | A     | 2009 | ILE  | Peptide |
| 1   | A     | 2016 | GLY  | Peptide |
| 1   | A     | 2071 | ASN  | Peptide |
| 1   | A     | 2115 | MET  | Peptide |
| 1   | A     | 2142 | GLU  | Peptide |
| 1   | A     | 2184 | ALA  | Peptide |
| 1   | A     | 2192 | THR  | Peptide |
| 1   | A     | 254  | ASP  | Peptide |
| 1   | A     | 260  | GLN  | Peptide |
| 1   | A     | 406  | ILE  | Peptide |
| 1   | A     | 73   | TRP  | Peptide |
| 1   | A     | 8    | PHE  | Peptide |
| 1   | A     | 989  | ARG  | Peptide |
| 1   | B     | 1269 | GLU  | Peptide |
| 1   | B     | 1287 | ILE  | Peptide |
| 1   | B     | 1310 | LYS  | Peptide |
| 1   | B     | 1461 | CYS  | Peptide |
| 1   | B     | 1639 | ASN  | Peptide |
| 1   | B     | 176  | VAL  | Peptide |
| 1   | B     | 179  | GLY  | Peptide |
| 1   | B     | 1816 | SER  | Peptide |
| 1   | B     | 1883 | ASN  | Peptide |
| 1   | B     | 190  | GLY  | Peptide |
| 1   | B     | 191  | GLN  | Peptide |
| 1   | B     | 251  | LEU  | Peptide |
| 1   | B     | 252  | THR  | Peptide |
| 1   | B     | 299  | TRP  | Peptide |
| 1   | B     | 306  | LYS  | Peptide |
| 1   | B     | 424  | LYS  | Peptide |
| 1   | B     | 464  | THR  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 670 | LEU  | Peptide |
| 1   | B     | 7   | SER  | Peptide |
| 1   | B     | 744 | CYS  | Peptide |
| 1   | B     | 749 | TYR  | Peptide |
| 1   | B     | 759 | LEU  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 8479  | 0        | 3697     | 386     | 0            |
| 1   | B     | 8469  | 0        | 3697     | 360     | 0            |
| All | All   | 16948 | 0        | 7394     | 745     | 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 31.

All (745) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1208:MET:O  | 1:A:1212:ALA:HB3 | 1.49                     | 1.10              |
| 1:A:405:PRO:HA  | 1:A:416:LEU:HA   | 1.39                     | 1.04              |
| 1:A:162:TYR:O   | 1:A:184:LEU:C    | 1.97                     | 1.02              |
| 1:B:1682:MET:O  | 1:B:1686:ARG:N   | 1.93                     | 1.01              |
| 1:A:1472:SER:O  | 1:A:1476:LYS:CB  | 2.10                     | 1.00              |
| 1:A:866:VAL:O   | 1:A:870:ALA:HB2  | 1.62                     | 1.00              |
| 1:A:1371:LEU:O  | 1:A:1375:ILE:N   | 1.94                     | 1.00              |
| 1:A:1605:ASP:O  | 1:A:1609:ALA:HB2 | 1.62                     | 1.00              |
| 1:B:8:PHE:HA    | 1:B:177:VAL:HA   | 1.42                     | 0.99              |
| 1:A:1208:MET:O  | 1:A:1212:ALA:CB  | 2.10                     | 0.98              |
| 1:A:2020:LEU:O  | 1:A:2024:ILE:N   | 1.96                     | 0.98              |
| 1:A:162:TYR:O   | 1:A:184:LEU:CA   | 2.11                     | 0.98              |
| 1:A:314:LEU:HA  | 1:A:357:SER:HA   | 1.47                     | 0.95              |
| 1:A:1125:ILE:O  | 1:A:1129:SER:CB  | 2.14                     | 0.94              |
| 1:A:581:MET:O   | 1:A:585:ILE:N    | 2.00                     | 0.94              |
| 1:A:1798:LEU:HA | 1:A:1802:GLY:HA3 | 1.50                     | 0.94              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:242:LEU:O   | 1:B:251:LEU:N    | 2.00                     | 0.94              |
| 1:A:243:PHE:HA  | 1:A:250:PHE:HA   | 1.50                     | 0.94              |
| 1:A:521:LYS:O   | 1:A:523:LEU:N    | 2.01                     | 0.93              |
| 1:A:1118:ASP:O  | 1:A:1122:LEU:N   | 2.01                     | 0.93              |
| 1:B:2040:THR:O  | 1:B:2044:GLN:CB  | 2.17                     | 0.93              |
| 1:A:1231:GLN:O  | 1:A:1235:ARG:CB  | 2.17                     | 0.92              |
| 1:A:1379:GLU:HA | 1:A:1382:ALA:HB3 | 1.47                     | 0.92              |
| 1:B:1417:GLU:O  | 1:B:1421:ALA:N   | 2.02                     | 0.91              |
| 1:A:708:ARG:O   | 1:A:712:VAL:N    | 2.03                     | 0.91              |
| 1:A:1210:ALA:O  | 1:A:1214:VAL:CB  | 2.19                     | 0.91              |
| 1:B:314:LEU:HA  | 1:B:357:SER:HA   | 1.52                     | 0.91              |
| 1:A:117:TYR:O   | 1:A:173:GLY:N    | 2.02                     | 0.91              |
| 1:A:458:GLY:O   | 1:A:462:LYS:CB   | 2.18                     | 0.91              |
| 1:A:981:ILE:O   | 1:A:985:ARG:CB   | 2.19                     | 0.90              |
| 1:A:2125:LYS:O  | 1:A:2129:MET:CB  | 2.20                     | 0.90              |
| 1:B:1095:GLN:O  | 1:B:1099:GLN:N   | 2.05                     | 0.90              |
| 1:B:467:GLN:O   | 1:B:470:ARG:N    | 2.04                     | 0.90              |
| 1:B:7:SER:O     | 1:B:178:ILE:N    | 2.04                     | 0.89              |
| 1:B:1214:VAL:O  | 1:B:1218:LEU:N   | 2.06                     | 0.89              |
| 1:A:1378:VAL:O  | 1:A:1382:ALA:HB2 | 1.73                     | 0.88              |
| 1:B:315:ALA:HA  | 1:B:366:SER:HA   | 1.55                     | 0.88              |
| 1:A:2083:LEU:O  | 1:A:2087:LEU:CB  | 2.22                     | 0.88              |
| 1:A:856:ASP:O   | 1:A:860:ASN:CB   | 2.22                     | 0.88              |
| 1:B:117:TYR:C   | 1:B:173:GLY:H    | 1.77                     | 0.88              |
| 1:A:1864:LYS:O  | 1:A:1868:GLN:N   | 2.07                     | 0.87              |
| 1:A:2189:ALA:O  | 1:A:2193:ALA:N   | 2.06                     | 0.87              |
| 1:A:1380:LEU:O  | 1:A:1384:CYS:CB  | 2.23                     | 0.86              |
| 1:B:981:ILE:O   | 1:B:985:ARG:CB   | 2.23                     | 0.86              |
| 1:A:2124:ILE:O  | 1:A:2128:TYR:CB  | 2.24                     | 0.86              |
| 1:A:19:ALA:N    | 1:A:25:GLY:O     | 2.09                     | 0.85              |
| 1:B:696:VAL:O   | 1:B:700:TRP:N    | 2.10                     | 0.85              |
| 1:B:2183:GLU:O  | 1:B:2187:PHE:CB  | 2.24                     | 0.85              |
| 1:B:686:ALA:O   | 1:B:689:ALA:HB3  | 1.77                     | 0.84              |
| 1:A:8:PHE:H     | 1:A:177:VAL:C    | 1.80                     | 0.84              |
| 1:B:19:ALA:HA   | 1:B:218:TRP:HA   | 1.58                     | 0.84              |
| 1:A:2036:LEU:O  | 1:A:2040:THR:CB  | 2.25                     | 0.84              |
| 1:A:162:TYR:O   | 1:A:184:LEU:HA   | 1.74                     | 0.84              |
| 1:B:244:HIS:O   | 1:B:248:GLU:N    | 2.10                     | 0.83              |
| 1:B:140:ALA:N   | 1:B:146:ALA:O    | 2.11                     | 0.83              |
| 1:B:130:LYS:HA  | 1:B:153:GLU:HA   | 1.58                     | 0.83              |
| 1:B:1212:ALA:O  | 1:B:1216:GLU:CB  | 2.26                     | 0.83              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1421:ALA:O  | 1:A:1425:PHE:CB  | 2.26                     | 0.83              |
| 1:B:1594:ARG:O  | 1:B:1598:ASN:CB  | 2.27                     | 0.83              |
| 1:B:391:ARG:HA  | 1:B:398:TRP:HA   | 1.59                     | 0.83              |
| 1:A:125:HIS:O   | 1:A:129:ASN:N    | 2.11                     | 0.83              |
| 1:A:1861:ASP:O  | 1:A:1865:VAL:CB  | 2.26                     | 0.83              |
| 1:B:103:ASN:O   | 1:B:107:ASN:CB   | 2.26                     | 0.83              |
| 1:B:865:GLU:O   | 1:B:869:LEU:CB   | 2.27                     | 0.82              |
| 1:A:1605:ASP:O  | 1:A:1609:ALA:CB  | 2.27                     | 0.82              |
| 1:A:354:SER:HA  | 1:A:419:GLY:HA3  | 1.61                     | 0.82              |
| 1:B:1096:ALA:O  | 1:B:1100:VAL:N   | 2.13                     | 0.82              |
| 1:A:2189:ALA:O  | 1:A:2192:THR:N   | 2.13                     | 0.82              |
| 1:A:621:LEU:O   | 1:A:625:ASN:N    | 2.10                     | 0.81              |
| 1:A:1849:ASP:O  | 1:A:1853:GLU:N   | 2.12                     | 0.81              |
| 1:A:298:TYR:HA  | 1:A:381:LEU:HA   | 1.61                     | 0.81              |
| 1:A:480:LEU:O   | 1:A:483:PHE:N    | 2.14                     | 0.81              |
| 1:B:392:HIS:N   | 1:B:397:THR:O    | 2.12                     | 0.81              |
| 1:A:975:ILE:O   | 1:A:979:GLN:CB   | 2.28                     | 0.81              |
| 1:A:1417:GLU:O  | 1:A:1421:ALA:N   | 2.10                     | 0.81              |
| 1:A:162:TYR:CB  | 1:A:185:ASN:O    | 2.29                     | 0.81              |
| 1:A:2188:TYR:O  | 1:A:2192:THR:CB  | 2.29                     | 0.81              |
| 1:B:392:HIS:O   | 1:B:396:ASN:N    | 2.13                     | 0.81              |
| 1:B:764:ILE:O   | 1:B:768:MET:CB   | 2.29                     | 0.81              |
| 1:A:1224:LYS:HA | 1:A:1270:ALA:HB3 | 1.63                     | 0.80              |
| 1:B:666:ILE:CB  | 1:B:670:LEU:H    | 1.93                     | 0.80              |
| 1:B:697:TRP:O   | 1:B:701:ARG:N    | 2.10                     | 0.80              |
| 1:A:866:VAL:O   | 1:A:870:ALA:CB   | 2.30                     | 0.80              |
| 1:B:767:CYS:O   | 1:B:771:GLU:CB   | 2.30                     | 0.80              |
| 1:A:251:LEU:HA  | 1:A:264:LEU:HA   | 1.64                     | 0.80              |
| 1:A:8:PHE:N     | 1:A:177:VAL:O    | 2.14                     | 0.79              |
| 1:B:670:LEU:HA  | 1:B:673:SER:H    | 1.47                     | 0.79              |
| 1:B:605:LEU:O   | 1:B:608:LYS:N    | 2.16                     | 0.79              |
| 1:B:163:ILE:HA  | 1:B:184:LEU:HA   | 1.63                     | 0.78              |
| 1:B:398:TRP:H   | 1:B:422:PRO:HA   | 1.47                     | 0.78              |
| 1:A:118:GLY:N   | 1:A:163:ILE:O    | 2.13                     | 0.78              |
| 1:A:1381:LEU:O  | 1:A:1385:THR:CB  | 2.32                     | 0.78              |
| 1:A:761:VAL:O   | 1:A:764:ILE:N    | 2.17                     | 0.78              |
| 1:A:1992:ASN:O  | 1:A:1994:THR:N   | 2.15                     | 0.78              |
| 1:A:1252:GLN:O  | 1:A:1256:HIS:CB  | 2.31                     | 0.78              |
| 1:B:61:CYS:CB   | 1:B:122:GLN:O    | 2.32                     | 0.78              |
| 1:B:162:TYR:CB  | 1:B:185:ASN:O    | 2.31                     | 0.78              |
| 1:A:252:THR:O   | 1:A:263:PHE:O    | 2.01                     | 0.77              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:A:1862:ARG:O | 1:A:1866:ALA:CB  | 2.33                     | 0.77              |
| 1:B:1813:ASN:O | 1:B:1815:SER:N   | 2.17                     | 0.77              |
| 1:A:1792:ALA:O | 1:A:1796:CYS:CB  | 2.31                     | 0.77              |
| 1:B:1632:PRO:O | 1:B:1635:LEU:N   | 2.17                     | 0.77              |
| 1:A:853:PRO:O  | 1:A:855:SER:N    | 2.17                     | 0.77              |
| 1:A:1862:ARG:O | 1:A:1866:ALA:HB3 | 1.85                     | 0.77              |
| 1:A:1126:VAL:O | 1:A:1130:GLU:CB  | 2.33                     | 0.76              |
| 1:B:15:CYS:HA  | 1:B:222:LEU:HA   | 1.67                     | 0.76              |
| 1:B:313:TYR:CB | 1:B:358:VAL:O    | 2.34                     | 0.76              |
| 1:A:666:ILE:CB | 1:A:670:LEU:H    | 1.98                     | 0.76              |
| 1:A:16:SER:O   | 1:A:221:VAL:N    | 2.19                     | 0.76              |
| 1:A:2035:THR:O | 1:A:2039:LEU:CB  | 2.34                     | 0.76              |
| 1:B:162:TYR:O  | 1:B:184:LEU:C    | 2.24                     | 0.76              |
| 1:A:194:HIS:H  | 1:A:211:SER:HA   | 1.51                     | 0.76              |
| 1:A:2116:ARG:O | 1:A:2120:LEU:N   | 2.18                     | 0.75              |
| 1:A:392:HIS:O  | 1:A:396:ASN:N    | 2.20                     | 0.75              |
| 1:A:1377:LEU:O | 1:A:1381:LEU:CB  | 2.34                     | 0.75              |
| 1:B:1795:GLN:O | 1:B:1799:ASP:N   | 2.20                     | 0.75              |
| 1:A:1795:GLN:O | 1:A:1799:ASP:N   | 2.19                     | 0.74              |
| 1:B:161:PHE:HA | 1:B:186:PRO:HA   | 1.68                     | 0.74              |
| 1:B:891:LEU:O  | 1:B:895:LEU:CB   | 2.35                     | 0.74              |
| 1:A:767:CYS:O  | 1:A:771:GLU:CB   | 2.35                     | 0.74              |
| 1:A:32:LEU:H   | 1:A:448:ASP:CB   | 2.01                     | 0.74              |
| 1:B:252:THR:O  | 1:B:262:VAL:HA   | 1.88                     | 0.74              |
| 1:A:254:ASP:O  | 1:A:261:HIS:CB   | 2.36                     | 0.74              |
| 1:B:185:ASN:HA | 1:B:192:PRO:HA   | 1.68                     | 0.74              |
| 1:B:15:CYS:HA  | 1:B:223:PHE:H    | 1.53                     | 0.73              |
| 1:B:252:THR:O  | 1:B:262:VAL:CA   | 2.36                     | 0.73              |
| 1:A:1848:GLU:O | 1:A:1850:LYS:N   | 2.18                     | 0.73              |
| 1:B:305:PHE:O  | 1:B:314:LEU:N    | 2.20                     | 0.73              |
| 1:A:2088:LYS:O | 1:A:2092:SER:N   | 2.22                     | 0.72              |
| 1:A:365:SER:HA | 1:A:394:CYS:CB   | 2.19                     | 0.72              |
| 1:A:2147:SER:O | 1:A:2151:VAL:CB  | 2.38                     | 0.72              |
| 1:B:162:TYR:O  | 1:B:184:LEU:HA   | 1.89                     | 0.72              |
| 1:A:212:VAL:O  | 1:A:214:CYS:N    | 2.21                     | 0.72              |
| 1:A:255:GLU:HA | 1:A:260:GLN:HA   | 1.72                     | 0.72              |
| 1:B:509:LEU:O  | 1:B:513:GLN:N    | 2.19                     | 0.72              |
| 1:B:982:LEU:O  | 1:B:986:LEU:N    | 2.23                     | 0.72              |
| 1:B:102:GLN:O  | 1:B:106:GLU:CB   | 2.37                     | 0.72              |
| 1:B:1818:ARG:O | 1:B:1821:HIS:N   | 2.22                     | 0.72              |
| 1:B:199:GLN:HA | 1:B:207:ASN:HA   | 1.71                     | 0.71              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:252:THR:HA  | 1:B:280:ALA:HA  | 1.72                     | 0.71              |
| 1:B:1052:LEU:O  | 1:B:1057:GLY:N  | 2.23                     | 0.71              |
| 1:B:315:ALA:HB3 | 1:B:356:VAL:O   | 1.89                     | 0.71              |
| 1:B:1422:TYR:O  | 1:B:1426:LEU:CB | 2.38                     | 0.71              |
| 1:A:474:THR:O   | 1:A:477:LEU:N   | 2.24                     | 0.71              |
| 1:A:15:CYS:HA   | 1:A:222:LEU:HA  | 1.72                     | 0.71              |
| 1:B:773:LEU:O   | 1:B:775:TYR:N   | 2.20                     | 0.71              |
| 1:A:741:ALA:HB2 | 1:A:876:PHE:HA  | 1.73                     | 0.71              |
| 1:A:253:CYS:C   | 1:A:261:HIS:O   | 2.29                     | 0.71              |
| 1:A:973:LYS:O   | 1:A:977:ILE:CB  | 2.39                     | 0.71              |
| 1:A:2021:GLY:O  | 1:A:2025:ASN:N  | 2.24                     | 0.71              |
| 1:A:181:LYS:HA  | 1:A:218:TRP:O   | 1.90                     | 0.70              |
| 1:B:2152:GLY:O  | 1:B:2156:TYR:CB | 2.39                     | 0.70              |
| 1:A:20:GLU:N    | 1:A:217:SER:O   | 2.22                     | 0.70              |
| 1:A:1371:LEU:O  | 1:A:1374:HIS:N  | 2.24                     | 0.70              |
| 1:A:1297:HIS:HA | 1:A:1301:THR:HA | 1.73                     | 0.70              |
| 1:A:102:GLN:O   | 1:A:106:GLU:CB  | 2.40                     | 0.70              |
| 1:A:1040:ILE:O  | 1:A:1043:GLY:N  | 2.25                     | 0.70              |
| 1:A:8:PHE:N     | 1:A:176:VAL:O   | 2.26                     | 0.69              |
| 1:B:104:GLU:O   | 1:B:108:ARG:CB  | 2.40                     | 0.69              |
| 1:B:1636:PHE:O  | 1:B:1638:GLU:N  | 2.23                     | 0.69              |
| 1:A:2189:ALA:C  | 1:A:2193:ALA:H  | 1.96                     | 0.69              |
| 1:A:253:CYS:O   | 1:A:261:HIS:O   | 2.10                     | 0.69              |
| 1:A:1178:GLU:O  | 1:A:1182:ARG:CB | 2.41                     | 0.69              |
| 1:A:1378:VAL:O  | 1:A:1382:ALA:CB | 2.40                     | 0.69              |
| 1:A:1118:ASP:O  | 1:A:1121:GLN:N  | 2.25                     | 0.69              |
| 1:A:2115:MET:O  | 1:A:2119:GLU:N  | 2.22                     | 0.69              |
| 1:A:307:HIS:O   | 1:A:311:GLY:N   | 2.26                     | 0.69              |
| 1:B:14:ILE:O    | 1:B:223:PHE:N   | 2.26                     | 0.68              |
| 1:B:55:ASP:HA   | 1:B:127:LYS:CB  | 2.23                     | 0.68              |
| 1:A:1294:HIS:O  | 1:A:1298:CYS:N  | 2.21                     | 0.68              |
| 1:B:162:TYR:O   | 1:B:184:LEU:CA  | 2.41                     | 0.68              |
| 1:B:853:PRO:O   | 1:B:855:SER:N   | 2.25                     | 0.68              |
| 1:A:874:ILE:O   | 1:A:878:PHE:N   | 2.26                     | 0.68              |
| 1:A:243:PHE:HA  | 1:A:250:PHE:CA  | 2.23                     | 0.68              |
| 1:B:1593:SER:O  | 1:B:1597:ARG:N  | 2.18                     | 0.68              |
| 1:A:2117:PRO:O  | 1:A:2121:VAL:CB | 2.41                     | 0.68              |
| 1:B:315:ALA:HB2 | 1:B:358:VAL:CB  | 2.23                     | 0.68              |
| 1:A:162:TYR:O   | 1:A:184:LEU:O   | 2.10                     | 0.67              |
| 1:B:1991:ASN:CB | 1:B:1998:LEU:HA | 2.25                     | 0.67              |
| 1:B:11:ILE:H    | 1:B:113:THR:C   | 1.98                     | 0.67              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:628:PRO:O   | 1:B:632:ASP:N    | 2.22                     | 0.67              |
| 1:B:2050:ASN:O  | 1:B:2054:ILE:CB  | 2.42                     | 0.67              |
| 1:A:390:LEU:O   | 1:A:398:TRP:HA   | 1.93                     | 0.67              |
| 1:B:398:TRP:O   | 1:B:421:SER:O    | 2.13                     | 0.67              |
| 1:B:476:LEU:O   | 1:B:479:ASP:N    | 2.28                     | 0.67              |
| 1:A:14:ILE:O    | 1:A:223:PHE:N    | 2.23                     | 0.67              |
| 1:B:8:PHE:HA    | 1:B:177:VAL:CA   | 2.22                     | 0.67              |
| 1:A:244:HIS:N   | 1:A:249:LYS:O    | 2.28                     | 0.67              |
| 1:A:255:GLU:HA  | 1:A:259:LYS:O    | 1.95                     | 0.67              |
| 1:A:769:SER:HA  | 1:A:779:ALA:HA   | 1.77                     | 0.67              |
| 1:A:1476:LYS:HA | 1:A:1884:LYS:HA  | 1.75                     | 0.66              |
| 1:A:391:ARG:HA  | 1:A:398:TRP:HA   | 1.77                     | 0.66              |
| 1:A:998:LYS:O   | 1:A:1007:GLN:HA  | 1.95                     | 0.66              |
| 1:B:421:SER:O   | 1:B:423:LEU:N    | 2.28                     | 0.66              |
| 1:B:135:ASN:CB  | 1:B:148:ARG:O    | 2.42                     | 0.66              |
| 1:B:279:LYS:HA  | 1:B:309:ALA:H    | 1.60                     | 0.66              |
| 1:A:255:GLU:CA  | 1:A:259:LYS:O    | 2.42                     | 0.66              |
| 1:B:1986:PHE:O  | 1:B:1990:GLN:N   | 2.29                     | 0.66              |
| 1:B:152:ASP:O   | 1:B:155:GLY:N    | 2.28                     | 0.66              |
| 1:B:223:PHE:HA  | 1:B:293:ARG:HA   | 1.76                     | 0.66              |
| 1:B:398:TRP:N   | 1:B:422:PRO:HA   | 2.10                     | 0.66              |
| 1:B:680:VAL:O   | 1:B:682:THR:N    | 2.28                     | 0.66              |
| 1:A:1062:ARG:O  | 1:A:1066:HIS:N   | 2.23                     | 0.66              |
| 1:A:7:SER:HA    | 1:A:177:VAL:N    | 2.11                     | 0.65              |
| 1:A:19:ALA:O    | 1:A:25:GLY:N     | 2.29                     | 0.65              |
| 1:B:1597:ARG:O  | 1:B:1601:GLU:CB  | 2.44                     | 0.65              |
| 1:A:1108:ASP:O  | 1:A:1112:TYR:N   | 2.26                     | 0.65              |
| 1:B:1225:ALA:H  | 1:B:1270:ALA:HB3 | 1.60                     | 0.65              |
| 1:A:118:GLY:H   | 1:A:163:ILE:C    | 2.00                     | 0.65              |
| 1:B:252:THR:CB  | 1:B:280:ALA:HA   | 2.27                     | 0.65              |
| 1:A:478:GLU:O   | 1:A:480:LEU:N    | 2.29                     | 0.65              |
| 1:A:179:GLY:HA2 | 1:A:220:ILE:O    | 1.96                     | 0.65              |
| 1:A:355:LEU:H   | 1:A:419:GLY:HA2  | 1.61                     | 0.64              |
| 1:B:621:LEU:O   | 1:B:625:ASN:N    | 2.30                     | 0.64              |
| 1:B:1850:LYS:O  | 1:B:1854:LYS:N   | 2.30                     | 0.64              |
| 1:A:2076:LEU:HA | 1:A:2080:ARG:CB  | 2.27                     | 0.64              |
| 1:A:61:CYS:CB   | 1:A:122:GLN:O    | 2.45                     | 0.64              |
| 1:A:32:LEU:CB   | 1:A:445:PHE:HA   | 2.28                     | 0.64              |
| 1:B:70:LYS:O    | 1:B:74:LYS:CB    | 2.46                     | 0.64              |
| 1:A:2123:VAL:O  | 1:A:2127:ALA:HB3 | 1.98                     | 0.63              |
| 1:A:100:LYS:O   | 1:A:103:ASN:N    | 2.31                     | 0.63              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:252:THR:CA  | 1:B:280:ALA:HA  | 2.27                     | 0.63              |
| 1:B:2091:ALA:O  | 1:B:2095:LEU:CB | 2.46                     | 0.63              |
| 1:A:16:SER:N    | 1:A:221:VAL:O   | 2.31                     | 0.63              |
| 1:B:1489:PHE:HA | 1:B:1493:PRO:C  | 2.18                     | 0.63              |
| 1:A:313:TYR:O   | 1:A:358:VAL:CB  | 2.46                     | 0.63              |
| 1:A:124:LEU:HA  | 1:A:131:TYR:HA  | 1.80                     | 0.63              |
| 1:A:253:CYS:CB  | 1:A:262:VAL:HA  | 2.28                     | 0.62              |
| 1:B:134:VAL:O   | 1:B:136:LYS:N   | 2.32                     | 0.62              |
| 1:B:125:HIS:N   | 1:B:130:LYS:O   | 2.25                     | 0.62              |
| 1:B:1986:PHE:O  | 1:B:1989:CYS:N  | 2.32                     | 0.62              |
| 1:B:132:LEU:HA  | 1:B:150:THR:O   | 1.99                     | 0.62              |
| 1:B:1966:GLN:O  | 1:B:1970:ARG:CB | 2.48                     | 0.62              |
| 1:B:138:LEU:O   | 1:B:148:ARG:N   | 2.22                     | 0.62              |
| 1:A:2168:GLU:O  | 1:A:2172:MET:CB | 2.48                     | 0.62              |
| 1:B:1820:PHE:C  | 1:B:1822:GLU:H  | 2.04                     | 0.62              |
| 1:A:404:ILE:O   | 1:A:417:LYS:N   | 2.33                     | 0.61              |
| 1:A:1033:ILE:HA | 1:A:1036:GLN:CB | 2.30                     | 0.61              |
| 1:B:789:HIS:O   | 1:B:791:ASP:N   | 2.33                     | 0.61              |
| 1:B:1269:GLU:HA | 1:B:1319:GLU:CB | 2.30                     | 0.61              |
| 1:A:7:SER:C     | 1:A:176:VAL:O   | 2.39                     | 0.61              |
| 1:B:1457:ILE:O  | 1:B:1459:ARG:N  | 2.33                     | 0.61              |
| 1:A:39:VAL:N    | 1:A:207:ASN:O   | 2.32                     | 0.61              |
| 1:A:888:THR:O   | 1:A:891:LEU:N   | 2.33                     | 0.61              |
| 1:B:666:ILE:H   | 1:B:667:GLU:HA  | 1.66                     | 0.61              |
| 1:B:118:GLY:H   | 1:B:163:ILE:C   | 2.04                     | 0.61              |
| 1:B:1849:ASP:O  | 1:B:1852:SER:N  | 2.34                     | 0.61              |
| 1:B:279:LYS:N   | 1:B:309:ALA:HB2 | 2.15                     | 0.61              |
| 1:A:69:GLN:O    | 1:A:73:TRP:CB   | 2.49                     | 0.61              |
| 1:B:125:HIS:O   | 1:B:129:ASN:N   | 2.33                     | 0.61              |
| 1:A:1848:GLU:C  | 1:A:1850:LYS:H  | 2.03                     | 0.60              |
| 1:A:666:ILE:N   | 1:A:667:GLU:HA  | 2.16                     | 0.60              |
| 1:A:683:GLY:O   | 1:A:685:ASN:N   | 2.34                     | 0.60              |
| 1:B:449:ALA:O   | 1:B:452:VAL:N   | 2.34                     | 0.60              |
| 1:B:1459:ARG:C  | 1:B:1461:CYS:H  | 2.04                     | 0.60              |
| 1:B:1051:ASP:O  | 1:B:1055:HIS:N  | 2.32                     | 0.60              |
| 1:B:2120:LEU:O  | 1:B:2123:VAL:N  | 2.34                     | 0.60              |
| 1:A:885:LEU:O   | 1:A:888:THR:N   | 2.34                     | 0.60              |
| 1:A:1030:PHE:O  | 1:A:1034:GLU:CB | 2.50                     | 0.60              |
| 1:B:1609:ALA:O  | 1:B:1613:ARG:CB | 2.50                     | 0.60              |
| 1:B:2061:GLY:O  | 1:B:2064:ILE:N  | 2.31                     | 0.60              |
| 1:A:1480:GLU:CB | 1:A:1882:GLY:H  | 2.15                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:1128:LYS:O  | 1:B:1132:TRP:CB  | 2.50                     | 0.60              |
| 1:B:692:ASP:O   | 1:B:696:VAL:N    | 2.35                     | 0.60              |
| 1:B:2188:TYR:O  | 1:B:2192:THR:CB  | 2.49                     | 0.60              |
| 1:A:130:LYS:HA  | 1:A:153:GLU:HA   | 1.83                     | 0.59              |
| 1:B:117:TYR:O   | 1:B:173:GLY:N    | 2.35                     | 0.59              |
| 1:A:103:ASN:O   | 1:A:107:ASN:CB   | 2.50                     | 0.59              |
| 1:A:1291:VAL:O  | 1:A:1295:PHE:N   | 2.35                     | 0.59              |
| 1:B:398:TRP:H   | 1:B:422:PRO:CA   | 2.13                     | 0.59              |
| 1:A:893:ALA:O   | 1:A:897:CYS:CB   | 2.51                     | 0.59              |
| 1:B:1231:GLN:HA | 1:B:1275:HIS:CB  | 2.33                     | 0.59              |
| 1:B:1231:GLN:O  | 1:B:1235:ARG:CB  | 2.51                     | 0.59              |
| 1:B:2157:ILE:O  | 1:B:2161:GLN:CB  | 2.51                     | 0.59              |
| 1:A:755:ILE:O   | 1:A:758:GLN:N    | 2.35                     | 0.59              |
| 1:B:313:TYR:O   | 1:B:357:SER:C    | 2.41                     | 0.59              |
| 1:B:691:GLU:O   | 1:B:695:GLU:N    | 2.35                     | 0.59              |
| 1:B:117:TYR:O   | 1:B:119:ASN:N    | 2.37                     | 0.58              |
| 1:B:962:LYS:O   | 1:B:966:MET:CB   | 2.51                     | 0.58              |
| 1:A:680:VAL:O   | 1:A:682:THR:N    | 2.34                     | 0.58              |
| 1:A:2020:LEU:O  | 1:A:2021:GLY:C   | 2.42                     | 0.58              |
| 1:A:1251:ASN:O  | 1:A:1255:LEU:CB  | 2.51                     | 0.58              |
| 1:A:1417:GLU:O  | 1:A:1420:ILE:N   | 2.36                     | 0.58              |
| 1:A:1453:PHE:O  | 1:A:1457:ILE:CB  | 2.52                     | 0.58              |
| 1:B:978:LEU:O   | 1:B:982:LEU:CB   | 2.52                     | 0.58              |
| 1:A:1208:MET:O  | 1:A:1212:ALA:HB2 | 2.02                     | 0.58              |
| 1:A:164:GLN:CB  | 1:A:183:VAL:O    | 2.52                     | 0.57              |
| 1:A:242:LEU:O   | 1:A:250:PHE:HA   | 2.04                     | 0.57              |
| 1:B:252:THR:O   | 1:B:262:VAL:C    | 2.42                     | 0.57              |
| 1:B:1489:PHE:HA | 1:B:1493:PRO:HA  | 1.86                     | 0.57              |
| 1:B:1839:GLN:O  | 1:B:1842:PHE:CB  | 2.52                     | 0.57              |
| 1:A:256:HIS:H   | 1:A:261:HIS:H    | 1.51                     | 0.57              |
| 1:B:45:ASP:O    | 1:B:49:PRO:HA    | 2.05                     | 0.57              |
| 1:A:978:LEU:O   | 1:A:982:LEU:CB   | 2.53                     | 0.56              |
| 1:A:125:HIS:N   | 1:A:130:LYS:O    | 2.38                     | 0.56              |
| 1:B:11:ILE:C    | 1:B:13:ASP:H     | 2.09                     | 0.56              |
| 1:B:233:ILE:HA  | 1:B:384:ARG:N    | 2.19                     | 0.56              |
| 1:B:399:VAL:HA  | 1:B:420:THR:HA   | 1.87                     | 0.56              |
| 1:A:30:LEU:CB   | 1:A:36:ARG:H     | 2.18                     | 0.56              |
| 1:A:1798:LEU:CA | 1:A:1802:GLY:HA3 | 2.30                     | 0.56              |
| 1:B:277:SER:O   | 1:B:280:ALA:HB3  | 2.06                     | 0.56              |
| 1:B:313:TYR:O   | 1:B:357:SER:CA   | 2.53                     | 0.56              |
| 1:B:253:CYS:HA  | 1:B:262:VAL:HA   | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:386:SER:O    | 1:B:432:ILE:N    | 2.29                     | 0.56              |
| 1:B:1849:ASP:O   | 1:B:1850:LYS:C   | 2.43                     | 0.56              |
| 1:B:1976:CYS:O   | 1:B:1979:HIS:N   | 2.39                     | 0.56              |
| 1:B:1200:GLN:O   | 1:B:1203:ARG:N   | 2.39                     | 0.56              |
| 1:B:1595:ASP:O   | 1:B:1599:ILE:CB  | 2.54                     | 0.56              |
| 1:B:856:ASP:O    | 1:B:860:ASN:CB   | 2.53                     | 0.56              |
| 1:A:563:SER:O    | 1:A:565:GLN:N    | 2.39                     | 0.56              |
| 1:A:233:ILE:HA   | 1:A:383:PRO:HA   | 1.86                     | 0.56              |
| 1:A:254:ASP:O    | 1:A:256:HIS:N    | 2.39                     | 0.56              |
| 1:A:256:HIS:H    | 1:A:261:HIS:N    | 2.03                     | 0.56              |
| 1:A:1048:THR:O   | 1:A:1050:LEU:N   | 2.36                     | 0.56              |
| 1:A:1476:LYS:CA  | 1:A:1884:LYS:HA  | 2.36                     | 0.56              |
| 1:B:2181:GLY:HA2 | 1:B:2184:ALA:HB3 | 1.88                     | 0.56              |
| 1:A:40:GLN:HA    | 1:A:206:CYS:HA   | 1.87                     | 0.55              |
| 1:A:252:THR:C    | 1:A:263:PHE:O    | 2.44                     | 0.55              |
| 1:A:551:HIS:O    | 1:A:554:ARG:N    | 2.37                     | 0.55              |
| 1:A:1682:MET:O   | 1:A:1686:ARG:N   | 2.39                     | 0.55              |
| 1:B:7:SER:O      | 1:B:178:ILE:C    | 2.44                     | 0.55              |
| 1:B:676:GLU:O    | 1:B:680:VAL:N    | 2.35                     | 0.55              |
| 1:A:617:THR:O    | 1:A:621:LEU:CB   | 2.55                     | 0.55              |
| 1:A:682:THR:O    | 1:A:686:ALA:HB3  | 2.07                     | 0.55              |
| 1:A:998:LYS:C    | 1:A:1007:GLN:HA  | 2.26                     | 0.55              |
| 1:B:1638:GLU:O   | 1:B:1640:THR:N   | 2.39                     | 0.55              |
| 1:A:263:PHE:CB   | 1:A:416:LEU:H    | 2.19                     | 0.55              |
| 1:A:457:ALA:HA   | 1:A:522:LEU:HA   | 1.88                     | 0.55              |
| 1:B:1378:VAL:O   | 1:B:1382:ALA:HB2 | 2.05                     | 0.55              |
| 1:A:297:GLY:O    | 1:A:381:LEU:HA   | 2.06                     | 0.55              |
| 1:A:1371:LEU:O   | 1:A:1372:MET:C   | 2.42                     | 0.55              |
| 1:A:1952:ALA:O   | 1:A:1954:ASP:N   | 2.40                     | 0.55              |
| 1:B:1286:GLU:O   | 1:B:1289:GLU:O   | 2.25                     | 0.55              |
| 1:B:1682:MET:CB  | 1:B:1687:GLY:H   | 2.19                     | 0.55              |
| 1:B:1797:HIS:O   | 1:B:1802:GLY:N   | 2.29                     | 0.55              |
| 1:A:704:ASN:C    | 1:A:706:GLU:H    | 2.10                     | 0.55              |
| 1:A:1864:LYS:O   | 1:A:1867:GLN:N   | 2.39                     | 0.55              |
| 1:A:7:SER:CB     | 1:A:179:GLY:N    | 2.69                     | 0.55              |
| 1:B:848:VAL:O    | 1:B:850:GLN:N    | 2.40                     | 0.55              |
| 1:B:2062:ILE:O   | 1:B:2066:THR:CB  | 2.55                     | 0.55              |
| 1:A:195:ALA:HB3  | 1:A:216:THR:CB   | 2.37                     | 0.55              |
| 1:B:680:VAL:C    | 1:B:682:THR:H    | 2.11                     | 0.55              |
| 1:A:40:GLN:CA    | 1:A:206:CYS:HA   | 2.37                     | 0.54              |
| 1:A:1317:LYS:HA  | 1:A:1323:ILE:CB  | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1476:LYS:CB  | 1:A:1883:ASN:HA  | 2.38                     | 0.54              |
| 1:B:117:TYR:C    | 1:B:119:ASN:H    | 2.11                     | 0.54              |
| 1:B:139:PRO:HA   | 1:B:147:MET:HA   | 1.89                     | 0.54              |
| 1:A:1862:ARG:O   | 1:A:1866:ALA:HB2 | 2.07                     | 0.54              |
| 1:B:127:LYS:C    | 1:B:129:ASN:N    | 2.57                     | 0.54              |
| 1:B:1129:SER:CB  | 1:B:1180:LEU:HA  | 2.38                     | 0.54              |
| 1:B:91:LYS:O     | 1:B:95:ALA:HB2   | 2.07                     | 0.54              |
| 1:A:11:ILE:H     | 1:A:113:THR:C    | 2.09                     | 0.54              |
| 1:B:863:THR:O    | 1:B:867:VAL:CB   | 2.55                     | 0.54              |
| 1:B:1093:VAL:HA  | 1:B:1176:VAL:N   | 2.22                     | 0.54              |
| 1:A:253:CYS:HA   | 1:A:263:PHE:H    | 1.73                     | 0.54              |
| 1:A:475:LYS:O    | 1:A:479:ASP:CB   | 2.56                     | 0.54              |
| 1:B:2185:LEU:HA  | 1:B:2188:TYR:CB  | 2.38                     | 0.54              |
| 1:B:1405:ILE:O   | 1:B:1408:VAL:N   | 2.41                     | 0.54              |
| 1:A:11:ILE:H     | 1:A:113:THR:N    | 2.06                     | 0.54              |
| 1:B:780:SER:O    | 1:B:783:ARG:N    | 2.40                     | 0.54              |
| 1:B:1235:ARG:O   | 1:B:1238:HIS:N   | 2.41                     | 0.54              |
| 1:B:1445:HIS:C   | 1:B:1447:TRP:H   | 2.11                     | 0.54              |
| 1:A:199:GLN:HA   | 1:A:207:ASN:HA   | 1.89                     | 0.54              |
| 1:B:1682:MET:O   | 1:B:1685:ASP:N   | 2.41                     | 0.54              |
| 1:A:45:ASP:N     | 1:A:48:ASN:O     | 2.36                     | 0.53              |
| 1:A:1682:MET:C   | 1:A:1685:ASP:H   | 2.12                     | 0.53              |
| 1:A:2020:LEU:O   | 1:A:2023:TYR:N   | 2.40                     | 0.53              |
| 1:B:1052:LEU:HA  | 1:B:1056:GLY:H   | 1.72                     | 0.53              |
| 1:A:123:LEU:O    | 1:A:132:LEU:N    | 2.36                     | 0.53              |
| 1:B:570:ASN:O    | 1:B:573:TYR:N    | 2.42                     | 0.53              |
| 1:A:1798:LEU:HA  | 1:A:1802:GLY:CA  | 2.30                     | 0.53              |
| 1:B:299:TRP:H    | 1:B:380:SER:C    | 2.10                     | 0.53              |
| 1:A:1682:MET:HA  | 1:A:1685:ASP:CB  | 2.39                     | 0.53              |
| 1:B:729:ILE:O    | 1:B:732:TYR:N    | 2.41                     | 0.53              |
| 1:B:1026:GLY:HA2 | 1:B:1594:ARG:CB  | 2.38                     | 0.53              |
| 1:B:1796:CYS:HA  | 1:B:1799:ASP:CB  | 2.39                     | 0.53              |
| 1:A:38:VAL:HA    | 1:A:208:GLU:HA   | 1.91                     | 0.53              |
| 1:B:62:PRO:O     | 1:B:64:ASN:N     | 2.42                     | 0.53              |
| 1:A:865:GLU:O    | 1:A:869:LEU:CB   | 2.57                     | 0.53              |
| 1:A:1209:GLY:O   | 1:A:1213:VAL:CB  | 2.57                     | 0.52              |
| 1:A:2010:CYS:O   | 1:A:2012:SER:N   | 2.43                     | 0.52              |
| 1:B:1211:HIS:O   | 1:B:1214:VAL:N   | 2.42                     | 0.52              |
| 1:B:1341:VAL:O   | 1:B:1345:TYR:N   | 2.42                     | 0.52              |
| 1:B:200:LEU:O    | 1:B:203:ASN:N    | 2.41                     | 0.52              |
| 1:B:1277:PHE:O   | 1:B:1280:ASN:N   | 2.43                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:17:LEU:HA   | 1:A:219:LYS:O   | 2.10                     | 0.52              |
| 1:B:10:HIS:H    | 1:B:13:ASP:CB   | 2.22                     | 0.52              |
| 1:B:163:ILE:O   | 1:B:164:GLN:O   | 2.27                     | 0.52              |
| 1:B:236:GLY:HA3 | 1:B:286:VAL:H   | 1.74                     | 0.52              |
| 1:A:85:ASP:HA   | 1:A:86:ALA:C    | 2.30                     | 0.52              |
| 1:B:127:LYS:C   | 1:B:129:ASN:H   | 2.11                     | 0.52              |
| 1:B:315:ALA:HA  | 1:B:366:SER:CA  | 2.35                     | 0.52              |
| 1:B:315:ALA:H   | 1:B:357:SER:HA  | 1.75                     | 0.52              |
| 1:B:577:GLN:O   | 1:B:581:MET:N   | 2.32                     | 0.52              |
| 1:A:1111:ASN:O  | 1:A:1115:ILE:N  | 2.43                     | 0.52              |
| 1:B:242:LEU:C   | 1:B:251:LEU:H   | 2.06                     | 0.52              |
| 1:A:1297:HIS:O  | 1:A:1301:THR:N  | 2.43                     | 0.52              |
| 1:B:1608:SER:O  | 1:B:1612:ASP:CB | 2.57                     | 0.52              |
| 1:B:2186:GLU:O  | 1:B:2189:ALA:N  | 2.41                     | 0.52              |
| 1:A:19:ALA:HA   | 1:A:217:SER:O   | 2.09                     | 0.52              |
| 1:A:684:GLU:O   | 1:A:687:LEU:CB  | 2.58                     | 0.52              |
| 1:A:977:ILE:O   | 1:A:981:ILE:CB  | 2.58                     | 0.52              |
| 1:A:2184:ALA:HA | 1:A:2187:PHE:CB | 2.40                     | 0.52              |
| 1:A:1986:PHE:O  | 1:A:1990:GLN:N  | 2.43                     | 0.52              |
| 1:A:2114:ASN:O  | 1:A:2116:ARG:N  | 2.43                     | 0.52              |
| 1:A:7:SER:HA    | 1:A:177:VAL:CA  | 2.40                     | 0.51              |
| 1:A:265:ARG:O   | 1:A:267:THR:N   | 2.44                     | 0.51              |
| 1:A:459:LYS:O   | 1:A:463:GLY:N   | 2.31                     | 0.51              |
| 1:B:136:LYS:HA  | 1:B:147:MET:CB  | 2.40                     | 0.51              |
| 1:A:854:PHE:O   | 1:A:857:LYS:N   | 2.41                     | 0.51              |
| 1:A:896:ASP:C   | 1:A:898:VAL:H   | 2.13                     | 0.51              |
| 1:B:117:TYR:HA  | 1:B:163:ILE:O   | 2.10                     | 0.51              |
| 1:B:654:LYS:O   | 1:B:658:ASN:N   | 2.39                     | 0.51              |
| 1:B:984:VAL:O   | 1:B:989:ARG:N   | 2.43                     | 0.51              |
| 1:B:421:SER:O   | 1:B:422:PRO:C   | 2.49                     | 0.51              |
| 1:A:316:ALA:HA  | 1:A:354:SER:O   | 2.10                     | 0.51              |
| 1:A:1341:VAL:O  | 1:A:1344:PHE:N  | 2.43                     | 0.51              |
| 1:B:242:LEU:O   | 1:B:250:PHE:HA  | 2.10                     | 0.51              |
| 1:B:1488:THR:O  | 1:B:1492:SER:N  | 2.42                     | 0.51              |
| 1:B:1850:LYS:O  | 1:B:1854:LYS:CB | 2.59                     | 0.51              |
| 1:A:1179:ILE:O  | 1:A:1183:LEU:CB | 2.58                     | 0.51              |
| 1:B:7:SER:N     | 1:B:177:VAL:CB  | 2.73                     | 0.51              |
| 1:B:867:VAL:O   | 1:B:870:ALA:N   | 2.43                     | 0.51              |
| 1:B:2063:ASP:HA | 1:B:2113:TYR:CB | 2.41                     | 0.51              |
| 1:A:19:ALA:O    | 1:A:24:ASN:HA   | 2.11                     | 0.51              |
| 1:A:399:VAL:HA  | 1:A:421:SER:H   | 1.76                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:2129:MET:O   | 1:B:2131:GLY:N  | 2.43                     | 0.51              |
| 1:A:692:ASP:O    | 1:A:696:VAL:N   | 2.43                     | 0.51              |
| 1:B:11:ILE:C     | 1:B:13:ASP:N    | 2.63                     | 0.51              |
| 1:A:1636:PHE:O   | 1:A:1638:GLU:N  | 2.44                     | 0.51              |
| 1:B:165:PRO:HA   | 1:B:182:VAL:HA  | 1.92                     | 0.51              |
| 1:B:885:LEU:C    | 1:B:888:THR:H   | 2.14                     | 0.51              |
| 1:B:1387:GLY:O   | 1:B:1389:ASN:N  | 2.44                     | 0.51              |
| 1:A:1085:ARG:O   | 1:A:1087:PHE:N  | 2.44                     | 0.50              |
| 1:A:100:LYS:O    | 1:A:101:LYS:C   | 2.48                     | 0.50              |
| 1:B:397:THR:HA   | 1:B:422:PRO:HA  | 1.93                     | 0.50              |
| 1:B:652:ILE:O    | 1:B:655:ALA:HB3 | 2.12                     | 0.50              |
| 1:A:2003:LEU:O   | 1:A:2007:ASP:CB | 2.60                     | 0.50              |
| 1:B:665:LEU:O    | 1:B:671:VAL:N   | 2.45                     | 0.50              |
| 1:B:1489:PHE:HA  | 1:B:1493:PRO:CA | 2.42                     | 0.50              |
| 1:B:1867:GLN:O   | 1:B:1871:LYS:N  | 2.27                     | 0.50              |
| 1:B:1095:GLN:O   | 1:B:1096:ALA:C  | 2.50                     | 0.50              |
| 1:A:221:VAL:O    | 1:A:222:LEU:O   | 2.29                     | 0.50              |
| 1:A:2018:GLY:C   | 1:A:2020:LEU:N  | 2.62                     | 0.50              |
| 1:B:1289:GLU:C   | 1:B:1291:VAL:N  | 2.64                     | 0.50              |
| 1:A:476:LEU:O    | 1:A:479:ASP:N   | 2.44                     | 0.50              |
| 1:A:1238:HIS:O   | 1:A:1240:PHE:N  | 2.45                     | 0.49              |
| 1:B:1636:PHE:C   | 1:B:1638:GLU:H  | 2.13                     | 0.49              |
| 1:B:1820:PHE:O   | 1:B:1822:GLU:N  | 2.45                     | 0.49              |
| 1:A:554:ARG:HA   | 1:A:557:TYR:CB  | 2.42                     | 0.49              |
| 1:A:2114:ASN:C   | 1:A:2116:ARG:N  | 2.66                     | 0.49              |
| 1:B:243:PHE:HA   | 1:B:249:LYS:O   | 2.11                     | 0.49              |
| 1:B:281:LEU:O    | 1:B:308:LEU:CB  | 2.60                     | 0.49              |
| 1:B:387:TYR:HA   | 1:B:431:ALA:HA  | 1.94                     | 0.49              |
| 1:B:2036:LEU:O   | 1:B:2040:THR:CB | 2.60                     | 0.49              |
| 1:A:391:ARG:HA   | 1:A:398:TRP:N   | 2.27                     | 0.49              |
| 1:A:2173:LEU:O   | 1:A:2177:GLY:N  | 2.45                     | 0.49              |
| 1:B:1115:ILE:C   | 1:B:1117:GLN:H  | 2.16                     | 0.49              |
| 1:B:1225:ALA:HB1 | 1:B:1226:GLU:HA | 1.94                     | 0.49              |
| 1:A:15:CYS:HA    | 1:A:223:PHE:N   | 2.27                     | 0.49              |
| 1:A:255:GLU:C    | 1:A:259:LYS:O   | 2.51                     | 0.49              |
| 1:A:1863:MET:O   | 1:A:1867:GLN:N  | 2.38                     | 0.49              |
| 1:A:2119:GLU:O   | 1:A:2123:VAL:CB | 2.60                     | 0.49              |
| 1:B:666:ILE:H    | 1:B:667:GLU:CA  | 2.26                     | 0.49              |
| 1:B:2007:ASP:O   | 1:B:2011:GLY:N  | 2.46                     | 0.49              |
| 1:B:279:LYS:H    | 1:B:309:ALA:HB2 | 1.76                     | 0.49              |
| 1:B:2044:GLN:C   | 1:B:2046:PRO:N  | 2.65                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:112:GLY:HA2  | 1:B:226:TRP:CB   | 2.43                     | 0.49              |
| 1:A:391:ARG:HA   | 1:A:398:TRP:CA   | 2.42                     | 0.49              |
| 1:B:1682:MET:C   | 1:B:1686:ARG:H   | 2.16                     | 0.49              |
| 1:A:1251:ASN:CB  | 1:A:1283:LEU:HA  | 2.43                     | 0.49              |
| 1:A:2019:LEU:O   | 1:A:2021:GLY:N   | 2.46                     | 0.49              |
| 1:B:763:LEU:O    | 1:B:767:CYS:CB   | 2.60                     | 0.49              |
| 1:B:860:ASN:O    | 1:B:861:LYS:C    | 2.51                     | 0.49              |
| 1:B:1127:GLU:O   | 1:B:1130:GLU:N   | 2.41                     | 0.49              |
| 1:A:2189:ALA:O   | 1:A:2191:HIS:N   | 2.45                     | 0.48              |
| 1:A:13:ASP:HA    | 1:A:226:TRP:N    | 2.28                     | 0.48              |
| 1:A:826:LYS:O    | 1:A:830:LYS:CB   | 2.61                     | 0.48              |
| 1:A:1872:ALA:O   | 1:A:1876:VAL:CB  | 2.61                     | 0.48              |
| 1:B:16:SER:N     | 1:B:221:VAL:O    | 2.30                     | 0.48              |
| 1:B:1843:PHE:O   | 1:B:1846:LEU:N   | 2.45                     | 0.48              |
| 1:A:39:VAL:C     | 1:A:207:ASN:H    | 2.16                     | 0.48              |
| 1:A:724:LYS:O    | 1:A:726:ASP:N    | 2.47                     | 0.48              |
| 1:A:2043:CYS:C   | 1:A:2097:ALA:HB1 | 2.34                     | 0.48              |
| 1:A:2043:CYS:O   | 1:A:2097:ALA:HB1 | 2.14                     | 0.48              |
| 1:B:298:TYR:HA   | 1:B:381:LEU:CA   | 2.43                     | 0.48              |
| 1:B:298:TYR:HA   | 1:B:381:LEU:HA   | 1.95                     | 0.48              |
| 1:B:986:LEU:C    | 1:B:988:TYR:H    | 2.16                     | 0.48              |
| 1:A:355:LEU:H    | 1:A:419:GLY:CA   | 2.27                     | 0.48              |
| 1:A:558:ARG:C    | 1:A:560:LEU:N    | 2.67                     | 0.48              |
| 1:A:2150:ASN:O   | 1:A:2153:HIS:N   | 2.46                     | 0.48              |
| 1:A:8:PHE:N      | 1:A:177:VAL:C    | 2.59                     | 0.48              |
| 1:A:1631:ARG:CB  | 1:A:1648:SER:H   | 2.26                     | 0.48              |
| 1:B:180:ASP:C    | 1:B:219:LYS:HA   | 2.34                     | 0.48              |
| 1:B:1634:LEU:O   | 1:B:1638:GLU:O   | 2.31                     | 0.48              |
| 1:A:781:PHE:O    | 1:A:784:LEU:N    | 2.46                     | 0.48              |
| 1:A:1270:ALA:HB2 | 1:A:1319:GLU:CB  | 2.44                     | 0.48              |
| 1:B:1199:LYS:C   | 1:B:1201:GLN:N   | 2.67                     | 0.48              |
| 1:B:233:ILE:CB   | 1:B:383:PRO:HA   | 2.44                     | 0.48              |
| 1:A:1049:PRO:O   | 1:A:1053:ASP:N   | 2.43                     | 0.47              |
| 1:A:225:LYS:H    | 1:A:228:ASP:CB   | 2.25                     | 0.47              |
| 1:A:1332:ALA:O   | 1:A:1335:VAL:N   | 2.42                     | 0.47              |
| 1:B:2015:GLY:O   | 1:B:2067:ALA:HB1 | 2.14                     | 0.47              |
| 1:A:15:CYS:HA    | 1:A:222:LEU:CA   | 2.42                     | 0.47              |
| 1:A:239:VAL:O    | 1:A:434:PRO:HA   | 2.14                     | 0.47              |
| 1:B:111:LEU:C    | 1:B:113:THR:H    | 2.18                     | 0.47              |
| 1:B:1061:LEU:O   | 1:B:1064:LEU:CB  | 2.63                     | 0.47              |
| 1:A:204:PRO:O    | 1:A:205:GLY:C    | 2.51                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1789:MET:N  | 1:B:1789:MET:N   | 2.62                     | 0.47              |
| 1:A:2068:LEU:O  | 1:A:2072:ASP:HA  | 2.14                     | 0.47              |
| 1:A:1341:VAL:O  | 1:A:1345:TYR:N   | 2.44                     | 0.47              |
| 1:B:365:SER:HA  | 1:B:394:CYS:CB   | 2.44                     | 0.47              |
| 1:B:680:VAL:C   | 1:B:682:THR:N    | 2.67                     | 0.47              |
| 1:B:617:THR:O   | 1:B:621:LEU:CB   | 2.63                     | 0.47              |
| 1:A:10:HIS:CB   | 1:A:112:GLY:HA2  | 2.45                     | 0.47              |
| 1:B:315:ALA:CB  | 1:B:358:VAL:H    | 2.27                     | 0.47              |
| 1:A:1980:ASN:HA | 1:A:2038:SER:HA  | 1.97                     | 0.47              |
| 1:B:15:CYS:CA   | 1:B:223:PHE:H    | 2.25                     | 0.47              |
| 1:B:696:VAL:O   | 1:B:697:TRP:C    | 2.53                     | 0.47              |
| 1:B:2184:ALA:O  | 1:B:2188:TYR:CB  | 2.62                     | 0.47              |
| 1:A:149:VAL:CB  | 1:A:210:ASN:HA   | 2.45                     | 0.46              |
| 1:A:576:LYS:O   | 1:A:578:PHE:N    | 2.48                     | 0.46              |
| 1:B:125:HIS:O   | 1:B:127:LYS:N    | 2.48                     | 0.46              |
| 1:A:869:LEU:O   | 1:A:873:LEU:CB   | 2.64                     | 0.46              |
| 1:B:305:PHE:O   | 1:B:313:TYR:HA   | 2.16                     | 0.46              |
| 1:A:98:LEU:O    | 1:A:101:LYS:N    | 2.48                     | 0.46              |
| 1:B:299:TRP:H   | 1:B:380:SER:CB   | 2.28                     | 0.46              |
| 1:B:620:SER:O   | 1:B:624:LYS:N    | 2.43                     | 0.46              |
| 1:B:1053:ASP:O  | 1:B:1057:GLY:HA3 | 2.16                     | 0.46              |
| 1:B:1880:ASP:C  | 1:B:1882:GLY:H   | 2.18                     | 0.46              |
| 1:B:1632:PRO:O  | 1:B:1634:LEU:N   | 2.49                     | 0.46              |
| 1:A:13:ASP:HA   | 1:A:225:LYS:C    | 2.36                     | 0.46              |
| 1:A:180:ASP:O   | 1:A:219:LYS:HA   | 2.15                     | 0.46              |
| 1:A:1973:GLN:O  | 1:A:1976:CYS:N   | 2.48                     | 0.46              |
| 1:B:1632:PRO:O  | 1:B:1636:PHE:N   | 2.41                     | 0.46              |
| 1:B:2197:ILE:HA | 1:B:2212:PRO:CA  | 2.46                     | 0.46              |
| 1:A:68:ALA:O    | 1:A:72:PHE:CB    | 2.63                     | 0.46              |
| 1:B:476:LEU:O   | 1:B:477:LEU:C    | 2.53                     | 0.46              |
| 1:B:1199:LYS:O  | 1:B:1202:GLN:N   | 2.47                     | 0.46              |
| 1:A:979:GLN:O   | 1:A:982:LEU:N    | 2.49                     | 0.46              |
| 1:A:1001:PHE:O  | 1:A:1003:GLU:N   | 2.44                     | 0.46              |
| 1:A:1271:VAL:O  | 1:A:1275:HIS:N   | 2.46                     | 0.46              |
| 1:B:117:TYR:CB  | 1:B:172:ILE:HA   | 2.46                     | 0.46              |
| 1:B:773:LEU:C   | 1:B:775:TYR:H    | 2.13                     | 0.46              |
| 1:A:1245:CYS:CB | 1:A:1285:SER:O   | 2.64                     | 0.45              |
| 1:B:131:TYR:O   | 1:B:152:ASP:O    | 2.34                     | 0.45              |
| 1:A:393:LEU:C   | 1:A:396:ASN:H    | 2.20                     | 0.45              |
| 1:A:659:PRO:O   | 1:A:661:ASN:N    | 2.48                     | 0.45              |
| 1:B:862:LEU:O   | 1:B:864:PHE:N    | 2.49                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:2147:SER:O  | 1:B:2151:VAL:CB  | 2.65                     | 0.45              |
| 1:A:1966:GLN:O  | 1:A:1970:ARG:CB  | 2.63                     | 0.45              |
| 1:B:594:THR:O   | 1:B:597:ALA:HB3  | 2.15                     | 0.45              |
| 1:B:1214:VAL:O  | 1:B:1215:LEU:C   | 2.55                     | 0.45              |
| 1:B:1843:PHE:O  | 1:B:1847:THR:N   | 2.45                     | 0.45              |
| 1:B:444:ASP:O   | 1:B:447:ASN:N    | 2.49                     | 0.45              |
| 1:A:616:ASP:O   | 1:A:620:SER:CB   | 2.65                     | 0.45              |
| 1:B:11:ILE:O    | 1:B:13:ASP:N     | 2.50                     | 0.45              |
| 1:B:356:VAL:O   | 1:B:358:VAL:N    | 2.50                     | 0.45              |
| 1:B:1986:PHE:O  | 1:B:1987:LEU:C   | 2.54                     | 0.45              |
| 1:A:140:ALA:HB2 | 1:A:147:MET:C    | 2.37                     | 0.45              |
| 1:B:15:CYS:HA   | 1:B:223:PHE:N    | 2.25                     | 0.45              |
| 1:B:183:VAL:O   | 1:B:185:ASN:N    | 2.44                     | 0.45              |
| 1:B:1847:THR:O  | 1:B:1850:LYS:N   | 2.50                     | 0.45              |
| 1:A:870:ALA:HA  | 1:A:873:LEU:CB   | 2.47                     | 0.45              |
| 1:A:1116:LYS:O  | 1:A:1117:GLN:C   | 2.55                     | 0.45              |
| 1:A:7:SER:CB    | 1:A:180:ASP:N    | 2.80                     | 0.45              |
| 1:A:253:CYS:HA  | 1:A:263:PHE:N    | 2.31                     | 0.45              |
| 1:A:716:ALA:O   | 1:A:718:ASP:N    | 2.50                     | 0.45              |
| 1:B:313:TYR:O   | 1:B:357:SER:HA   | 2.17                     | 0.45              |
| 1:A:445:PHE:O   | 1:A:449:ALA:HB2  | 2.17                     | 0.45              |
| 1:B:1218:LEU:C  | 1:B:1220:ILE:H   | 2.20                     | 0.45              |
| 1:A:480:LEU:C   | 1:A:483:PHE:H    | 2.20                     | 0.44              |
| 1:A:1197:SER:O  | 1:A:1200:GLN:N   | 2.50                     | 0.44              |
| 1:B:279:LYS:CA  | 1:B:309:ALA:HB2  | 2.47                     | 0.44              |
| 1:B:397:THR:CA  | 1:B:422:PRO:HA   | 2.47                     | 0.44              |
| 1:B:648:THR:O   | 1:B:651:LEU:N    | 2.49                     | 0.44              |
| 1:B:1820:PHE:C  | 1:B:1822:GLU:N   | 2.69                     | 0.44              |
| 1:B:2202:ARG:CB | 1:B:2206:GLN:HA  | 2.47                     | 0.44              |
| 1:A:40:GLN:N    | 1:A:206:CYS:HA   | 2.31                     | 0.44              |
| 1:B:121:ILE:O   | 1:B:160:TRP:HA   | 2.17                     | 0.44              |
| 1:B:1682:MET:O  | 1:B:1685:ASP:C   | 2.54                     | 0.44              |
| 1:B:116:GLN:HA  | 1:B:175:SER:HA   | 1.99                     | 0.44              |
| 1:B:118:GLY:N   | 1:B:163:ILE:C    | 2.69                     | 0.44              |
| 1:A:370:LEU:HA  | 1:A:389:ARG:O    | 2.17                     | 0.44              |
| 1:A:399:VAL:HA  | 1:A:420:THR:HA   | 2.00                     | 0.44              |
| 1:A:838:GLU:O   | 1:A:840:VAL:N    | 2.50                     | 0.44              |
| 1:A:2044:GLN:HA | 1:A:2097:ALA:HB1 | 1.99                     | 0.44              |
| 1:B:89:LEU:O    | 1:B:93:HIS:CB    | 2.65                     | 0.44              |
| 1:B:1211:HIS:O  | 1:B:1213:VAL:N   | 2.50                     | 0.44              |
| 1:A:1682:MET:CA | 1:A:1686:ARG:H   | 2.31                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:521:LYS:O   | 1:B:524:GLN:N    | 2.51                     | 0.44              |
| 1:A:399:VAL:HA  | 1:A:421:SER:N    | 2.31                     | 0.44              |
| 1:A:558:ARG:C   | 1:A:560:LEU:H    | 2.21                     | 0.44              |
| 1:A:1476:LYS:HA | 1:A:1884:LYS:CA  | 2.47                     | 0.44              |
| 1:B:179:GLY:HA2 | 1:B:220:ILE:O    | 2.18                     | 0.44              |
| 1:B:1682:MET:C  | 1:B:1685:ASP:H   | 2.21                     | 0.44              |
| 1:B:113:THR:O   | 1:B:114:VAL:C    | 2.56                     | 0.44              |
| 1:B:117:TYR:C   | 1:B:119:ASN:N    | 2.70                     | 0.44              |
| 1:A:398:TRP:O   | 1:A:421:SER:CB   | 2.66                     | 0.44              |
| 1:A:690:GLY:O   | 1:A:691:GLU:C    | 2.56                     | 0.44              |
| 1:A:979:GLN:O   | 1:A:983:ASN:N    | 2.41                     | 0.44              |
| 1:A:2126:LYS:O  | 1:A:2130:GLN:CB  | 2.66                     | 0.44              |
| 1:B:1178:GLU:O  | 1:B:1182:ARG:CB  | 2.66                     | 0.44              |
| 1:B:2186:GLU:O  | 1:B:2189:ALA:HB3 | 2.17                     | 0.44              |
| 1:A:1680:GLU:C  | 1:A:1682:MET:N   | 2.71                     | 0.44              |
| 1:A:1795:GLN:HA | 1:A:1798:LEU:CB  | 2.48                     | 0.44              |
| 1:B:440:VAL:O   | 1:B:443:LEU:N    | 2.51                     | 0.44              |
| 1:B:893:ALA:O   | 1:B:896:ASP:N    | 2.51                     | 0.44              |
| 1:B:1252:GLN:O  | 1:B:1255:LEU:N   | 2.51                     | 0.44              |
| 1:B:2029:VAL:O  | 1:B:2030:ALA:C   | 2.55                     | 0.44              |
| 1:B:2186:GLU:C  | 1:B:2189:ALA:H   | 2.19                     | 0.44              |
| 1:A:645:ILE:O   | 1:A:648:THR:N    | 2.51                     | 0.43              |
| 1:A:1295:PHE:C  | 1:A:1297:HIS:N   | 2.72                     | 0.43              |
| 1:A:1848:GLU:C  | 1:A:1850:LYS:N   | 2.64                     | 0.43              |
| 1:A:1420:ILE:O  | 1:A:1424:ASN:CB  | 2.67                     | 0.43              |
| 1:B:118:GLY:C   | 1:B:163:ILE:H    | 2.21                     | 0.43              |
| 1:B:755:ILE:O   | 1:B:758:GLN:N    | 2.50                     | 0.43              |
| 1:A:978:LEU:HA  | 1:A:981:ILE:CB   | 2.49                     | 0.43              |
| 1:B:1289:GLU:O  | 1:B:1291:VAL:N   | 2.51                     | 0.43              |
| 1:A:7:SER:HA    | 1:A:177:VAL:C    | 2.38                     | 0.43              |
| 1:A:20:GLU:HA   | 1:A:24:ASN:HA    | 2.00                     | 0.43              |
| 1:A:551:HIS:C   | 1:A:554:ARG:H    | 2.22                     | 0.43              |
| 1:A:715:LEU:O   | 1:A:716:ALA:C    | 2.57                     | 0.43              |
| 1:B:1682:MET:CA | 1:B:1686:ARG:H   | 2.32                     | 0.43              |
| 1:B:572:GLU:O   | 1:B:574:ILE:N    | 2.52                     | 0.43              |
| 1:B:719:ALA:C   | 1:B:722:GLY:H    | 2.22                     | 0.43              |
| 1:B:1682:MET:CB | 1:B:1687:GLY:N   | 2.82                     | 0.43              |
| 1:A:7:SER:CB    | 1:A:179:GLY:H    | 2.31                     | 0.43              |
| 1:A:1376:HIS:O  | 1:A:1380:LEU:CB  | 2.66                     | 0.43              |
| 1:A:1883:ASN:HA | 1:A:1884:LYS:HA  | 1.75                     | 0.43              |
| 1:B:402:THR:CB  | 1:B:418:ILE:HA   | 2.48                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:13:ASP:HA   | 1:A:226:TRP:HA  | 2.00                     | 0.43              |
| 1:A:117:TYR:C   | 1:A:172:ILE:HA  | 2.39                     | 0.43              |
| 1:A:659:PRO:C   | 1:A:661:ASN:H   | 2.21                     | 0.43              |
| 1:A:761:VAL:O   | 1:A:762:ASP:C   | 2.56                     | 0.43              |
| 1:B:670:LEU:HA  | 1:B:673:SER:CB  | 2.48                     | 0.43              |
| 1:A:8:PHE:H     | 1:A:177:VAL:CA  | 2.31                     | 0.43              |
| 1:B:860:ASN:O   | 1:B:863:THR:N   | 2.51                     | 0.43              |
| 1:B:1849:ASP:O  | 1:B:1850:LYS:O  | 2.36                     | 0.43              |
| 1:A:862:LEU:O   | 1:A:863:THR:C   | 2.55                     | 0.43              |
| 1:A:1417:GLU:O  | 1:A:1418:VAL:C  | 2.57                     | 0.43              |
| 1:A:1477:TYR:HA | 1:A:1881:LEU:O  | 2.19                     | 0.43              |
| 1:A:85:ASP:HA   | 1:A:86:ALA:O    | 2.18                     | 0.43              |
| 1:A:480:LEU:O   | 1:A:481:VAL:C   | 2.57                     | 0.42              |
| 1:A:715:LEU:O   | 1:A:717:GLN:N   | 2.51                     | 0.42              |
| 1:B:118:GLY:H   | 1:B:164:GLN:N   | 2.17                     | 0.42              |
| 1:B:181:LYS:HA  | 1:B:218:TRP:O   | 2.19                     | 0.42              |
| 1:B:1818:ARG:C  | 1:B:1820:PHE:N  | 2.72                     | 0.42              |
| 1:B:2061:GLY:C  | 1:B:2064:ILE:H  | 2.19                     | 0.42              |
| 1:A:11:ILE:O    | 1:A:112:GLY:N   | 2.52                     | 0.42              |
| 1:A:101:LYS:O   | 1:A:104:GLU:N   | 2.49                     | 0.42              |
| 1:A:391:ARG:HA  | 1:A:397:THR:C   | 2.39                     | 0.42              |
| 1:A:1375:ILE:HA | 1:A:1378:VAL:CB | 2.49                     | 0.42              |
| 1:B:1457:ILE:C  | 1:B:1459:ARG:N  | 2.72                     | 0.42              |
| 1:B:1649:GLY:O  | 1:B:1650:GLY:C  | 2.55                     | 0.42              |
| 1:B:133:THR:O   | 1:B:149:VAL:HA  | 2.19                     | 0.42              |
| 1:B:278:SER:O   | 1:B:279:LYS:C   | 2.58                     | 0.42              |
| 1:A:598:LEU:O   | 1:A:599:LEU:C   | 2.57                     | 0.42              |
| 1:A:2189:ALA:O  | 1:A:2190:LYS:C  | 2.58                     | 0.42              |
| 1:B:773:LEU:C   | 1:B:775:TYR:N   | 2.72                     | 0.42              |
| 1:B:134:VAL:HA  | 1:B:149:VAL:CB  | 2.49                     | 0.42              |
| 1:B:315:ALA:CA  | 1:B:366:SER:HA  | 2.39                     | 0.42              |
| 1:B:1080:LEU:O  | 1:B:1084:PHE:N  | 2.35                     | 0.42              |
| 1:A:354:SER:CA  | 1:A:419:GLY:HA3 | 2.40                     | 0.42              |
| 1:A:982:LEU:O   | 1:A:986:LEU:N   | 2.36                     | 0.42              |
| 1:A:1369:SER:C  | 1:A:1371:LEU:N  | 2.73                     | 0.42              |
| 1:B:622:VAL:O   | 1:B:626:ARG:HA  | 2.20                     | 0.42              |
| 1:B:781:PHE:O   | 1:B:784:LEU:N   | 2.51                     | 0.42              |
| 1:A:680:VAL:C   | 1:A:682:THR:H   | 2.21                     | 0.42              |
| 1:B:1813:ASN:O  | 1:B:1814:ALA:C  | 2.58                     | 0.42              |
| 1:B:1880:ASP:O  | 1:B:1882:GLY:N  | 2.44                     | 0.42              |
| 1:A:19:ALA:HA   | 1:A:218:TRP:HA  | 2.02                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:92:LEU:O    | 1:A:95:ALA:HB3   | 2.19                     | 0.42              |
| 1:A:252:THR:N   | 1:A:263:PHE:O    | 2.52                     | 0.42              |
| 1:A:355:LEU:N   | 1:A:418:ILE:O    | 2.53                     | 0.42              |
| 1:A:789:HIS:O   | 1:A:791:ASP:N    | 2.52                     | 0.42              |
| 1:A:1270:ALA:O  | 1:A:1272:THR:N   | 2.48                     | 0.42              |
| 1:A:2183:GLU:HA | 1:A:2186:GLU:CB  | 2.50                     | 0.42              |
| 1:A:666:ILE:N   | 1:A:667:GLU:CA   | 2.80                     | 0.42              |
| 1:B:690:GLY:O   | 1:B:691:GLU:C    | 2.58                     | 0.42              |
| 1:A:648:THR:O   | 1:A:651:LEU:N    | 2.53                     | 0.41              |
| 1:A:1793:GLU:HA | 1:A:1796:CYS:CB  | 2.50                     | 0.41              |
| 1:B:250:PHE:O   | 1:B:264:LEU:HA   | 2.20                     | 0.41              |
| 1:A:16:SER:C    | 1:A:221:VAL:H    | 2.22                     | 0.41              |
| 1:A:191:GLN:CB  | 1:A:212:VAL:HA   | 2.50                     | 0.41              |
| 1:B:263:PHE:CB  | 1:B:416:LEU:O    | 2.68                     | 0.41              |
| 1:A:18:TYR:O    | 1:A:218:TRP:HA   | 2.21                     | 0.41              |
| 1:A:1381:LEU:HA | 1:A:1384:CYS:CB  | 2.50                     | 0.41              |
| 1:A:2123:VAL:O  | 1:A:2127:ALA:CB  | 2.64                     | 0.41              |
| 1:B:62:PRO:O    | 1:B:63:MET:C     | 2.58                     | 0.41              |
| 1:B:1093:VAL:O  | 1:B:1096:ALA:HB3 | 2.20                     | 0.41              |
| 1:B:1199:LYS:O  | 1:B:1200:GLN:C   | 2.58                     | 0.41              |
| 1:B:91:LYS:O    | 1:B:95:ALA:CB    | 2.66                     | 0.41              |
| 1:B:305:PHE:C   | 1:B:314:LEU:H    | 2.15                     | 0.41              |
| 1:B:1236:LEU:O  | 1:B:1237:ALA:C   | 2.58                     | 0.41              |
| 1:B:1633:GLU:HA | 1:B:1636:PHE:CB  | 2.50                     | 0.41              |
| 1:B:1840:HIS:O  | 1:B:1841:SER:C   | 2.58                     | 0.41              |
| 1:A:1118:ASP:O  | 1:A:1119:LEU:C   | 2.59                     | 0.41              |
| 1:B:756:SER:O   | 1:B:760:ASP:HA   | 2.20                     | 0.41              |
| 1:B:1080:LEU:O  | 1:B:1083:LEU:CB  | 2.68                     | 0.41              |
| 1:A:166:PHE:N   | 1:A:182:VAL:HA   | 2.35                     | 0.41              |
| 1:A:724:LYS:C   | 1:A:726:ASP:H    | 2.22                     | 0.41              |
| 1:A:1836:THR:HA | 1:A:1839:GLN:CB  | 2.50                     | 0.41              |
| 1:B:253:CYS:O   | 1:B:279:LYS:CB   | 2.68                     | 0.41              |
| 1:B:862:LEU:O   | 1:B:863:THR:C    | 2.59                     | 0.41              |
| 1:B:1062:ARG:O  | 1:B:1063:VAL:C   | 2.59                     | 0.41              |
| 1:A:772:ASN:O   | 1:A:773:LEU:C    | 2.57                     | 0.41              |
| 1:B:251:LEU:HA  | 1:B:264:LEU:HA   | 2.03                     | 0.41              |
| 1:B:2197:ILE:HA | 1:B:2212:PRO:CB  | 2.51                     | 0.41              |
| 1:A:86:ALA:O    | 1:A:88:LEU:N     | 2.54                     | 0.41              |
| 1:A:861:LYS:O   | 1:A:864:PHE:N    | 2.54                     | 0.41              |
| 1:A:1061:LEU:HA | 1:A:1101:GLN:CB  | 2.50                     | 0.41              |
| 1:A:1207:ASN:C  | 1:A:1209:GLY:N   | 2.73                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1211:HIS:O  | 1:A:1215:LEU:CB  | 2.68                     | 0.41              |
| 1:B:1106:SER:O  | 1:B:1107:GLN:CB  | 2.69                     | 0.41              |
| 1:A:509:LEU:O   | 1:A:513:GLN:N    | 2.54                     | 0.41              |
| 1:A:708:ARG:O   | 1:A:709:SER:C    | 2.59                     | 0.41              |
| 1:B:675:PHE:O   | 1:B:679:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:1245:CYS:CB | 1:A:1341:VAL:H   | 2.34                     | 0.41              |
| 1:B:706:GLU:O   | 1:B:708:ARG:N    | 2.44                     | 0.41              |
| 1:A:368:PHE:HA  | 1:A:392:HIS:HA   | 2.04                     | 0.40              |
| 1:A:1953:LYS:O  | 1:A:1954:ASP:C   | 2.59                     | 0.40              |
| 1:B:1657:LYS:O  | 1:B:1660:LYS:N   | 2.44                     | 0.40              |
| 1:B:1678:LEU:HA | 1:B:1827:ALA:HA  | 2.02                     | 0.40              |
| 1:A:243:PHE:O   | 1:A:430:PHE:CB   | 2.69                     | 0.40              |
| 1:B:24:ASN:O    | 1:B:41:PRO:HA    | 2.22                     | 0.40              |
| 1:B:740:PHE:O   | 1:B:742:ARG:N    | 2.55                     | 0.40              |
| 1:B:1214:VAL:O  | 1:B:1217:LEU:N   | 2.55                     | 0.40              |
| 1:B:1824:ILE:O  | 1:B:1827:ALA:HB3 | 2.20                     | 0.40              |
| 1:B:1966:GLN:C  | 1:B:1970:ARG:H   | 2.25                     | 0.40              |
| 1:A:251:LEU:CA  | 1:A:264:LEU:HA   | 2.42                     | 0.40              |
| 1:A:255:GLU:HA  | 1:A:261:HIS:H    | 1.86                     | 0.40              |
| 1:A:406:ILE:N   | 1:A:415:MET:O    | 2.55                     | 0.40              |
| 1:A:580:PHE:O   | 1:A:581:MET:C    | 2.59                     | 0.40              |
| 1:A:896:ASP:C   | 1:A:898:VAL:N    | 2.74                     | 0.40              |
| 1:A:1954:ASP:O  | 1:A:1955:ASP:C   | 2.60                     | 0.40              |
| 1:B:1459:ARG:C  | 1:B:1461:CYS:N   | 2.72                     | 0.40              |
| 1:B:1682:MET:CB | 1:B:1686:ARG:H   | 2.34                     | 0.40              |
| 1:A:100:LYS:O   | 1:A:103:ASN:CB   | 2.70                     | 0.40              |
| 1:A:1134:TYR:O  | 1:A:1230:MET:N   | 2.52                     | 0.40              |
| 1:A:1680:GLU:C  | 1:A:1682:MET:H   | 2.24                     | 0.40              |
| 1:B:2211:VAL:O  | 1:B:2212:PRO:C   | 2.59                     | 0.40              |
| 1:A:17:LEU:CB   | 1:A:220:ILE:HA   | 2.52                     | 0.40              |
| 1:A:157:GLU:C   | 1:A:159:SER:N    | 2.75                     | 0.40              |
| 1:B:986:LEU:C   | 1:B:988:TYR:N    | 2.75                     | 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 X-ray entries followed by that with respect to entries

of similar resolution.

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     | 1682/2217 (76%) | 1265 (75%) | 296 (18%) | 121 (7%) | 1           | 14 |
| 1   | B     | 1680/2217 (76%) | 1193 (71%) | 337 (20%) | 150 (9%) | 1           | 11 |
| All | All   | 3362/4434 (76%) | 2458 (73%) | 633 (19%) | 271 (8%) | 1           | 12 |

All (271) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 86   | ALA  |
| 1   | A     | 87   | VAL  |
| 1   | A     | 213  | ASN  |
| 1   | A     | 222  | LEU  |
| 1   | A     | 226  | TRP  |
| 1   | A     | 255  | GLU  |
| 1   | A     | 266  | THR  |
| 1   | A     | 478  | GLU  |
| 1   | A     | 479  | ASP  |
| 1   | A     | 502  | PRO  |
| 1   | A     | 522  | LEU  |
| 1   | A     | 598  | LEU  |
| 1   | A     | 628  | PRO  |
| 1   | A     | 659  | PRO  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 681  | SER  |
| 1   | A     | 744  | CYS  |
| 1   | A     | 899  | HIS  |
| 1   | A     | 990  | ILE  |
| 1   | A     | 1239 | GLU  |
| 1   | A     | 1264 | ASN  |
| 1   | A     | 1370 | PRO  |
| 1   | A     | 1400 | LEU  |
| 1   | A     | 1637 | PRO  |
| 1   | A     | 1849 | ASP  |
| 1   | A     | 1864 | LYS  |
| 1   | A     | 1885 | LYS  |
| 1   | A     | 1966 | GLN  |
| 1   | A     | 1993 | LYS  |
| 1   | A     | 2013 | THR  |
| 1   | A     | 2046 | PRO  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2071       | ASN         |
| 1          | A            | 2104       | ASP         |
| 1          | A            | 2143       | ASP         |
| 1          | A            | 2178       | GLN         |
| 1          | A            | 2210       | PRO         |
| 1          | B            | 38         | VAL         |
| 1          | B            | 113        | THR         |
| 1          | B            | 164        | GLN         |
| 1          | B            | 165        | PRO         |
| 1          | B            | 223        | PHE         |
| 1          | B            | 293        | ARG         |
| 1          | B            | 300        | ASN         |
| 1          | B            | 357        | SER         |
| 1          | B            | 405        | PRO         |
| 1          | B            | 513        | GLN         |
| 1          | B            | 628        | PRO         |
| 1          | B            | 659        | PRO         |
| 1          | B            | 666        | ILE         |
| 1          | B            | 681        | SER         |
| 1          | B            | 696        | VAL         |
| 1          | B            | 741        | ALA         |
| 1          | B            | 744        | CYS         |
| 1          | B            | 760        | ASP         |
| 1          | B            | 773        | LEU         |
| 1          | B            | 774        | PRO         |
| 1          | B            | 854        | PHE         |
| 1          | B            | 990        | ILE         |
| 1          | B            | 999        | ARG         |
| 1          | B            | 1008       | SER         |
| 1          | B            | 1095       | GLN         |
| 1          | B            | 1096       | ALA         |
| 1          | B            | 1107       | GLN         |
| 1          | B            | 1214       | VAL         |
| 1          | B            | 1220       | ILE         |
| 1          | B            | 1285       | SER         |
| 1          | B            | 1292       | VAL         |
| 1          | B            | 1300       | GLU         |
| 1          | B            | 1311       | PHE         |
| 1          | B            | 1400       | LEU         |
| 1          | B            | 1458       | CYS         |
| 1          | B            | 1462       | ASN         |
| 1          | B            | 1463       | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 1492       | SER         |
| 1          | B            | 1637       | PRO         |
| 1          | B            | 1814       | ALA         |
| 1          | B            | 1966       | GLN         |
| 1          | B            | 1967       | PRO         |
| 1          | B            | 1984       | GLN         |
| 1          | B            | 2046       | PRO         |
| 1          | B            | 2075       | PRO         |
| 1          | B            | 2117       | PRO         |
| 1          | B            | 2129       | MET         |
| 1          | B            | 2210       | PRO         |
| 1          | A            | 52         | LYS         |
| 1          | A            | 175        | SER         |
| 1          | A            | 177        | VAL         |
| 1          | A            | 564        | GLN         |
| 1          | A            | 600        | HIS         |
| 1          | A            | 684        | GLU         |
| 1          | A            | 716        | ALA         |
| 1          | A            | 717        | GLN         |
| 1          | A            | 725        | GLU         |
| 1          | A            | 740        | PHE         |
| 1          | A            | 854        | PHE         |
| 1          | A            | 1027       | ALA         |
| 1          | A            | 1095       | GLN         |
| 1          | A            | 1267       | ILE         |
| 1          | A            | 1288       | ASN         |
| 1          | A            | 1346       | ASN         |
| 1          | A            | 1347       | ASP         |
| 1          | A            | 1349       | ALA         |
| 1          | A            | 1372       | MET         |
| 1          | A            | 1435       | VAL         |
| 1          | A            | 1458       | CYS         |
| 1          | A            | 1461       | CYS         |
| 1          | A            | 1464       | THR         |
| 1          | A            | 1865       | VAL         |
| 1          | A            | 1881       | LEU         |
| 1          | A            | 1984       | GLN         |
| 1          | A            | 2011       | GLY         |
| 1          | A            | 2021       | GLY         |
| 1          | A            | 2115       | MET         |
| 1          | A            | 2146       | ALA         |
| 1          | A            | 2148       | PRO         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 12         | GLY         |
| 1          | B            | 63         | MET         |
| 1          | B            | 75         | ALA         |
| 1          | B            | 118        | GLY         |
| 1          | B            | 135        | ASN         |
| 1          | B            | 221        | VAL         |
| 1          | B            | 307        | HIS         |
| 1          | B            | 313        | TYR         |
| 1          | B            | 380        | SER         |
| 1          | B            | 381        | LEU         |
| 1          | B            | 414        | VAL         |
| 1          | B            | 422        | PRO         |
| 1          | B            | 423        | LEU         |
| 1          | B            | 450        | SER         |
| 1          | B            | 484        | VAL         |
| 1          | B            | 573        | TYR         |
| 1          | B            | 603        | ARG         |
| 1          | B            | 640        | SER         |
| 1          | B            | 665        | LEU         |
| 1          | B            | 767        | CYS         |
| 1          | B            | 790        | VAL         |
| 1          | B            | 849        | CYS         |
| 1          | B            | 893        | ALA         |
| 1          | B            | 1460       | ALA         |
| 1          | B            | 1461       | CYS         |
| 1          | B            | 1639       | ASN         |
| 1          | B            | 1797       | HIS         |
| 1          | B            | 1801       | GLU         |
| 1          | B            | 1817       | ASP         |
| 1          | B            | 1850       | LYS         |
| 1          | B            | 2146       | ALA         |
| 1          | A            | 100        | LYS         |
| 1          | A            | 227        | SER         |
| 1          | A            | 396        | ASN         |
| 1          | A            | 405        | PRO         |
| 1          | A            | 413        | PRO         |
| 1          | A            | 450        | SER         |
| 1          | A            | 604        | LYS         |
| 1          | A            | 1061       | LEU         |
| 1          | A            | 1086       | HIS         |
| 1          | A            | 1462       | ASN         |
| 1          | A            | 1630       | HIS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1820       | PHE         |
| 1          | A            | 1953       | LYS         |
| 1          | A            | 2060       | ASN         |
| 1          | A            | 2165       | HIS         |
| 1          | B            | 66         | TYR         |
| 1          | B            | 114        | VAL         |
| 1          | B            | 126        | LEU         |
| 1          | B            | 264        | LEU         |
| 1          | B            | 379        | ASP         |
| 1          | B            | 434        | PRO         |
| 1          | B            | 514        | ASN         |
| 1          | B            | 521        | LYS         |
| 1          | B            | 682        | THR         |
| 1          | B            | 686        | ALA         |
| 1          | B            | 707        | ILE         |
| 1          | B            | 722        | GLY         |
| 1          | B            | 776        | ASP         |
| 1          | B            | 993        | LEU         |
| 1          | B            | 1002       | ASP         |
| 1          | B            | 1116       | LYS         |
| 1          | B            | 1200       | GLN         |
| 1          | B            | 1241       | LEU         |
| 1          | B            | 1268       | LEU         |
| 1          | B            | 1388       | LYS         |
| 1          | B            | 1391       | TYR         |
| 1          | B            | 1821       | HIS         |
| 1          | B            | 2060       | ASN         |
| 1          | B            | 2085       | LEU         |
| 1          | B            | 2130       | GLN         |
| 1          | B            | 2165       | HIS         |
| 1          | B            | 2205       | GLU         |
| 1          | A            | 40         | GLN         |
| 1          | A            | 51         | LYS         |
| 1          | A            | 447        | ASN         |
| 1          | A            | 599        | LEU         |
| 1          | A            | 704        | ASN         |
| 1          | A            | 1096       | ALA         |
| 1          | A            | 1221       | PRO         |
| 1          | A            | 1299       | ILE         |
| 1          | A            | 1887       | ASP         |
| 1          | A            | 2202       | ARG         |
| 1          | B            | 41         | PRO         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 279        | LYS         |
| 1          | B            | 684        | GLU         |
| 1          | B            | 694        | GLU         |
| 1          | B            | 699        | PHE         |
| 1          | B            | 778        | ARG         |
| 1          | B            | 887        | LEU         |
| 1          | B            | 968        | MET         |
| 1          | B            | 982        | LEU         |
| 1          | B            | 1198       | ARG         |
| 1          | B            | 1211       | HIS         |
| 1          | B            | 1290       | ARG         |
| 1          | B            | 1632       | PRO         |
| 1          | B            | 1881       | LEU         |
| 1          | B            | 2070       | LEU         |
| 1          | A            | 602        | ASN         |
| 1          | A            | 645        | ILE         |
| 1          | A            | 790        | VAL         |
| 1          | A            | 852        | PHE         |
| 1          | A            | 895        | LEU         |
| 1          | A            | 897        | CYS         |
| 1          | A            | 1275       | HIS         |
| 1          | A            | 1463       | ASN         |
| 1          | A            | 2020       | LEU         |
| 1          | A            | 2190       | LYS         |
| 1          | A            | 2215       | CYS         |
| 1          | B            | 230        | LYS         |
| 1          | B            | 285        | GLU         |
| 1          | B            | 424        | LYS         |
| 1          | B            | 439        | GLU         |
| 1          | B            | 473        | VAL         |
| 1          | B            | 522        | LEU         |
| 1          | B            | 703        | SER         |
| 1          | B            | 863        | THR         |
| 1          | B            | 1271       | VAL         |
| 1          | B            | 1996       | TYR         |
| 1          | B            | 2029       | VAL         |
| 1          | B            | 2147       | SER         |
| 1          | B            | 2207       | ILE         |
| 1          | B            | 2209       | PHE         |
| 1          | A            | 120        | VAL         |
| 1          | A            | 705        | LYS         |
| 1          | A            | 715        | LEU         |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1369 | SER  |
| 1   | A     | 1466 | ASP  |
| 1   | A     | 1991 | ASN  |
| 1   | A     | 2147 | SER  |
| 1   | B     | 418  | ILE  |
| 1   | B     | 680  | VAL  |
| 1   | B     | 1466 | ASP  |
| 1   | B     | 1651 | PHE  |
| 1   | A     | 38   | VAL  |
| 1   | A     | 178  | ILE  |
| 1   | A     | 383  | PRO  |
| 1   | B     | 191  | GLN  |
| 1   | B     | 367  | ILE  |
| 1   | B     | 1299 | ILE  |
| 1   | A     | 559  | VAL  |
| 1   | A     | 707  | ILE  |
| 1   | A     | 1874 | VAL  |
| 1   | A     | 2062 | ILE  |
| 1   | B     | 1291 | VAL  |
| 1   | B     | 1341 | VAL  |
| 1   | B     | 1370 | PRO  |
| 1   | A     | 1418 | VAL  |
| 1   | B     | 179  | GLY  |
| 1   | B     | 1631 | ARG  |
| 1   | A     | 894  | ILE  |
| 1   | A     | 1838 | ILE  |
| 1   | A     | 1967 | PRO  |
| 1   | B     | 212  | VAL  |
| 1   | B     | 2045 | GLY  |
| 1   | B     | 186  | PRO  |

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| 1   | A     | 1710/2217 (77%) | 0.34   | 184 (10%) <b>5</b> <b>9</b>  | 0, 157, 428, 888      | 0     |
| 1   | B     | 1708/2217 (77%) | 0.29   | 175 (10%) <b>6</b> <b>10</b> | 0, 136, 432, 776      | 0     |
| All | All   | 3418/4434 (77%) | 0.31   | 359 (10%) <b>6</b> <b>9</b>  | 0, 147, 430, 888      | 0     |

All (359) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 2102 | ARG  | 18.5 |
| 1   | A     | 2103 | HIS  | 16.7 |
| 1   | A     | 2101 | SER  | 13.2 |
| 1   | A     | 2107 | ASN  | 13.0 |
| 1   | A     | 1395 | LYS  | 11.4 |
| 1   | A     | 1387 | GLY  | 11.0 |
| 1   | B     | 1442 | THR  | 10.8 |
| 1   | B     | 1439 | GLU  | 10.8 |
| 1   | A     | 2104 | ASP  | 10.7 |
| 1   | B     | 2216 | GLU  | 10.5 |
| 1   | B     | 1443 | SER  | 10.5 |
| 1   | B     | 1438 | LYS  | 10.4 |
| 1   | B     | 1437 | MET  | 10.3 |
| 1   | A     | 1396 | CYS  | 10.1 |
| 1   | A     | 1385 | THR  | 9.7  |
| 1   | B     | 1436 | GLU  | 9.5  |
| 1   | A     | 2105 | SER  | 9.4  |
| 1   | B     | 588  | ASP  | 9.4  |
| 1   | B     | 1326 | CYS  | 9.0  |
| 1   | A     | 1458 | CYS  | 9.0  |
| 1   | B     | 1329 | MET  | 8.8  |
| 1   | A     | 1388 | LYS  | 8.6  |
| 1   | A     | 2106 | GLU  | 8.6  |
| 1   | A     | 1454 | LEU  | 8.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 1457       | ILE         | 8.3         |
| 1          | B            | 2018       | GLY         | 7.9         |
| 1          | B            | 1328       | ASP         | 7.8         |
| 1          | B            | 2019       | LEU         | 7.7         |
| 1          | A            | 2099       | MET         | 7.6         |
| 1          | B            | 639        | VAL         | 7.5         |
| 1          | A            | 2142       | GLU         | 7.4         |
| 1          | A            | 2140       | ASN         | 7.3         |
| 1          | A            | 2141       | GLY         | 7.2         |
| 1          | B            | 2163       | ALA         | 7.0         |
| 1          | A            | 1386       | GLU         | 7.0         |
| 1          | B            | 585        | ILE         | 7.0         |
| 1          | B            | 2215       | CYS         | 6.9         |
| 1          | B            | 463        | GLY         | 6.9         |
| 1          | B            | 2205       | GLU         | 6.8         |
| 1          | B            | 1370       | PRO         | 6.7         |
| 1          | B            | 2020       | LEU         | 6.6         |
| 1          | A            | 1389       | ASN         | 6.6         |
| 1          | B            | 584        | GLN         | 6.6         |
| 1          | B            | 1389       | ASN         | 6.5         |
| 1          | A            | 1384       | CYS         | 6.5         |
| 1          | A            | 1455       | VAL         | 6.5         |
| 1          | B            | 1413       | ASP         | 6.4         |
| 1          | A            | 215        | ASN         | 6.3         |
| 1          | A            | 1456       | ASP         | 6.2         |
| 1          | B            | 2164       | ARG         | 6.2         |
| 1          | B            | 638        | CYS         | 6.2         |
| 1          | A            | 2210       | PRO         | 6.1         |
| 1          | B            | 1327       | GLN         | 6.1         |
| 1          | A            | 1468       | LYS         | 6.1         |
| 1          | B            | 1416       | PRO         | 6.1         |
| 1          | B            | 1307       | GLN         | 6.0         |
| 1          | B            | 582        | GLN         | 6.0         |
| 1          | A            | 1026       | GLY         | 6.0         |
| 1          | B            | 1325       | LYS         | 6.0         |
| 1          | B            | 1369       | SER         | 5.9         |
| 1          | B            | 462        | LYS         | 5.9         |
| 1          | B            | 2206       | GLN         | 5.8         |
| 1          | B            | 1415       | ILE         | 5.7         |
| 1          | B            | 1385       | THR         | 5.7         |
| 1          | B            | 1440       | ILE         | 5.7         |
| 1          | A            | 2196       | GLU         | 5.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 2143       | ASP         | 5.6         |
| 1          | B            | 1444       | ASN         | 5.5         |
| 1          | A            | 309        | ALA         | 5.5         |
| 1          | A            | 2100       | GLU         | 5.5         |
| 1          | A            | 2098       | ILE         | 5.5         |
| 1          | A            | 1027       | ALA         | 5.4         |
| 1          | B            | 1429       | CYS         | 5.4         |
| 1          | B            | 1388       | LYS         | 5.4         |
| 1          | B            | 1414       | CYS         | 5.3         |
| 1          | B            | 1387       | GLY         | 5.3         |
| 1          | B            | 1465       | SER         | 5.3         |
| 1          | A            | 2108       | ALA         | 5.3         |
| 1          | A            | 1177       | LYS         | 5.2         |
| 1          | A            | 305        | PHE         | 5.2         |
| 1          | B            | 583        | LYS         | 5.2         |
| 1          | B            | 586        | GLY         | 5.2         |
| 1          | A            | 2042       | TYR         | 5.1         |
| 1          | B            | 1834       | GLY         | 5.1         |
| 1          | B            | 2023       | TYR         | 5.1         |
| 1          | A            | 1984       | GLN         | 5.1         |
| 1          | A            | 1178       | GLU         | 5.1         |
| 1          | B            | 1330       | VAL         | 5.1         |
| 1          | A            | 1368       | ASN         | 5.0         |
| 1          | B            | 1427       | ASN         | 5.0         |
| 1          | A            | 2198       | VAL         | 4.9         |
| 1          | A            | 1367       | GLU         | 4.9         |
| 1          | B            | 1835       | ASN         | 4.9         |
| 1          | A            | 1451       | GLU         | 4.9         |
| 1          | B            | 1428       | HIS         | 4.9         |
| 1          | A            | 310        | THR         | 4.8         |
| 1          | B            | 1386       | GLU         | 4.8         |
| 1          | A            | 37         | CYS         | 4.8         |
| 1          | B            | 1348       | ARG         | 4.8         |
| 1          | A            | 2043       | CYS         | 4.7         |
| 1          | B            | 195        | ALA         | 4.7         |
| 1          | B            | 1430       | TYR         | 4.7         |
| 1          | B            | 459        | LYS         | 4.6         |
| 1          | B            | 587        | TYR         | 4.6         |
| 1          | B            | 1431       | VAL         | 4.6         |
| 1          | B            | 640        | SER         | 4.6         |
| 1          | B            | 194        | HIS         | 4.5         |
| 1          | A            | 2197       | ILE         | 4.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 2209       | PHE         | 4.4         |
| 1          | B            | 2204       | MET         | 4.4         |
| 1          | A            | 1398       | SER         | 4.4         |
| 1          | B            | 589        | VAL         | 4.4         |
| 1          | A            | 209        | VAL         | 4.4         |
| 1          | A            | 1132       | TRP         | 4.4         |
| 1          | A            | 1394       | ILE         | 4.4         |
| 1          | A            | 2050       | ASN         | 4.3         |
| 1          | A            | 2110       | ARG         | 4.3         |
| 1          | A            | 987        | ASP         | 4.3         |
| 1          | A            | 1414       | CYS         | 4.2         |
| 1          | B            | 461        | GLU         | 4.2         |
| 1          | B            | 1333       | GLU         | 4.2         |
| 1          | B            | 1441       | TYR         | 4.1         |
| 1          | B            | 23         | THR         | 4.1         |
| 1          | B            | 2217       | PHE         | 4.1         |
| 1          | A            | 1983       | LEU         | 4.0         |
| 1          | A            | 2047       | CYS         | 4.0         |
| 1          | A            | 1642       | ALA         | 4.0         |
| 1          | B            | 1350       | SER         | 4.0         |
| 1          | A            | 1887       | ASP         | 4.0         |
| 1          | B            | 581        | MET         | 4.0         |
| 1          | A            | 1397       | ASN         | 4.0         |
| 1          | B            | 1349       | ALA         | 4.0         |
| 1          | B            | 2017       | LEU         | 4.0         |
| 1          | A            | 1288       | ASN         | 4.0         |
| 1          | B            | 1306       | VAL         | 3.9         |
| 1          | A            | 753        | ASN         | 3.9         |
| 1          | B            | 2207       | ILE         | 3.9         |
| 1          | B            | 1833       | GLY         | 3.9         |
| 1          | A            | 900        | VAL         | 3.9         |
| 1          | A            | 283        | GLU         | 3.9         |
| 1          | B            | 2165       | HIS         | 3.8         |
| 1          | A            | 2046       | PRO         | 3.8         |
| 1          | B            | 2160       | HIS         | 3.8         |
| 1          | A            | 879        | TYR         | 3.8         |
| 1          | A            | 1888       | ASP         | 3.8         |
| 1          | B            | 1305       | ASN         | 3.7         |
| 1          | B            | 405        | PRO         | 3.7         |
| 1          | B            | 403        | ASN         | 3.7         |
| 1          | B            | 1002       | ASP         | 3.7         |
| 1          | A            | 2051       | GLN         | 3.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 2139       | GLU         | 3.6         |
| 1          | B            | 1466       | ASP         | 3.6         |
| 1          | A            | 195        | ALA         | 3.6         |
| 1          | A            | 2048       | HIS         | 3.6         |
| 1          | A            | 307        | HIS         | 3.6         |
| 1          | B            | 402        | THR         | 3.6         |
| 1          | B            | 1405       | ILE         | 3.6         |
| 1          | A            | 196        | SER         | 3.6         |
| 1          | A            | 1467       | ARG         | 3.5         |
| 1          | A            | 216        | THR         | 3.5         |
| 1          | A            | 1459       | ARG         | 3.5         |
| 1          | B            | 2074       | ASN         | 3.5         |
| 1          | A            | 306        | LYS         | 3.5         |
| 1          | B            | 1373       | TYR         | 3.5         |
| 1          | A            | 308        | LEU         | 3.5         |
| 1          | A            | 2199       | ARG         | 3.5         |
| 1          | B            | 404        | ILE         | 3.4         |
| 1          | B            | 2138       | GLY         | 3.4         |
| 1          | A            | 1492       | SER         | 3.4         |
| 1          | A            | 2045       | GLY         | 3.4         |
| 1          | B            | 25         | GLY         | 3.4         |
| 1          | A            | 880        | ASN         | 3.4         |
| 1          | A            | 2052       | ASN         | 3.3         |
| 1          | B            | 295        | GLY         | 3.3         |
| 1          | B            | 418        | ILE         | 3.3         |
| 1          | A            | 1434       | GLU         | 3.3         |
| 1          | A            | 1310       | LYS         | 3.3         |
| 1          | A            | 2029       | VAL         | 3.2         |
| 1          | A            | 1491       | SER         | 3.2         |
| 1          | A            | 754        | GLU         | 3.2         |
| 1          | A            | 2165       | HIS         | 3.2         |
| 1          | B            | 1371       | LEU         | 3.2         |
| 1          | A            | 2137       | ASP         | 3.2         |
| 1          | A            | 2109       | GLU         | 3.2         |
| 1          | B            | 1417       | GLU         | 3.2         |
| 1          | B            | 1310       | LYS         | 3.2         |
| 1          | A            | 1279       | ASN         | 3.2         |
| 1          | A            | 1438       | LYS         | 3.2         |
| 1          | A            | 1280       | ASN         | 3.2         |
| 1          | A            | 878        | PHE         | 3.2         |
| 1          | B            | 2166       | ASN         | 3.2         |
| 1          | A            | 285        | GLU         | 3.2         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 142        | LEU         | 3.2         |
| 1          | A            | 2144       | GLY         | 3.1         |
| 1          | B            | 1324       | LYS         | 3.1         |
| 1          | A            | 314        | LEU         | 3.1         |
| 1          | A            | 1436       | GLU         | 3.1         |
| 1          | A            | 2027       | LYS         | 3.1         |
| 1          | A            | 2095       | LEU         | 3.1         |
| 1          | B            | 460        | LEU         | 3.1         |
| 1          | A            | 2097       | ALA         | 3.1         |
| 1          | B            | 2203       | THR         | 3.1         |
| 1          | A            | 210        | ASN         | 3.1         |
| 1          | B            | 66         | TYR         | 3.0         |
| 1          | B            | 2139       | GLU         | 3.0         |
| 1          | B            | 2162       | LEU         | 3.0         |
| 1          | A            | 1982       | ASP         | 3.0         |
| 1          | B            | 24         | ASN         | 3.0         |
| 1          | A            | 1392       | THR         | 3.0         |
| 1          | B            | 1372       | MET         | 3.0         |
| 1          | A            | 1441       | TYR         | 3.0         |
| 1          | B            | 464        | THR         | 3.0         |
| 1          | A            | 1493       | PRO         | 3.0         |
| 1          | A            | 1435       | VAL         | 3.0         |
| 1          | B            | 2079       | LYS         | 3.0         |
| 1          | A            | 1488       | THR         | 3.0         |
| 1          | A            | 409        | GLU         | 2.9         |
| 1          | B            | 2202       | ARG         | 2.9         |
| 1          | B            | 2161       | GLN         | 2.9         |
| 1          | B            | 1467       | ARG         | 2.9         |
| 1          | A            | 1433       | THR         | 2.9         |
| 1          | A            | 2138       | GLY         | 2.9         |
| 1          | A            | 1289       | GLU         | 2.9         |
| 1          | B            | 28         | SER         | 2.9         |
| 1          | A            | 129        | ASN         | 2.9         |
| 1          | A            | 2200       | LEU         | 2.9         |
| 1          | B            | 1435       | VAL         | 2.9         |
| 1          | B            | 1384       | CYS         | 2.9         |
| 1          | A            | 1089       | GLN         | 2.8         |
| 1          | A            | 135        | ASN         | 2.8         |
| 1          | A            | 626        | ARG         | 2.8         |
| 1          | B            | 1177       | LYS         | 2.8         |
| 1          | B            | 579        | GLY         | 2.8         |
| 1          | A            | 627        | GLU         | 2.8         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 2028       | ASN         | 2.8         |
| 1          | A            | 304        | ARG         | 2.8         |
| 1          | A            | 2161       | GLN         | 2.8         |
| 1          | B            | 704        | ASN         | 2.8         |
| 1          | A            | 1415       | ILE         | 2.8         |
| 1          | A            | 52         | LYS         | 2.8         |
| 1          | A            | 751        | ALA         | 2.8         |
| 1          | A            | 1439       | GLU         | 2.7         |
| 1          | B            | 578        | PHE         | 2.7         |
| 1          | B            | 1829       | ALA         | 2.7         |
| 1          | B            | 2193       | ALA         | 2.7         |
| 1          | A            | 1989       | CYS         | 2.7         |
| 1          | A            | 208        | GLU         | 2.7         |
| 1          | A            | 2041       | GLU         | 2.7         |
| 1          | A            | 38         | VAL         | 2.7         |
| 1          | B            | 267        | THR         | 2.7         |
| 1          | B            | 1404       | ASP         | 2.6         |
| 1          | B            | 85         | ASP         | 2.6         |
| 1          | B            | 1464       | THR         | 2.6         |
| 1          | B            | 2194       | GLN         | 2.6         |
| 1          | A            | 311        | GLY         | 2.6         |
| 1          | B            | 2201       | ASP         | 2.6         |
| 1          | A            | 1300       | GLU         | 2.6         |
| 1          | A            | 143        | GLU         | 2.6         |
| 1          | A            | 1179       | ILE         | 2.6         |
| 1          | A            | 1099       | GLN         | 2.6         |
| 1          | B            | 2159       | ALA         | 2.6         |
| 1          | B            | 2024       | ILE         | 2.6         |
| 1          | A            | 282        | TRP         | 2.6         |
| 1          | B            | 417        | LYS         | 2.6         |
| 1          | A            | 377        | GLY         | 2.6         |
| 1          | B            | 1681       | MET         | 2.6         |
| 1          | B            | 1003       | GLU         | 2.5         |
| 1          | A            | 1889       | GLU         | 2.5         |
| 1          | A            | 2211       | VAL         | 2.5         |
| 1          | A            | 1278       | MET         | 2.5         |
| 1          | A            | 1437       | MET         | 2.5         |
| 1          | A            | 1242       | GLN         | 2.5         |
| 1          | B            | 1304       | ARG         | 2.5         |
| 1          | A            | 2166       | ASN         | 2.5         |
| 1          | B            | 1303       | GLY         | 2.5         |
| 1          | A            | 1086       | HIS         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 2049       | GLU         | 2.5         |
| 1          | A            | 899        | HIS         | 2.5         |
| 1          | B            | 213        | ASN         | 2.5         |
| 1          | B            | 196        | SER         | 2.4         |
| 1          | B            | 458        | GLY         | 2.4         |
| 1          | B            | 1302       | HIS         | 2.4         |
| 1          | B            | 1432       | ASP         | 2.4         |
| 1          | B            | 969        | ASP         | 2.4         |
| 1          | B            | 1004       | SER         | 2.4         |
| 1          | A            | 1180       | LEU         | 2.4         |
| 1          | A            | 1360       | SER         | 2.4         |
| 1          | A            | 1489       | PHE         | 2.4         |
| 1          | A            | 1243       | ASN         | 2.4         |
| 1          | B            | 1390       | VAL         | 2.4         |
| 1          | B            | 580        | PHE         | 2.4         |
| 1          | B            | 660        | THR         | 2.4         |
| 1          | A            | 1886       | LYS         | 2.4         |
| 1          | B            | 1346       | ASN         | 2.3         |
| 1          | B            | 1679       | ARG         | 2.3         |
| 1          | A            | 1416       | PRO         | 2.3         |
| 1          | B            | 661        | ASN         | 2.3         |
| 1          | A            | 51         | LYS         | 2.3         |
| 1          | A            | 2112       | LEU         | 2.3         |
| 1          | B            | 2045       | GLY         | 2.3         |
| 1          | A            | 2044       | GLN         | 2.3         |
| 1          | B            | 294        | GLY         | 2.3         |
| 1          | B            | 1339       | GLU         | 2.3         |
| 1          | A            | 1133       | VAL         | 2.3         |
| 1          | A            | 1452       | ASN         | 2.3         |
| 1          | A            | 752        | ILE         | 2.3         |
| 1          | A            | 2096       | LEU         | 2.3         |
| 1          | B            | 1001       | PHE         | 2.3         |
| 1          | B            | 1300       | GLU         | 2.3         |
| 1          | A            | 1462       | ASN         | 2.3         |
| 1          | A            | 1641       | ASP         | 2.3         |
| 1          | A            | 2082       | ASP         | 2.3         |
| 1          | B            | 575        | ALA         | 2.3         |
| 1          | B            | 1830       | LEU         | 2.3         |
| 1          | B            | 1832       | GLU         | 2.2         |
| 1          | A            | 1329       | MET         | 2.2         |
| 1          | B            | 2146       | ALA         | 2.2         |
| 1          | B            | 1456       | ASP         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1347 | ASP  | 2.2  |
| 1   | B     | 1605 | ASP  | 2.2  |
| 1   | A     | 826  | LYS  | 2.2  |
| 1   | B     | 1243 | ASN  | 2.2  |
| 1   | B     | 2046 | PRO  | 2.2  |
| 1   | B     | 1988 | ARG  | 2.2  |
| 1   | B     | 1053 | ASP  | 2.2  |
| 1   | A     | 145  | ASN  | 2.2  |
| 1   | B     | 419  | GLY  | 2.2  |
| 1   | A     | 27   | ILE  | 2.2  |
| 1   | A     | 1352 | GLN  | 2.2  |
| 1   | A     | 571  | GLN  | 2.2  |
| 1   | B     | 2002 | THR  | 2.2  |
| 1   | A     | 141  | LEU  | 2.2  |
| 1   | B     | 2080 | ARG  | 2.2  |
| 1   | B     | 52   | LYS  | 2.1  |
| 1   | B     | 2001 | GLU  | 2.1  |
| 1   | B     | 1434 | GLU  | 2.1  |
| 1   | B     | 401  | SER  | 2.1  |
| 1   | B     | 1412 | GLU  | 2.1  |
| 1   | B     | 960  | PRO  | 2.1  |
| 1   | A     | 1366 | ASP  | 2.1  |
| 1   | B     | 137  | ARG  | 2.1  |
| 1   | A     | 2026 | GLU  | 2.1  |
| 1   | B     | 27   | ILE  | 2.1  |
| 1   | A     | 1277 | PHE  | 2.1  |
| 1   | A     | 1333 | GLU  | 2.1  |
| 1   | A     | 1461 | CYS  | 2.1  |
| 1   | A     | 2030 | ALA  | 2.1  |
| 1   | A     | 2160 | HIS  | 2.1  |
| 1   | B     | 2021 | GLY  | 2.1  |
| 1   | B     | 2073 | ILE  | 2.0  |
| 1   | A     | 1985 | ASN  | 2.0  |
| 1   | B     | 210  | ASN  | 2.0  |
| 1   | A     | 697  | TRP  | 2.0  |
| 1   | A     | 2212 | PRO  | 2.0  |
| 1   | B     | 1029 | ASP  | 2.0  |
| 1   | B     | 1461 | CYS  | 2.0  |
| 1   | A     | 378  | GLY  | 2.0  |
| 1   | B     | 1402 | LEU  | 2.0  |
| 1   | A     | 827  | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.