



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 05:35 pm GMT

PDB ID : 6ZH2  
EMDB ID : EMD-11211  
Title : Cryo-EM structure of DNA-PKcs (State 1)  
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.  
Deposited on : 2020-06-20  
Resolution : 3.92 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

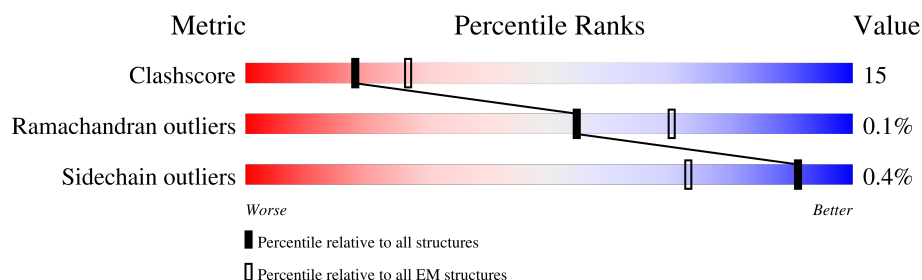
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

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

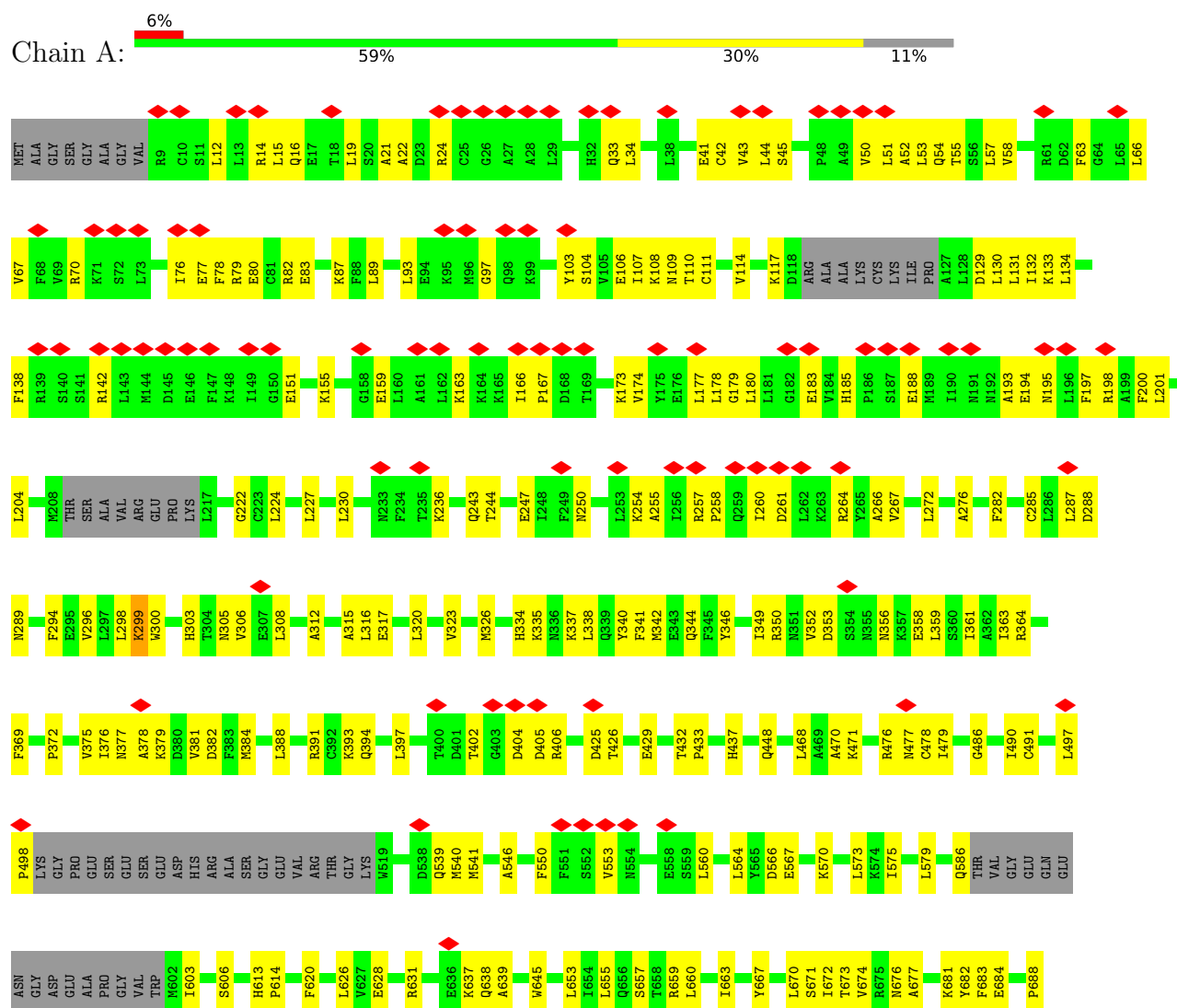
| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 4156   |                  |



### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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





|       |       |       |     |     |       |       |       |       |       |       |
|-------|-------|-------|-----|-----|-------|-------|-------|-------|-------|-------|
| L2812 | L2929 | H3070 | PRO | GLN | Q2432 | L2349 | D2269 | A2173 | W2089 | L1939 |
| F2813 | L2933 | L3073 | SER | GLY | R2433 | L2349 | D2269 | A2173 | R2090 | TYR   |
| D2821 | L2933 | L3078 | SER | THR | V2434 | Q2352 | N2270 | E2175 | R2091 | TYR   |
| E2828 | R2940 | E3085 | SER | GLN | C2435 | Q2353 | G2273 | G2178 | E2092 | ALA   |
|       |       |       | LEU | THR | I2438 | W2356 | I2274 |       | C2093 | ALA   |
|       |       |       | LEU | ARG | R2522 | E2357 |       |       | L2097 | SER   |
|       |       |       | LEU | THR | N2523 | E2357 |       |       | L2100 | THR   |
|       |       |       | PHE | THR | Y2440 | K2441 |       |       | V2101 | LEU   |
|       |       |       | ALA | GLN | R2529 | D2358 |       |       | M2104 | GLU   |
|       |       |       | HIS | GLU | R2530 | K2359 |       |       | L1977 | GLU   |
|       |       |       | LVS | GLY | M2442 | N2283 |       |       | F1978 | GLU   |
|       |       |       | ARG | GLY | M2443 | D2284 |       |       | N1980 | GLN   |
|       |       |       | ARG | SER | M2444 | L2285 |       |       | F1979 | SER   |
|       |       |       | SER | LEU | R2538 | W2365 |       |       | N1981 | ASP   |
|       |       |       | GLU | LEU | L2539 | T2368 |       |       | K1985 | PHE   |
|       |       |       | GLU | ALA | L2540 | K2369 |       |       | ARG   | ARG   |
|       |       |       | ARG | ALA | A2541 | D2448 |       |       | THR   | THR   |
|       |       |       | LEU | ARG | V2449 | A2375 |       |       | GLY   | GLY   |
|       |       |       | GLM | TRP | N2543 | D2376 |       |       | GLU   | VAL   |
|       |       |       | ARG | PRO | L2451 | R2377 |       |       | GLU   | GLN   |
|       |       |       | ALA | VAL |       | F2378 |       |       | ASP   | PRO   |
|       |       |       | PRO | ALA | L2454 | W2379 |       |       | VAL   | VAL   |
|       |       |       | LEU | GLY | L2455 | N2380 |       |       | GLU   | GLN   |
|       |       |       | LEU | GLN | L2456 | P2457 |       |       | ASP   | PHE   |
|       |       |       | LVS | ILE | L2554 | V2381 |       |       | PRO   | PRO   |
|       |       |       | SER | ILE | L2555 | V2382 |       |       | TYR   | VAL   |
|       |       |       | VAL | ARG | V2458 | F2383 |       |       | GLU   | GLU   |
|       |       |       | GLY | ALA |       | F2384 |       |       | ASP   | SER   |
|       |       |       | PRO | THR | E2471 |       |       |       | VAL   | VAL   |
|       |       |       | ASP | GLN | Q2472 | K2388 |       |       | P2119 | TYR   |
|       |       |       | PHE | GLN | M2473 | L2389 |       |       | R2214 | TYR   |
|       |       |       | GLY | GLN | V2474 | A2302 |       |       | R2190 | SER   |
|       |       |       | LVS | HIS | N2475 | L2303 |       |       | D2121 | SER   |
|       |       |       | ARG | ASP | S2569 | H2390 |       |       | D2122 | GLN   |
|       |       |       | LVS | PHE | V2572 | K2394 |       |       | F2218 | ASP   |
|       |       |       | GLY | THR | P2573 | C2397 |       |       | K2312 | GLU   |
|       |       |       | LEU | LEU | N2574 | L2398 |       |       | S2194 | ARG   |
|       |       |       | LEU | THR | P2575 | V2314 |       |       | W2125 | PRO   |
|       |       |       | PRO | GLN | N2576 | Y2316 |       |       | H2130 | LVS   |
|       |       |       | GLY | THR | M2576 | E2399 |       |       | L2133 | LVS   |
|       |       |       | ASP | ALA | F2577 | V2401 |       |       | GLY   | TYR   |
|       |       |       | GLU | ASP | V2586 | V2405 |       |       | ILE   | ILE   |
|       |       |       | VAL | GLY | F2586 |       |       |       | P2139 | GLU   |
|       |       |       | ASN | ARG | Y2589 | T2409 |       |       | L2140 | ILE   |
|       |       |       | LVS | SER |       | E2410 |       |       | N2141 | ARG   |
|       |       |       | VAL | PHE | D2592 | L2411 |       |       | L2142 | ARG   |
|       |       |       | LVS | ASP | S2593 | Y2412 |       |       | GLU   | GLU   |
|       |       |       | GLY | TRP | D2594 | F2413 |       |       | R2143 | ALA   |
|       |       |       | ALA | LEU | T2595 | Q2414 |       |       | F2145 | ARG   |
|       |       |       | ALA | THR | D2596 | L2415 |       |       | L2146 | ASP   |
|       |       |       | GLY | GLY | N2493 | D2492 |       |       | A2147 | GLU   |
|       |       |       | ARG | SER | D2494 | N2493 |       |       | K2148 | ALA   |
|       |       |       | THR | SER | S2495 | R2332 |       |       | L2149 | VAL   |
|       |       |       | ASP | THR | Q2496 | R2333 |       |       | HIS   | GLY   |
|       |       |       | LEU | ASP | F2499 | K2334 |       |       | ASP   | ASP   |
|       |       |       | LEU | PRO | W2601 | F2420 |       |       | VAL   | SER   |
|       |       |       | ARG | LEU | V2607 | V2421 |       |       | T2152 | VAL   |
|       |       |       | ARG | VAL | GLU   | W2422 |       |       | T2153 | GLY   |
|       |       |       | LEU | VAL | V2607 | V2423 |       |       | R2158 | LEU   |
|       |       |       | ARG | VAL | THR   | M2424 |       |       | F2257 | GLU   |
|       |       |       | ARG | HIS | V2505 | R2425 |       |       | W2163 | PRO   |
|       |       |       | ARG | THR | GLN   | H2426 |       |       | K2259 | TYR   |
|       |       |       | PHE | SER | ALA   | R2431 |       |       | F2260 | MET   |
|       |       |       |     |     |       |       |       |       | M2085 | SER   |
|       |       |       |     |     |       |       |       |       | L2168 |       |
|       |       |       |     |     |       |       |       |       | A2172 |       |



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 38575                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 53.95                                   | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.199                                   | Depositor |
| Minimum map value                    | -0.071                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.011                                   | Depositor |
| Recommended contour level            | 0.055                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 280.36002, 280.36002, 280.36002         | wwPDB     |
| Map dimensions                       | 430, 430, 430                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.652, 0.652, 0.652                     | Depositor |



## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.27         | 0/29777     | 0.44        | 0/40278     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 29313 | 0        | 29356    | 863     | 0            |
| All | All   | 29313 | 0        | 29356    | 863     | 0            |

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

All (863) 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:3472:ILE:HA   | 1:A:3479:THR:HG21 | 1.22                     | 1.15              |
| 1:A:3472:ILE:HG23 | 1:A:3479:THR:HB   | 1.38                     | 1.02              |
| 1:A:3472:ILE:HA   | 1:A:3479:THR:CG2  | 1.93                     | 0.98              |
| 1:A:2085:MET:N    | 1:A:2184:TYR:HH   | 1.76                     | 0.84              |
| 1:A:3475:TYR:HB3  | 1:A:3478:GLU:OE2  | 1.77                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:264:ARG:HH11  | 1:A:267:VAL:HG23  | 1.47                     | 0.79              |
| 1:A:3612:ARG:HD3  | 1:A:3799:ARG:HH12 | 1.47                     | 0.79              |
| 1:A:1586:SER:HB2  | 1:A:1632:TRP:HE1  | 1.49                     | 0.78              |
| 1:A:14:ARG:HE     | 1:A:2390:HIS:HB3  | 1.51                     | 0.75              |
| 1:A:138:PHE:HA    | 1:A:142:ARG:HB2   | 1.68                     | 0.74              |
| 1:A:3684:SER:HB2  | 1:A:3685:PRO:HD3  | 1.69                     | 0.74              |
| 1:A:3319:ASN:HA   | 1:A:3323:PHE:HB3  | 1.71                     | 0.72              |
| 1:A:3026:ASP:OD1  | 1:A:3028:ASN:ND2  | 2.21                     | 0.72              |
| 1:A:2477:LEU:HA   | 1:A:2480:ILE:HG22 | 1.72                     | 0.72              |
| 1:A:76:ILE:O      | 1:A:79:ARG:HB3    | 1.89                     | 0.72              |
| 1:A:1690:GLY:HA2  | 1:A:1693:VAL:HG12 | 1.72                     | 0.72              |
| 1:A:3596:LEU:HD23 | 1:A:3601:VAL:HA   | 1.70                     | 0.72              |
| 1:A:138:PHE:HB3   | 1:A:180:LEU:HD23  | 1.71                     | 0.72              |
| 1:A:3680:LEU:HD23 | 1:A:3682:GLU:H    | 1.55                     | 0.71              |
| 1:A:356:ASN:HD22  | 1:A:404:ASP:HB3   | 1.55                     | 0.71              |
| 1:A:2383:PHE:O    | 1:A:2418:LYS:NZ   | 2.24                     | 0.71              |
| 1:A:3472:ILE:CA   | 1:A:3479:THR:HG21 | 2.13                     | 0.71              |
| 1:A:2158:ARG:HG2  | 1:A:2196:TRP:HE1  | 1.55                     | 0.70              |
| 1:A:3298:LEU:HD12 | 1:A:3333:THR:HG23 | 1.72                     | 0.70              |
| 1:A:4085:LYS:O    | 1:A:4092:GLN:NE2  | 2.24                     | 0.70              |
| 1:A:2595:TRP:O    | 1:A:2596:ARG:NH2  | 2.23                     | 0.70              |
| 1:A:3392:ALA:HB1  | 1:A:3409:VAL:HG23 | 1.72                     | 0.70              |
| 1:A:1267:TYR:HD2  | 1:A:1290:LEU:HD22 | 1.55                     | 0.70              |
| 1:A:3450:MET:HG3  | 1:A:3468:LEU:HD11 | 1.73                     | 0.70              |
| 1:A:1075:ARG:NH2  | 1:A:1117:ASP:OD2  | 2.25                     | 0.70              |
| 1:A:3699:LEU:HG   | 1:A:3719:ILE:HD13 | 1.74                     | 0.69              |
| 1:A:3668:LEU:O    | 1:A:3672:LYS:NZ   | 2.26                     | 0.69              |
| 1:A:3284:SER:HB3  | 1:A:3301:LEU:HD22 | 1.74                     | 0.69              |
| 1:A:1775:GLU:OE2  | 1:A:1822:ARG:NH1  | 2.27                     | 0.68              |
| 1:A:3589:SER:O    | 1:A:3593:ARG:HB2  | 1.93                     | 0.68              |
| 1:A:166:ILE:HG13  | 1:A:167:PRO:HD3   | 1.76                     | 0.67              |
| 1:A:1813:SER:OG   | 1:A:1816:ARG:NH2  | 2.27                     | 0.67              |
| 1:A:3459:ASN:OD1  | 1:A:3462:ARG:NH2  | 2.27                     | 0.67              |
| 1:A:1549:SER:OG   | 1:A:1550:VAL:N    | 2.28                     | 0.67              |
| 1:A:3425:ARG:NH2  | 1:A:4003:ASP:OD2  | 2.27                     | 0.67              |
| 1:A:3616:ALA:O    | 1:A:3629:ARG:NH2  | 2.27                     | 0.67              |
| 1:A:683:PHE:HD2   | 1:A:737:PRO:HG3   | 1.60                     | 0.67              |
| 1:A:3653:ARG:HH21 | 1:A:3655:LYS:HD2  | 1.59                     | 0.67              |
| 1:A:1087:ARG:HG2  | 1:A:1090:ARG:HH11 | 1.59                     | 0.67              |
| 1:A:1663:THR:HG22 | 1:A:1664:SER:H    | 1.60                     | 0.67              |
| 1:A:264:ARG:HH12  | 1:A:266:ALA:HB3   | 1.59                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:637:LYS:NZ    | 1:A:638:GLN:O     | 2.27                     | 0.66              |
| 1:A:1479:VAL:HA   | 1:A:1482:GLU:HB3  | 1.76                     | 0.66              |
| 1:A:3416:LEU:HD21 | 1:A:3445:LEU:HD21 | 1.77                     | 0.66              |
| 1:A:393:LYS:HG3   | 1:A:397:LEU:HD12  | 1.78                     | 0.66              |
| 1:A:2183:HIS:CE1  | 1:A:2185:MET:HB2  | 2.30                     | 0.66              |
| 1:A:3354:ASP:O    | 1:A:3357:ARG:HB3  | 1.96                     | 0.66              |
| 1:A:3663:THR:HA   | 1:A:3666:LEU:HD12 | 1.78                     | 0.66              |
| 1:A:3713:PRO:O    | 1:A:3716:HIS:NE2  | 2.29                     | 0.65              |
| 1:A:1889:VAL:O    | 1:A:1909:ASN:ND2  | 2.29                     | 0.65              |
| 1:A:3546:SER:O    | 1:A:3550:LYS:NZ   | 2.26                     | 0.65              |
| 1:A:721:TYR:HB3   | 1:A:725:LEU:HB2   | 1.78                     | 0.65              |
| 1:A:2890:ILE:O    | 1:A:2894:GLU:HG2  | 1.97                     | 0.65              |
| 1:A:255:ALA:HB1   | 1:A:258:PRO:HB3   | 1.77                     | 0.65              |
| 1:A:50:VAL:O      | 1:A:53:LEU:HB2    | 1.96                     | 0.64              |
| 1:A:258:PRO:HB2   | 1:A:299:LYS:HZ3   | 1.62                     | 0.64              |
| 1:A:2844:LEU:HB3  | 1:A:2875:ALA:HB1  | 1.79                     | 0.64              |
| 1:A:402:THR:HG23  | 1:A:406:ARG:HH11  | 1.62                     | 0.64              |
| 1:A:3027:LEU:HA   | 1:A:3031:TRP:HZ3  | 1.63                     | 0.64              |
| 1:A:2380:ASN:OD1  | 1:A:2381:ALA:N    | 2.30                     | 0.64              |
| 1:A:1637:SER:O    | 1:A:1642:LYS:NZ   | 2.31                     | 0.64              |
| 1:A:2255:LEU:O    | 1:A:2259:LYS:NZ   | 2.28                     | 0.64              |
| 1:A:381:VAL:HA    | 1:A:384:MET:HE2   | 1.78                     | 0.63              |
| 1:A:1285:GLU:HG2  | 1:A:1287:GLN:H    | 1.63                     | 0.63              |
| 1:A:3302:LYS:O    | 1:A:3306:LEU:N    | 2.29                     | 0.63              |
| 1:A:335:LYS:HE2   | 1:A:376:ILE:HD11  | 1.81                     | 0.63              |
| 1:A:2489:SER:OG   | 1:A:2490:GLU:OE1  | 2.17                     | 0.63              |
| 1:A:915:THR:HB    | 1:A:968:VAL:HG11  | 1.80                     | 0.63              |
| 1:A:3058:ASP:OD1  | 1:A:3059:GLN:N    | 2.32                     | 0.63              |
| 1:A:3095:ASP:OD2  | 1:A:3098:ARG:NH2  | 2.32                     | 0.62              |
| 1:A:3472:ILE:HG23 | 1:A:3479:THR:CB   | 2.23                     | 0.62              |
| 1:A:2178:GLY:O    | 1:A:2183:HIS:NE2  | 2.32                     | 0.62              |
| 1:A:3049:LEU:HD13 | 1:A:3085:GLU:HB2  | 1.80                     | 0.62              |
| 1:A:3522:THR:HG22 | 1:A:3529:ILE:HG21 | 1.81                     | 0.62              |
| 1:A:936:SER:OG    | 1:A:2773:ARG:NH1  | 2.33                     | 0.62              |
| 1:A:1607:GLU:OE2  | 1:A:1614:GLN:NE2  | 2.32                     | 0.62              |
| 1:A:3702:PRO:HB2  | 1:A:3794:VAL:HG11 | 1.82                     | 0.62              |
| 1:A:1328:GLU:HB2  | 1:A:1386:ILE:HD12 | 1.82                     | 0.62              |
| 1:A:93:LEU:O      | 1:A:97:GLY:N      | 2.33                     | 0.62              |
| 1:A:3270:ASP:HB3  | 1:A:3314:SER:HB3  | 1.82                     | 0.62              |
| 1:A:1791:CYS:HB2  | 1:A:1835:ALA:HB2  | 1.81                     | 0.62              |
| 1:A:405:ASP:OD2   | 1:A:1737:ASN:ND2  | 2.33                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2140:LEU:HA   | 1:A:2143:ARG:HE   | 1.65                     | 0.62              |
| 1:A:2288:TYR:O    | 1:A:2291:GLN:NE2  | 2.33                     | 0.62              |
| 1:A:3385:LEU:HB3  | 1:A:3416:LEU:HD13 | 1.81                     | 0.62              |
| 1:A:258:PRO:HB2   | 1:A:299:LYS:NZ    | 2.15                     | 0.61              |
| 1:A:3292:GLY:HA2  | 1:A:3348:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:3737:ARG:NH1  | 1:A:3807:GLU:OE2  | 2.34                     | 0.61              |
| 1:A:1397:ASP:O    | 1:A:1401:ASN:ND2  | 2.33                     | 0.61              |
| 1:A:2085:MET:HG3  | 1:A:2088:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:2933:ILE:HD11 | 1:A:3121:LEU:HD22 | 1.80                     | 0.61              |
| 1:A:3288:SER:O    | 1:A:3289:ARG:NE   | 2.33                     | 0.61              |
| 1:A:746:ARG:O     | 1:A:746:ARG:NH1   | 2.34                     | 0.61              |
| 1:A:2384:PHE:O    | 1:A:2388:LYS:NZ   | 2.34                     | 0.61              |
| 1:A:287:LEU:HD21  | 1:A:326:MET:HE1   | 1.81                     | 0.61              |
| 1:A:2123:PRO:HB2  | 1:A:2125:TRP:CD1  | 2.36                     | 0.61              |
| 1:A:2977:ASN:O    | 1:A:2979:GLN:NE2  | 2.33                     | 0.61              |
| 1:A:1250:LEU:HD23 | 1:A:1252:ALA:H    | 1.66                     | 0.61              |
| 1:A:1640:GLU:OE1  | 1:A:1640:GLU:N    | 2.32                     | 0.61              |
| 1:A:323:VAL:HG11  | 1:A:341:PHE:HE2   | 1.65                     | 0.61              |
| 1:A:377:ASN:OD1   | 1:A:378:ALA:N     | 2.31                     | 0.61              |
| 1:A:1299:GLU:N    | 1:A:1299:GLU:OE1  | 2.32                     | 0.61              |
| 1:A:1809:ASP:O    | 1:A:1816:ARG:NH1  | 2.34                     | 0.61              |
| 1:A:2273:GLY:O    | 1:A:2277:LEU:N    | 2.28                     | 0.61              |
| 1:A:628:GLU:OE1   | 1:A:631:ARG:NH2   | 2.33                     | 0.60              |
| 1:A:2326:ILE:O    | 1:A:2330:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:1771:GLN:H    | 1:A:1822:ARG:HH12 | 1.50                     | 0.60              |
| 1:A:767:GLU:O     | 1:A:771:ASN:ND2   | 2.34                     | 0.60              |
| 1:A:2101:VAL:HG21 | 1:A:2153:THR:HG21 | 1.84                     | 0.60              |
| 1:A:891:ARG:NH2   | 1:A:957:PRO:O     | 2.33                     | 0.60              |
| 1:A:803:SER:O     | 1:A:852:ARG:NH1   | 2.34                     | 0.60              |
| 1:A:78:PHE:O      | 1:A:82:ARG:N      | 2.29                     | 0.60              |
| 1:A:1754:GLN:HA   | 1:A:1785:ILE:HD11 | 1.84                     | 0.60              |
| 1:A:3118:ASP:OD1  | 1:A:3119:VAL:N    | 2.35                     | 0.60              |
| 1:A:1150:LYS:NZ   | 1:A:1161:ALA:O    | 2.35                     | 0.59              |
| 1:A:2940:ARG:HG2  | 1:A:2957:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:3011:LEU:HD23 | 1:A:3047:SER:HB3  | 1.83                     | 0.59              |
| 1:A:3774:ILE:HD11 | 1:A:3997:LEU:HD23 | 1.83                     | 0.59              |
| 1:A:891:ARG:HH12  | 1:A:957:PRO:HG2   | 1.67                     | 0.59              |
| 1:A:3094:ASP:OD1  | 1:A:3192:LYS:NZ   | 2.34                     | 0.59              |
| 1:A:1007:VAL:HA   | 1:A:1010:LEU:HD23 | 1.82                     | 0.59              |
| 1:A:2254:ARG:NH1  | 1:A:2299:TYR:OH   | 2.35                     | 0.59              |
| 1:A:4083:GLY:HA3  | 1:A:4090:ARG:HH21 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:674:VAL:O     | 1:A:677:ALA:HB3   | 2.03                     | 0.59              |
| 1:A:774:GLU:OE2   | 1:A:854:ARG:NH2   | 2.36                     | 0.59              |
| 1:A:1151:ARG:HB2  | 1:A:1163:LEU:HB2  | 1.84                     | 0.59              |
| 1:A:1696:LEU:HD11 | 1:A:1710:LEU:HD21 | 1.85                     | 0.58              |
| 1:A:888:ARG:HH21  | 1:A:3889:ARG:HH21 | 1.51                     | 0.58              |
| 1:A:3501:HIS:O    | 1:A:3504:ALA:HB3  | 2.03                     | 0.58              |
| 1:A:1139:GLU:O    | 1:A:1142:HIS:ND1  | 2.35                     | 0.58              |
| 1:A:1243:TYR:HA   | 1:A:1245:ARG:HH12 | 1.67                     | 0.58              |
| 1:A:3410:ILE:HD11 | 1:A:3456:LEU:HD13 | 1.86                     | 0.58              |
| 1:A:3500:SER:OG   | 1:A:3763:ARG:NH2  | 2.36                     | 0.58              |
| 1:A:33:GLN:OE1    | 1:A:33:GLN:N      | 2.36                     | 0.58              |
| 1:A:77:GLU:O      | 1:A:80:GLU:HG3    | 2.04                     | 0.58              |
| 1:A:287:LEU:HD23  | 1:A:337:LYS:HE2   | 1.85                     | 0.58              |
| 1:A:2810:SER:HA   | 1:A:2861:ILE:HD11 | 1.86                     | 0.58              |
| 1:A:1401:ASN:OD1  | 1:A:1404:LYS:NZ   | 2.34                     | 0.58              |
| 1:A:2313:LYS:HA   | 1:A:2316:TYR:HE1  | 1.66                     | 0.58              |
| 1:A:3626:GLY:HA3  | 1:A:3684:SER:O    | 2.04                     | 0.58              |
| 1:A:2145:PHE:HD1  | 1:A:2146:LEU:HD22 | 1.68                     | 0.58              |
| 1:A:2369:LYS:HZ2  | 1:A:2399:GLU:HG2  | 1.68                     | 0.58              |
| 1:A:3228:SER:O    | 1:A:3232:ARG:NE   | 2.36                     | 0.58              |
| 1:A:479:ILE:HG22  | 1:A:567:GLU:HG2   | 1.86                     | 0.57              |
| 1:A:1949:ILE:HG23 | 1:A:2100:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:3622:ALA:HB3  | 1:A:3625:LEU:HB2  | 1.86                     | 0.57              |
| 1:A:349:ILE:HD11  | 1:A:391:ARG:HG3   | 1.86                     | 0.57              |
| 1:A:3229:SER:HA   | 1:A:3232:ARG:HH21 | 1.69                     | 0.57              |
| 1:A:3328:ILE:HD12 | 1:A:3412:ALA:HA   | 1.87                     | 0.57              |
| 1:A:1664:SER:HA   | 1:A:1668:PHE:H    | 1.69                     | 0.57              |
| 1:A:2786:LYS:O    | 1:A:2789:SER:N    | 2.37                     | 0.57              |
| 1:A:3875:GLU:OE2  | 1:A:4127:TRP:HA   | 2.04                     | 0.57              |
| 1:A:1448:LEU:HD21 | 1:A:1514:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:3365:SER:HA   | 1:A:3380:ARG:HH11 | 1.70                     | 0.57              |
| 1:A:3464:LYS:NZ   | 1:A:4000:ASN:OD1  | 2.38                     | 0.57              |
| 1:A:41:GLU:HA     | 1:A:44:LEU:HB3    | 1.86                     | 0.57              |
| 1:A:849:GLU:OE2   | 1:A:3108:GLN:NE2  | 2.32                     | 0.57              |
| 1:A:2246:LYS:HG3  | 1:A:2285:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:2519:LEU:O    | 1:A:2523:ASN:ND2  | 2.38                     | 0.57              |
| 1:A:688:PRO:HB2   | 1:A:701:TYR:HE2   | 1.70                     | 0.56              |
| 1:A:868:LYS:HD2   | 1:A:3126:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:1930:GLU:HG2  | 1:A:1932:GLN:HG2  | 1.86                     | 0.56              |
| 1:A:1936:ARG:HD3  | 1:A:1939:LEU:HD12 | 1.87                     | 0.56              |
| 1:A:3597:ALA:HA   | 1:A:3656:LEU:HD13 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:631:ARG:HG3   | 1:A:672:ILE:HG21  | 1.87                     | 0.56              |
| 1:A:1039:TRP:HA   | 1:A:1042:LYS:HG2  | 1.87                     | 0.56              |
| 1:A:1248:PHE:HZ   | 1:A:1308:ALA:H    | 1.52                     | 0.56              |
| 1:A:1297:PHE:HD2  | 1:A:1298:LEU:HD12 | 1.70                     | 0.56              |
| 1:A:2213:ASN:O    | 1:A:2217:ASN:ND2  | 2.38                     | 0.56              |
| 1:A:3183:ILE:HG13 | 1:A:3242:MET:HG3  | 1.87                     | 0.56              |
| 1:A:67:VAL:HA     | 1:A:70:ARG:HB2    | 1.87                     | 0.56              |
| 1:A:346:TYR:HB3   | 1:A:350:ARG:HH12  | 1.70                     | 0.56              |
| 1:A:1367:HIS:HD2  | 1:A:1370:ARG:HH11 | 1.54                     | 0.56              |
| 1:A:3332:THR:HA   | 1:A:3335:ARG:HG2  | 1.86                     | 0.56              |
| 1:A:2254:ARG:HH11 | 1:A:2293:GLY:HA3  | 1.70                     | 0.56              |
| 1:A:2962:ARG:NH2  | 1:A:2964:ASP:OD2  | 2.38                     | 0.56              |
| 1:A:1267:TYR:CD2  | 1:A:1290:LEU:HD22 | 2.38                     | 0.56              |
| 1:A:1715:GLU:HA   | 1:A:1718:ILE:HG12 | 1.88                     | 0.56              |
| 1:A:2529:THR:OG1  | 1:A:2530:ARG:NH1  | 2.38                     | 0.56              |
| 1:A:2573:PRO:O    | 1:A:2786:LYS:NZ   | 2.34                     | 0.56              |
| 1:A:3733:ARG:HH22 | 1:A:4022:LYS:HB2  | 1.70                     | 0.56              |
| 1:A:3866:GLU:OE1  | 1:A:3866:GLU:N    | 2.34                     | 0.56              |
| 1:A:1786:ALA:O    | 1:A:1794:GLN:NE2  | 2.39                     | 0.56              |
| 1:A:1916:ILE:O    | 1:A:1920:TYR:HB2  | 2.05                     | 0.56              |
| 1:A:2303:LEU:HG   | 1:A:2323:LEU:HD21 | 1.88                     | 0.56              |
| 1:A:394:GLN:NE2   | 1:A:1685:ASP:OD2  | 2.38                     | 0.56              |
| 1:A:404:ASP:H     | 1:A:1732:GLY:HA2  | 1.71                     | 0.56              |
| 1:A:1299:GLU:O    | 1:A:1304:HIS:ND1  | 2.38                     | 0.56              |
| 1:A:3090:TYR:HA   | 1:A:3093:GLN:HG2  | 1.88                     | 0.56              |
| 1:A:2332:GLU:OE2  | 1:A:2333:ARG:NH2  | 2.39                     | 0.55              |
| 1:A:2485:ARG:NH2  | 1:A:2529:THR:O    | 2.33                     | 0.55              |
| 1:A:1855:PHE:HB3  | 1:A:1858:LEU:HD21 | 1.87                     | 0.55              |
| 1:A:12:LEU:HA     | 1:A:15:LEU:HB3    | 1.88                     | 0.55              |
| 1:A:42:CYS:SG     | 1:A:43:VAL:N      | 2.79                     | 0.55              |
| 1:A:3243:ILE:HD11 | 1:A:3255:ALA:HA   | 1.88                     | 0.55              |
| 1:A:109:ASN:OD1   | 1:A:110:THR:N     | 2.39                     | 0.55              |
| 1:A:317:GLU:OE1   | 1:A:364:ARG:NH1   | 2.39                     | 0.55              |
| 1:A:358:GLU:HA    | 1:A:361:ILE:HD12  | 1.89                     | 0.55              |
| 1:A:1072:ALA:HA   | 1:A:1075:ARG:HH21 | 1.70                     | 0.55              |
| 1:A:1356:TRP:HA   | 1:A:1359:LEU:HD13 | 1.88                     | 0.55              |
| 1:A:2919:ASP:OD1  | 1:A:2920:VAL:N    | 2.39                     | 0.55              |
| 1:A:972:LEU:HD13  | 1:A:984:TYR:HE2   | 1.72                     | 0.55              |
| 1:A:3863:ASN:N    | 1:A:3866:GLU:OE2  | 2.30                     | 0.55              |
| 1:A:108:LYS:HA    | 1:A:111:CYS:SG    | 2.47                     | 0.55              |
| 1:A:1646:LEU:HD21 | 1:A:1692:ALA:HB2  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3653:ARG:HH12 | 1:A:3659:PHE:HA   | 1.72                     | 0.55              |
| 1:A:799:TYR:O     | 1:A:852:ARG:NE    | 2.41                     | 0.54              |
| 1:A:1071:ASN:OD1  | 1:A:1073:PHE:N    | 2.37                     | 0.54              |
| 1:A:2093:CYS:HB2  | 1:A:2097:LEU:HD23 | 1.88                     | 0.54              |
| 1:A:1439:PRO:O    | 1:A:1442:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:12:LEU:O      | 1:A:16:GLN:HG3    | 2.07                     | 0.54              |
| 1:A:1281:VAL:HG23 | 1:A:1282:LEU:HG   | 1.88                     | 0.54              |
| 1:A:1407:LYS:HE2  | 1:A:1463:LEU:HG   | 1.89                     | 0.54              |
| 1:A:2207:LYS:HA   | 1:A:2210:VAL:HB   | 1.89                     | 0.54              |
| 1:A:2426:HIS:O    | 1:A:2432:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:3243:ILE:HD13 | 1:A:3258:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:111:CYS:SG    | 1:A:134:LEU:HD21  | 2.47                     | 0.54              |
| 1:A:2365:ASN:O    | 1:A:2369:LYS:HG2  | 2.07                     | 0.54              |
| 1:A:3849:LYS:HZ3  | 1:A:3851:ASP:HB2  | 1.72                     | 0.54              |
| 1:A:3596:LEU:HB3  | 1:A:3601:VAL:HG22 | 1.90                     | 0.54              |
| 1:A:2821:ASP:N    | 1:A:2821:ASP:OD1  | 2.40                     | 0.54              |
| 1:A:3603:LYS:HB3  | 1:A:3606:ILE:HB   | 1.89                     | 0.54              |
| 1:A:708:VAL:HG22  | 1:A:740:ILE:HG23  | 1.89                     | 0.54              |
| 1:A:3366:SER:OG   | 1:A:3368:GLU:OE2  | 2.25                     | 0.54              |
| 1:A:3723:ASP:OD1  | 1:A:3724:GLU:N    | 2.41                     | 0.54              |
| 1:A:305:ASN:OD1   | 1:A:306:VAL:N     | 2.41                     | 0.54              |
| 1:A:1672:PHE:HE1  | 1:A:1710:LEU:HD12 | 1.72                     | 0.54              |
| 1:A:1855:PHE:HE1  | 1:A:1867:ILE:HG22 | 1.73                     | 0.54              |
| 1:A:179:GLY:HA3   | 1:A:230:LEU:HD22  | 1.90                     | 0.53              |
| 1:A:294:PHE:HE1   | 1:A:320:LEU:HD21  | 1.72                     | 0.53              |
| 1:A:1857:LYS:HD2  | 1:A:1862:THR:HB   | 1.91                     | 0.53              |
| 1:A:1218:SER:O    | 1:A:1221:ILE:HG22 | 2.08                     | 0.53              |
| 1:A:1391:VAL:HG23 | 1:A:1392:MET:SD   | 2.48                     | 0.53              |
| 1:A:2834:GLN:O    | 1:A:2838:GLN:HG2  | 2.08                     | 0.53              |
| 1:A:4064:LEU:HD13 | 1:A:4077:TYR:HB3  | 1.88                     | 0.53              |
| 1:A:2857:CYS:O    | 1:A:2861:ILE:HG12 | 2.08                     | 0.53              |
| 1:A:478:CYS:SG    | 1:A:479:ILE:N     | 2.82                     | 0.53              |
| 1:A:2965:TYR:HB2  | 1:A:3005:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:3880:ALA:O    | 1:A:3966:GLN:NE2  | 2.41                     | 0.53              |
| 1:A:1301:ILE:HD12 | 1:A:1334:LYS:HG3  | 1.89                     | 0.53              |
| 1:A:1840:PHE:CD1  | 1:A:1880:MET:HG2  | 2.44                     | 0.53              |
| 1:A:3164:TRP:O    | 1:A:3186:ARG:NH1  | 2.38                     | 0.53              |
| 1:A:1834:ASP:OD1  | 1:A:1834:ASP:N    | 2.41                     | 0.53              |
| 1:A:1930:GLU:OE1  | 1:A:1937:ARG:NH2  | 2.41                     | 0.53              |
| 1:A:2227:LYS:HB3  | 1:A:2230:VAL:HG12 | 1.91                     | 0.53              |
| 1:A:2313:LYS:HA   | 1:A:2316:TYR:CE1  | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3169:PRO:HG2  | 1:A:3179:TRP:CE2  | 2.44                     | 0.53              |
| 1:A:1086:TYR:CD2  | 1:A:1087:ARG:HG3  | 2.43                     | 0.53              |
| 1:A:1367:HIS:CD2  | 1:A:1370:ARG:HH11 | 2.27                     | 0.53              |
| 1:A:1509:GLN:OE1  | 1:A:1509:GLN:N    | 2.34                     | 0.53              |
| 1:A:2435:CYS:O    | 1:A:2439:ILE:HG12 | 2.09                     | 0.53              |
| 1:A:978:GLN:OE1   | 1:A:981:ARG:NH1   | 2.41                     | 0.53              |
| 1:A:2312:TYR:HB2  | 1:A:2315:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:359:LEU:O     | 1:A:363:ILE:HG12  | 2.09                     | 0.52              |
| 1:A:3066:ASP:O    | 1:A:3070:HIS:ND1  | 2.41                     | 0.52              |
| 1:A:1105:VAL:HA   | 1:A:1108:MET:HE2  | 1.91                     | 0.52              |
| 1:A:1609:ALA:O    | 1:A:1611:GLN:NE2  | 2.42                     | 0.52              |
| 1:A:2439:ILE:HD12 | 1:A:2454:LEU:HD11 | 1.90                     | 0.52              |
| 1:A:3989:ARG:NH1  | 1:A:4100:GLU:OE2  | 2.42                     | 0.52              |
| 1:A:1342:MET:HE1  | 1:A:1372:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:3321:LEU:HD13 | 1:A:3324:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:51:LEU:O      | 1:A:54:GLN:HB2    | 2.09                     | 0.52              |
| 1:A:1893:GLU:OE2  | 1:A:1895:LYS:NZ   | 2.42                     | 0.52              |
| 1:A:3575:LEU:HD13 | 1:A:3802:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:3747:GLU:N    | 1:A:3747:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:789:TYR:HA    | 1:A:792:ILE:HG12  | 1.91                     | 0.52              |
| 1:A:2540:LEU:HD21 | 1:A:2832:ILE:HG23 | 1.91                     | 0.52              |
| 1:A:3243:ILE:HG12 | 1:A:3259:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:155:LYS:NZ    | 1:A:159:GLU:HB2   | 2.24                     | 0.52              |
| 1:A:1805:PHE:HD1  | 1:A:1816:ARG:HG2  | 1.73                     | 0.52              |
| 1:A:546:ALA:HA    | 1:A:550:PHE:HE1   | 1.75                     | 0.52              |
| 1:A:1019:ASP:N    | 1:A:1020:PRO:HD2  | 2.25                     | 0.52              |
| 1:A:1398:VAL:HA   | 1:A:1401:ASN:HD22 | 1.75                     | 0.52              |
| 1:A:539:GLN:N     | 1:A:539:GLN:OE1   | 2.43                     | 0.52              |
| 1:A:2543:ASN:HB3  | 1:A:2843:PHE:HZ   | 1.75                     | 0.52              |
| 1:A:342:MET:HE1   | 1:A:369:PHE:HB3   | 1.91                     | 0.52              |
| 1:A:1353:PRO:HB2  | 1:A:1356:TRP:HB2  | 1.91                     | 0.52              |
| 1:A:2394:LYS:HB3  | 1:A:2431:ARG:HH21 | 1.75                     | 0.52              |
| 1:A:2494:ASP:OD1  | 1:A:2495:SER:N    | 2.43                     | 0.52              |
| 1:A:3612:ARG:HD3  | 1:A:3799:ARG:NH1  | 2.21                     | 0.52              |
| 1:A:3681:LYS:HE2  | 1:A:3681:LYS:HA   | 1.92                     | 0.52              |
| 1:A:131:LEU:HD11  | 1:A:173:LYS:HB3   | 1.92                     | 0.52              |
| 1:A:1703:THR:HA   | 1:A:1707:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:2245:TRP:HB3  | 1:A:2249:LEU:HD23 | 1.91                     | 0.52              |
| 1:A:3582:GLU:OE2  | 1:A:3582:GLU:N    | 2.33                     | 0.52              |
| 1:A:948:MET:HG2   | 1:A:955:ALA:N     | 2.26                     | 0.51              |
| 1:A:1397:ASP:OD1  | 1:A:1398:VAL:N    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1443:VAL:HB   | 1:A:1447:ARG:HH22 | 1.75                     | 0.51              |
| 1:A:1504:ASP:OD1  | 1:A:1507:CYS:N    | 2.39                     | 0.51              |
| 1:A:1623:LEU:HB3  | 1:A:1666:GLY:HA3  | 1.93                     | 0.51              |
| 1:A:1709:GLU:O    | 1:A:1712:ARG:HG2  | 2.09                     | 0.51              |
| 1:A:1945:TYR:O    | 1:A:1949:ILE:HG12 | 2.09                     | 0.51              |
| 1:A:14:ARG:NE     | 1:A:2390:HIS:HB3  | 2.22                     | 0.51              |
| 1:A:653:LEU:O     | 1:A:657:SER:N     | 2.36                     | 0.51              |
| 1:A:891:ARG:N     | 1:A:908:ASP:OD2   | 2.42                     | 0.51              |
| 1:A:1153:LEU:HD21 | 1:A:1160:SER:HA   | 1.91                     | 0.51              |
| 1:A:1529:VAL:HG21 | 1:A:1582:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:2139:PRO:HD2  | 1:A:2142:ILE:HD12 | 1.91                     | 0.51              |
| 1:A:2594:ASP:OD1  | 1:A:2594:ASP:N    | 2.43                     | 0.51              |
| 1:A:560:LEU:HG    | 1:A:564:LEU:HD23  | 1.91                     | 0.51              |
| 1:A:1248:PHE:HZ   | 1:A:1307:ILE:HA   | 1.76                     | 0.51              |
| 1:A:1575:LEU:HD11 | 1:A:1617:LYS:HG2  | 1.92                     | 0.51              |
| 1:A:1828:LEU:O    | 1:A:1883:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:2149:LEU:O    | 1:A:2153:THR:HG22 | 2.10                     | 0.51              |
| 1:A:2184:TYR:HA   | 1:A:2187:VAL:HB   | 1.93                     | 0.51              |
| 1:A:108:LYS:NZ    | 1:A:151:GLU:OE1   | 2.40                     | 0.51              |
| 1:A:3879:PRO:O    | 1:A:3965:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:41:GLU:O      | 1:A:45:SER:OG     | 2.22                     | 0.51              |
| 1:A:197:PHE:CD1   | 1:A:227:LEU:HD21  | 2.45                     | 0.51              |
| 1:A:1338:VAL:O    | 1:A:1342:MET:HG2  | 2.11                     | 0.51              |
| 1:A:2493:ASN:H    | 1:A:2496:GLN:HE22 | 1.57                     | 0.51              |
| 1:A:2839:ASP:OD1  | 1:A:2842:ARG:NH2  | 2.40                     | 0.51              |
| 1:A:288:ASP:OD1   | 1:A:289:ASN:N     | 2.43                     | 0.51              |
| 1:A:376:ILE:HG23  | 1:A:377:ASN:H     | 1.76                     | 0.51              |
| 1:A:959:TYR:H     | 1:A:1004:GLN:HE22 | 1.57                     | 0.51              |
| 1:A:1005:ASP:O    | 1:A:1007:VAL:N    | 2.39                     | 0.51              |
| 1:A:1747:LEU:HD21 | 1:A:1778:PHE:CE1  | 2.46                     | 0.51              |
| 1:A:1754:GLN:HE22 | 1:A:1789:GLY:HA3  | 1.75                     | 0.51              |
| 1:A:2175:GLU:N    | 1:A:2175:GLU:OE1  | 2.44                     | 0.51              |
| 1:A:2283:ASN:HB3  | 1:A:2285:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:2379:MET:HA   | 1:A:2382:VAL:HG12 | 1.92                     | 0.51              |
| 1:A:2474:TYR:O    | 1:A:2478:MET:HG2  | 2.10                     | 0.51              |
| 1:A:3544:ASP:OD1  | 1:A:3547:THR:N    | 2.33                     | 0.51              |
| 1:A:3553:GLU:OE1  | 1:A:3553:GLU:N    | 2.42                     | 0.51              |
| 1:A:800:LEU:HA    | 1:A:852:ARG:HH21  | 1.76                     | 0.51              |
| 1:A:879:MET:O     | 1:A:3933:GLU:HB2  | 2.10                     | 0.51              |
| 1:A:1413:ASP:O    | 1:A:1417:THR:HG23 | 2.11                     | 0.51              |
| 1:A:1843:ILE:HG22 | 1:A:1847:ALA:HB2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2133:LEU:HD21 | 1:A:2146:LEU:HB3  | 1.92                     | 0.51              |
| 1:A:3134:ALA:O    | 1:A:3138:ILE:HG12 | 2.11                     | 0.51              |
| 1:A:3957:GLU:OE2  | 1:A:4124:TRP:NE1  | 2.44                     | 0.51              |
| 1:A:201:LEU:HD23  | 1:A:204:LEU:HD12  | 1.93                     | 0.50              |
| 1:A:566:ASP:OD1   | 1:A:645:TRP:NE1   | 2.40                     | 0.50              |
| 1:A:448:GLN:OE1   | 1:A:448:GLN:N     | 2.43                     | 0.50              |
| 1:A:1482:GLU:O    | 1:A:1486:LEU:HB2  | 2.11                     | 0.50              |
| 1:A:1866:GLN:HA   | 1:A:1869:LYS:HE2  | 1.92                     | 0.50              |
| 1:A:3236:PHE:CE2  | 1:A:3262:LEU:HD21 | 2.46                     | 0.50              |
| 1:A:250:ASN:O     | 1:A:254:LYS:HB2   | 2.11                     | 0.50              |
| 1:A:1149:LYS:NZ   | 1:A:1150:LYS:O    | 2.45                     | 0.50              |
| 1:A:3619:ASP:O    | 1:A:3621:LYS:N    | 2.36                     | 0.50              |
| 1:A:4050:LYS:HE3  | 1:A:4059:ILE:HG21 | 1.91                     | 0.50              |
| 1:A:1220:LEU:O    | 1:A:1223:THR:HG22 | 2.11                     | 0.50              |
| 1:A:2258:GLU:N    | 1:A:2258:GLU:OE1  | 2.45                     | 0.50              |
| 1:A:3169:PRO:HD3  | 1:A:3182:ILE:HD11 | 1.92                     | 0.50              |
| 1:A:12:LEU:HD11   | 1:A:44:LEU:HD22   | 1.92                     | 0.50              |
| 1:A:660:LEU:HB3   | 1:A:663:ILE:HG12  | 1.93                     | 0.50              |
| 1:A:1638:PRO:HB2  | 1:A:1641:THR:HG23 | 1.93                     | 0.50              |
| 1:A:1848:ILE:O    | 1:A:1852:LYS:N    | 2.45                     | 0.50              |
| 1:A:2257:PHE:O    | 1:A:2261:SER:OG   | 2.26                     | 0.50              |
| 1:A:2349:LEU:O    | 1:A:2353:GLN:N    | 2.43                     | 0.50              |
| 1:A:2448:PRO:HA   | 1:A:2451:LEU:HB3  | 1.93                     | 0.50              |
| 1:A:681:LYS:HB3   | 1:A:684:GLU:HB2   | 1.94                     | 0.50              |
| 1:A:1323:SER:OG   | 1:A:1326:GLU:OE2  | 2.29                     | 0.50              |
| 1:A:3532:PRO:HA   | 1:A:3535:ILE:HG22 | 1.94                     | 0.50              |
| 1:A:1367:HIS:CD2  | 1:A:1370:ARG:HD3  | 2.47                     | 0.50              |
| 1:A:1693:VAL:O    | 1:A:1696:LEU:HD23 | 2.12                     | 0.50              |
| 1:A:1179:PRO:HB3  | 1:A:1259:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:1588:ASP:OD1  | 1:A:1589:ASN:N    | 2.44                     | 0.50              |
| 1:A:2782:ASP:OD1  | 1:A:2783:ILE:N    | 2.45                     | 0.50              |
| 1:A:272:LEU:HD21  | 1:A:312:ALA:HA    | 1.94                     | 0.49              |
| 1:A:372:PRO:HA    | 1:A:375:VAL:HG22  | 1.93                     | 0.49              |
| 1:A:1880:MET:HE3  | 1:A:1884:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:2319:ALA:O    | 1:A:2323:LEU:HD23 | 2.12                     | 0.49              |
| 1:A:3636:PHE:CE2  | 1:A:3669:LYS:HB3  | 2.47                     | 0.49              |
| 1:A:3778:ASP:OD1  | 1:A:3781:CYS:N    | 2.34                     | 0.49              |
| 1:A:1935:GLU:OE1  | 1:A:1935:GLU:N    | 2.30                     | 0.49              |
| 1:A:2563:LEU:HD23 | 1:A:2795:GLN:HB2  | 1.95                     | 0.49              |
| 1:A:3496:ILE:HB   | 1:A:3707:GLY:HA2  | 1.94                     | 0.49              |
| 1:A:3580:ASN:HB2  | 1:A:3583:LEU:HD23 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2471:GLU:OE2  | 1:A:2475:ASN:ND2  | 2.44                     | 0.49              |
| 1:A:1195:VAL:HG11 | 1:A:1204:PRO:HA   | 1.95                     | 0.49              |
| 1:A:1369:MET:HA   | 1:A:1372:LEU:HB3  | 1.94                     | 0.49              |
| 1:A:1491:ILE:HG13 | 1:A:1492:ALA:N    | 2.27                     | 0.49              |
| 1:A:1866:GLN:O    | 1:A:1870:LYS:HG3  | 2.11                     | 0.49              |
| 1:A:3120:LEU:HD13 | 1:A:3896:ALA:HA   | 1.93                     | 0.49              |
| 1:A:2190:VAL:HA   | 1:A:2193:ILE:HG22 | 1.93                     | 0.49              |
| 1:A:2538:ARG:NH1  | 1:A:2561:PHE:O    | 2.42                     | 0.49              |
| 1:A:3065:ILE:O    | 1:A:3069:MET:N    | 2.36                     | 0.49              |
| 1:A:486:GLY:O     | 1:A:490:ILE:HG12  | 2.13                     | 0.49              |
| 1:A:352:VAL:HG11  | 1:A:1735:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:382:ASP:OD1   | 1:A:382:ASP:N     | 2.42                     | 0.49              |
| 1:A:3058:ASP:OD1  | 1:A:3060:SER:N    | 2.37                     | 0.49              |
| 1:A:3148:GLN:N    | 1:A:3148:GLN:OE1  | 2.46                     | 0.49              |
| 1:A:200:PHE:CZ    | 1:A:224:LEU:HB3   | 2.48                     | 0.49              |
| 1:A:883:TYR:HB3   | 1:A:3896:ALA:HB2  | 1.94                     | 0.49              |
| 1:A:1064:TYR:CG   | 1:A:1106:ILE:HD13 | 2.47                     | 0.49              |
| 1:A:3413:TYR:CD1  | 1:A:3449:LYS:HD3  | 2.47                     | 0.49              |
| 1:A:247:GLU:HB2   | 1:A:282:PHE:CD1   | 2.48                     | 0.49              |
| 1:A:1351:THR:HG23 | 1:A:1353:PRO:HD2  | 1.95                     | 0.49              |
| 1:A:1472:SER:OG   | 1:A:1473:THR:N    | 2.45                     | 0.49              |
| 1:A:2414:GLN:O    | 1:A:2418:LYS:HG2  | 2.13                     | 0.49              |
| 1:A:4086:ASP:OD1  | 1:A:4086:ASP:N    | 2.43                     | 0.49              |
| 1:A:2130:HIS:NE2  | 1:A:2163:HIS:O    | 2.39                     | 0.49              |
| 1:A:4020:MET:HG2  | 1:A:4027:TRP:CE2  | 2.48                     | 0.49              |
| 1:A:352:VAL:HG11  | 1:A:1735:ARG:HD2  | 1.95                     | 0.48              |
| 1:A:575:ILE:O     | 1:A:579:LEU:HG    | 2.13                     | 0.48              |
| 1:A:2577:PHE:O    | 1:A:2784:GLN:NE2  | 2.46                     | 0.48              |
| 1:A:4090:ARG:NH2  | 1:A:4113:ASP:OD2  | 2.42                     | 0.48              |
| 1:A:1607:GLU:O    | 1:A:1611:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:1838:GLU:O    | 1:A:1842:THR:OG1  | 2.25                     | 0.48              |
| 1:A:3592:VAL:HA   | 1:A:3595:GLU:HG2  | 1.95                     | 0.48              |
| 1:A:1221:ILE:HD11 | 1:A:1288:SER:HA   | 1.95                     | 0.48              |
| 1:A:1373:VAL:HG21 | 1:A:1418:HIS:HB3  | 1.94                     | 0.48              |
| 1:A:1775:GLU:O    | 1:A:1779:GLN:HG2  | 2.12                     | 0.48              |
| 1:A:3653:ARG:HD2  | 1:A:3655:LYS:HD2  | 1.94                     | 0.48              |
| 1:A:709:LYS:O     | 1:A:713:GLU:HG2   | 2.12                     | 0.48              |
| 1:A:2369:LYS:NZ   | 1:A:2399:GLU:HG2  | 2.28                     | 0.48              |
| 1:A:3681:LYS:HB3  | 1:A:3724:GLU:HA   | 1.96                     | 0.48              |
| 1:A:106:GLU:HA    | 1:A:109:ASN:ND2   | 2.28                     | 0.48              |
| 1:A:1601:LEU:HD13 | 1:A:1651:LYS:HB3  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:859:LEU:HD11  | 1:A:870:LEU:HD22  | 1.96                     | 0.48              |
| 1:A:2330:VAL:HG11 | 1:A:2338:GLU:HB3  | 1.94                     | 0.48              |
| 1:A:1112:ALA:HB1  | 1:A:1180:GLN:HG2  | 1.95                     | 0.48              |
| 1:A:1488:TYR:CD1  | 1:A:1531:LEU:HD21 | 2.49                     | 0.48              |
| 1:A:1854:ARG:HE   | 1:A:1855:PHE:H    | 1.61                     | 0.48              |
| 1:A:1865:THR:OG1  | 1:A:1866:GLN:OE1  | 2.31                     | 0.48              |
| 1:A:1909:ASN:OD1  | 1:A:1910:GLU:N    | 2.47                     | 0.48              |
| 1:A:3953:LEU:HD22 | 1:A:4026:SER:HB3  | 1.96                     | 0.48              |
| 1:A:429:GLU:OE1   | 1:A:429:GLU:N     | 2.42                     | 0.48              |
| 1:A:672:ILE:HG13  | 1:A:673:THR:N     | 2.28                     | 0.48              |
| 1:A:1416:GLU:HB3  | 1:A:1420:ARG:HH22 | 1.79                     | 0.48              |
| 1:A:67:VAL:HB     | 1:A:82:ARG:HH22   | 1.78                     | 0.48              |
| 1:A:3066:ASP:HA   | 1:A:3069:MET:HB2  | 1.95                     | 0.48              |
| 1:A:3868:VAL:HG23 | 1:A:4114:PRO:HB2  | 1.96                     | 0.48              |
| 1:A:1348:LEU:O    | 1:A:1351:THR:HG22 | 2.13                     | 0.48              |
| 1:A:1503:LEU:HD22 | 1:A:1508:LYS:HB2  | 1.96                     | 0.48              |
| 1:A:1657:SER:O    | 1:A:1660:SER:OG   | 2.27                     | 0.48              |
| 1:A:1825:LEU:HD22 | 1:A:1879:VAL:HG11 | 1.96                     | 0.48              |
| 1:A:3085:GLU:OE1  | 1:A:3085:GLU:N    | 2.40                     | 0.48              |
| 1:A:3611:GLU:OE1  | 1:A:3611:GLU:N    | 2.45                     | 0.48              |
| 1:A:358:GLU:N     | 1:A:358:GLU:OE1   | 2.46                     | 0.47              |
| 1:A:1712:ARG:HA   | 1:A:1715:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:261:ASP:N     | 1:A:261:ASP:OD1   | 2.47                     | 0.47              |
| 1:A:437:HIS:NE2   | 1:A:6017:UNK:O    | 2.46                     | 0.47              |
| 1:A:603:ILE:HD11  | 1:A:1031:ARG:HG2  | 1.96                     | 0.47              |
| 1:A:1427:SER:HA   | 1:A:1430:GLU:OE2  | 2.14                     | 0.47              |
| 1:A:1772:HIS:HB3  | 1:A:1775:GLU:HG3  | 1.96                     | 0.47              |
| 1:A:1790:SER:O    | 1:A:1794:GLN:HG3  | 2.14                     | 0.47              |
| 1:A:2172:ALA:HB1  | 1:A:2215:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:104:SER:HA    | 1:A:107:ILE:HD12  | 1.96                     | 0.47              |
| 1:A:1728:GLU:OE1  | 1:A:1728:GLU:N    | 2.30                     | 0.47              |
| 1:A:1854:ARG:HE   | 1:A:1855:PHE:N    | 2.12                     | 0.47              |
| 1:A:200:PHE:O     | 1:A:204:LEU:HG    | 2.15                     | 0.47              |
| 1:A:1445:ARG:H    | 1:A:1445:ARG:HD2  | 1.80                     | 0.47              |
| 1:A:1636:ASP:OD1  | 1:A:1636:ASP:N    | 2.46                     | 0.47              |
| 1:A:2890:ILE:HD11 | 1:A:2929:LEU:HB3  | 1.95                     | 0.47              |
| 1:A:3786:LEU:HB3  | 1:A:3910:LEU:HD22 | 1.95                     | 0.47              |
| 1:A:432:THR:OG1   | 1:A:433:PRO:HD3   | 2.14                     | 0.47              |
| 1:A:476:ARG:CZ    | 1:A:477:ASN:HA    | 2.44                     | 0.47              |
| 1:A:2269:ASP:OD1  | 1:A:2270:ASN:N    | 2.47                     | 0.47              |
| 1:A:2420:PHE:O    | 1:A:2423:VAL:HG22 | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2424:MET:HB3  | 1:A:2435:CYS:SG   | 2.54                     | 0.47              |
| 1:A:3176:MET:HG3  | 1:A:3254:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:50:VAL:HA     | 1:A:53:LEU:HD23   | 1.96                     | 0.47              |
| 1:A:89:LEU:HD11   | 1:A:133:LYS:HD3   | 1.96                     | 0.47              |
| 1:A:129:ASP:O     | 1:A:133:LYS:HE3   | 2.14                     | 0.47              |
| 1:A:163:LYS:NZ    | 1:A:167:PRO:O     | 2.39                     | 0.47              |
| 1:A:222:GLY:HA2   | 1:A:267:VAL:HG13  | 1.96                     | 0.47              |
| 1:A:1578:ALA:O    | 1:A:1582:LEU:HD23 | 2.15                     | 0.47              |
| 1:A:1873:TYR:HA   | 1:A:1876:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:2828:GLU:O    | 1:A:2832:ILE:HG12 | 2.15                     | 0.47              |
| 1:A:1513:GLY:O    | 1:A:1516:GLU:HG2  | 2.15                     | 0.47              |
| 1:A:1880:MET:O    | 1:A:1884:LEU:HD13 | 2.14                     | 0.47              |
| 1:A:1900:PHE:HZ   | 1:A:1906:THR:HA   | 1.78                     | 0.47              |
| 1:A:1909:ASN:ND2  | 1:A:1912:THR:HG23 | 2.29                     | 0.47              |
| 1:A:1951:VAL:O    | 1:A:1955:VAL:HG12 | 2.15                     | 0.47              |
| 1:A:3303:THR:HA   | 1:A:3306:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:3357:ARG:O    | 1:A:3360:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:3531:TYR:HB2  | 1:A:3532:PRO:HD3  | 1.97                     | 0.47              |
| 1:A:3667:LEU:HA   | 1:A:3670:MET:SD   | 2.55                     | 0.47              |
| 1:A:4027:TRP:HE3  | 1:A:4030:GLU:HB3  | 1.79                     | 0.47              |
| 1:A:1202:ARG:HE   | 1:A:1207:TRP:HA   | 1.80                     | 0.47              |
| 1:A:1949:ILE:HD12 | 1:A:2100:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:2219:LEU:O    | 1:A:2223:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:2455:LEU:HD12 | 1:A:2458:VAL:HB   | 1.97                     | 0.47              |
| 1:A:3588:TRP:CD1  | 1:A:3613:MET:HG2  | 2.50                     | 0.47              |
| 1:A:3685:PRO:HG2  | 1:A:3687:MET:HB3  | 1.96                     | 0.47              |
| 1:A:174:VAL:O     | 1:A:177:LEU:HG    | 2.14                     | 0.47              |
| 1:A:1018:VAL:HG13 | 1:A:1018:VAL:O    | 2.15                     | 0.47              |
| 1:A:1304:HIS:HB3  | 1:A:1307:ILE:O    | 2.15                     | 0.47              |
| 1:A:1378:GLU:OE1  | 1:A:1381:SER:HB3  | 2.14                     | 0.47              |
| 1:A:2168:LEU:HB3  | 1:A:2189:ILE:HD11 | 1.95                     | 0.47              |
| 1:A:3698:GLU:OE1  | 1:A:3698:GLU:N    | 2.40                     | 0.47              |
| 1:A:3757:ASP:N    | 1:A:3757:ASP:OD1  | 2.48                     | 0.47              |
| 1:A:2397:CYS:O    | 1:A:2401:VAL:HG23 | 2.14                     | 0.46              |
| 1:A:4035:GLU:HG3  | 1:A:4036:LYS:HZ2  | 1.80                     | 0.46              |
| 1:A:1069:HIS:CD2  | 1:A:1074:LYS:HD2  | 2.50                     | 0.46              |
| 1:A:2472:GLN:O    | 1:A:2476:ILE:HG12 | 2.14                     | 0.46              |
| 1:A:83:GLU:HG2    | 1:A:87:LYS:HZ3    | 1.80                     | 0.46              |
| 1:A:130:LEU:O     | 1:A:133:LYS:NZ    | 2.39                     | 0.46              |
| 1:A:901:MET:HG2   | 1:A:903:PRO:HD3   | 1.97                     | 0.46              |
| 1:A:1019:ASP:OD1  | 1:A:1026:ARG:NH1  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3653:ARG:HG3  | 1:A:3659:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:655:LEU:HG    | 1:A:1389:VAL:HG12 | 1.98                     | 0.46              |
| 1:A:2886:GLN:O    | 1:A:2890:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:3066:ASP:OD1  | 1:A:3067:LYS:N    | 2.49                     | 0.46              |
| 1:A:3864:ARG:NH1  | 1:A:4084:SER:HB2  | 2.30                     | 0.46              |
| 1:A:905:ILE:HG13  | 1:A:2811:SER:HB3  | 1.97                     | 0.46              |
| 1:A:1783:ARG:HG2  | 1:A:1830:HIS:CE1  | 2.51                     | 0.46              |
| 1:A:2369:LYS:HE2  | 1:A:2369:LYS:HA   | 1.97                     | 0.46              |
| 1:A:2424:MET:O    | 1:A:2432:GLN:NE2  | 2.48                     | 0.46              |
| 1:A:3497:SER:HB3  | 1:A:3707:GLY:HA3  | 1.98                     | 0.46              |
| 1:A:606:SER:HB2   | 1:A:1080:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:1700:THR:HG21 | 1:A:1753:SER:OG   | 2.15                     | 0.46              |
| 1:A:1864:ASP:O    | 1:A:1867:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:2104:MET:HA   | 1:A:2107:SER:HB3  | 1.98                     | 0.46              |
| 1:A:2197:THR:HG21 | 1:A:2244:CYS:HB3  | 1.98                     | 0.46              |
| 1:A:4074:PHE:HD2  | 1:A:4075:ARG:HD2  | 1.80                     | 0.46              |
| 1:A:15:LEU:O      | 1:A:19:LEU:HG     | 2.15                     | 0.46              |
| 1:A:1100:VAL:HG11 | 1:A:1145:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:2542:LEU:HD21 | 1:A:2558:ALA:HB1  | 1.98                     | 0.46              |
| 1:A:3607:GLU:N    | 1:A:3607:GLU:OE1  | 2.49                     | 0.46              |
| 1:A:52:ALA:O      | 1:A:55:THR:OG1    | 2.25                     | 0.46              |
| 1:A:276:ALA:HA    | 1:A:315:ALA:HA    | 1.97                     | 0.46              |
| 1:A:1639:LEU:O    | 1:A:1643:MET:HG3  | 2.16                     | 0.46              |
| 1:A:2575:PRO:O    | 1:A:2577:PHE:N    | 2.49                     | 0.46              |
| 1:A:3027:LEU:HA   | 1:A:3031:TRP:CZ3  | 2.46                     | 0.46              |
| 1:A:886:TRP:CZ3   | 1:A:911:LEU:HB3   | 2.51                     | 0.45              |
| 1:A:1225:GLU:HB2  | 1:A:1235:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:2274:ILE:HG23 | 1:A:2322:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:3097:ASP:OD1  | 1:A:3098:ARG:N    | 2.44                     | 0.45              |
| 1:A:3321:LEU:HA   | 1:A:3324:ARG:HH11 | 1.81                     | 0.45              |
| 1:A:3855:TYR:HA   | 1:A:3858:MET:HB3  | 1.99                     | 0.45              |
| 1:A:356:ASN:O     | 1:A:359:LEU:HB3   | 2.15                     | 0.45              |
| 1:A:991:LEU:HD22  | 1:A:995:PHE:HE2   | 1.81                     | 0.45              |
| 1:A:1186:LYS:O    | 1:A:1190:LEU:HD23 | 2.16                     | 0.45              |
| 1:A:1381:SER:OG   | 1:A:1382:ILE:N    | 2.50                     | 0.45              |
| 1:A:1437:TYR:HE2  | 1:A:1511:ALA:HB2  | 1.81                     | 0.45              |
| 1:A:1880:MET:HE3  | 1:A:1884:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:3006:ALA:HB3  | 1:A:3257:LYS:HD3  | 1.98                     | 0.45              |
| 1:A:3356:ALA:O    | 1:A:3359:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:303:HIS:CE1   | 1:A:305:ASN:HB2   | 2.52                     | 0.45              |
| 1:A:1934:LEU:O    | 1:A:1938:ARG:N    | 2.41                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2893:LEU:HD23 | 1:A:2893:LEU:HA   | 1.83                     | 0.45              |
| 1:A:201:LEU:HA    | 1:A:204:LEU:HD12  | 1.99                     | 0.45              |
| 1:A:573:LEU:HD23  | 1:A:573:LEU:HA    | 1.83                     | 0.45              |
| 1:A:1496:GLU:HG3  | 1:A:1498:GLN:OE1  | 2.17                     | 0.45              |
| 1:A:3371:GLU:OE1  | 1:A:3371:GLU:N    | 2.32                     | 0.45              |
| 1:A:3496:ILE:HD11 | 1:A:3521:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:55:THR:O      | 1:A:58:VAL:HG22   | 2.15                     | 0.45              |
| 1:A:236:LYS:HG3   | 1:A:243:GLN:HG3   | 1.98                     | 0.45              |
| 1:A:1067:ALA:O    | 1:A:1075:ARG:HG2  | 2.16                     | 0.45              |
| 1:A:1470:SER:HB2  | 1:A:1476:HIS:CG   | 2.51                     | 0.45              |
| 1:A:1709:GLU:OE1  | 1:A:1709:GLU:N    | 2.44                     | 0.45              |
| 1:A:1864:ASP:HA   | 1:A:1867:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:3478:GLU:CD   | 1:A:3478:GLU:H    | 2.19                     | 0.45              |
| 1:A:3992:ARG:NH1  | 1:A:4103:GLN:OE1  | 2.49                     | 0.45              |
| 1:A:967:PRO:HG3   | 1:A:1010:LEU:HD12 | 1.97                     | 0.45              |
| 1:A:1303:MET:N    | 1:A:1303:MET:SD   | 2.90                     | 0.45              |
| 1:A:1449:ALA:HA   | 1:A:1452:VAL:HG12 | 1.99                     | 0.45              |
| 1:A:2319:ALA:HA   | 1:A:2322:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:3512:VAL:HA   | 1:A:3515:GLN:OE1  | 2.16                     | 0.45              |
| 1:A:1412:LYS:O    | 1:A:1415:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:1438:GLY:N    | 1:A:1445:ARG:HH12 | 2.15                     | 0.45              |
| 1:A:1825:LEU:HD11 | 1:A:1875:LYS:HD3  | 1.98                     | 0.45              |
| 1:A:1887:ASP:N    | 1:A:1887:ASP:OD1  | 2.48                     | 0.45              |
| 1:A:3190:LEU:HD13 | 1:A:3235:LYS:HZ3  | 1.81                     | 0.45              |
| 1:A:3393:GLU:OE1  | 1:A:3393:GLU:N    | 2.45                     | 0.45              |
| 1:A:174:VAL:HG23  | 1:A:177:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:1082:PHE:HA   | 1:A:1085:ILE:HG12 | 1.99                     | 0.45              |
| 1:A:2540:LEU:HG   | 1:A:2832:ILE:HD12 | 1.97                     | 0.45              |
| 1:A:3008:TRP:CH2  | 1:A:3050:LYS:HG3  | 2.51                     | 0.45              |
| 1:A:3027:LEU:HD11 | 1:A:3060:SER:HB2  | 1.99                     | 0.45              |
| 1:A:3462:ARG:NH2  | 1:A:3708:ARG:HG2  | 2.32                     | 0.45              |
| 1:A:3496:ILE:HA   | 1:A:3499:ILE:HG12 | 1.99                     | 0.45              |
| 1:A:860:GLY:HA3   | 1:A:3136:THR:OG1  | 2.17                     | 0.45              |
| 1:A:1438:GLY:H    | 1:A:1445:ARG:HH12 | 1.65                     | 0.45              |
| 1:A:1714:LEU:O    | 1:A:1718:ILE:HG23 | 2.16                     | 0.45              |
| 1:A:2092:GLU:H    | 1:A:2092:GLU:CD   | 2.18                     | 0.45              |
| 1:A:2340:SER:O    | 1:A:2344:LEU:HD23 | 2.17                     | 0.45              |
| 1:A:3701:ILE:O    | 1:A:3704:GLN:HG2  | 2.16                     | 0.45              |
| 1:A:194:GLU:H     | 1:A:194:GLU:CD    | 2.21                     | 0.45              |
| 1:A:2376:ASP:OD1  | 1:A:2377:ARG:N    | 2.50                     | 0.45              |
| 1:A:2438:ILE:O    | 1:A:2442:MET:HG3  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2586:PHE:HB2  | 1:A:2776:ARG:HH21 | 1.81                     | 0.45              |
| 1:A:2897:LEU:HD23 | 1:A:2897:LEU:HA   | 1.83                     | 0.45              |
| 1:A:103:TYR:CE2   | 1:A:107:ILE:HD11  | 2.53                     | 0.44              |
| 1:A:163:LYS:HD2   | 1:A:163:LYS:HA    | 1.79                     | 0.44              |
| 1:A:1203:SER:H    | 1:A:1206:LEU:HD12 | 1.83                     | 0.44              |
| 1:A:2813:PHE:HZ   | 1:A:2836:LEU:HD13 | 1.82                     | 0.44              |
| 1:A:3190:LEU:HD13 | 1:A:3235:LYS:HB2  | 1.99                     | 0.44              |
| 1:A:3557:ARG:HG2  | 1:A:3561:LYS:HZ2  | 1.82                     | 0.44              |
| 1:A:771:ASN:OD1   | 1:A:854:ARG:NH2   | 2.50                     | 0.44              |
| 1:A:2434:VAL:O    | 1:A:2438:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:3511:ALA:O    | 1:A:3514:VAL:HG22 | 2.16                     | 0.44              |
| 1:A:53:LEU:O      | 1:A:57:LEU:N      | 2.48                     | 0.44              |
| 1:A:296:VAL:O     | 1:A:299:LYS:HG3   | 2.18                     | 0.44              |
| 1:A:781:ASP:OD1   | 1:A:782:ARG:N     | 2.51                     | 0.44              |
| 1:A:1886:LYS:HD2  | 1:A:1955:VAL:O    | 2.18                     | 0.44              |
| 1:A:3459:ASN:O    | 1:A:3463:LEU:HG   | 2.17                     | 0.44              |
| 1:A:3673:ASP:OD1  | 1:A:3673:ASP:N    | 2.50                     | 0.44              |
| 1:A:659:ARG:HE    | 1:A:660:LEU:HD23  | 1.81                     | 0.44              |
| 1:A:682:TYR:CZ    | 1:A:700:LYS:HG2   | 2.52                     | 0.44              |
| 1:A:1627:LYS:HA   | 1:A:1627:LYS:HD2  | 1.69                     | 0.44              |
| 1:A:1747:LEU:HD22 | 1:A:1762:MET:HE1  | 1.99                     | 0.44              |
| 1:A:2318:ALA:O    | 1:A:2321:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:363:ILE:HD12  | 1:A:388:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:1309:ALA:HA   | 1:A:1315:THR:HG21 | 1.99                     | 0.44              |
| 1:A:1358:LEU:HD11 | 1:A:1410:PRO:HG2  | 1.99                     | 0.44              |
| 1:A:2898:LEU:HD21 | 1:A:3973:PRO:HG3  | 1.99                     | 0.44              |
| 1:A:3285:HIS:NE2  | 1:A:3333:THR:OG1  | 2.38                     | 0.44              |
| 1:A:3589:SER:O    | 1:A:3593:ARG:CB   | 2.62                     | 0.44              |
| 1:A:4113:ASP:HB3  | 1:A:4116:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:3274:VAL:HA   | 1:A:3277:VAL:HG12 | 2.00                     | 0.44              |
| 1:A:3295:GLU:O    | 1:A:3299:THR:HG23 | 2.17                     | 0.44              |
| 1:A:3578:LEU:HD21 | 1:A:3681:LYS:HZ1  | 1.82                     | 0.44              |
| 1:A:3819:THR:HA   | 1:A:3889:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:4056:PRO:HG3  | 1:A:4107:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:683:PHE:CD2   | 1:A:737:PRO:HG3   | 2.47                     | 0.44              |
| 1:A:848:LEU:O     | 1:A:852:ARG:HG3   | 2.18                     | 0.44              |
| 1:A:1367:HIS:HD2  | 1:A:1370:ARG:HD3  | 1.82                     | 0.44              |
| 1:A:3065:ILE:HD12 | 1:A:3078:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:3875:GLU:HB3  | 1:A:3965:ARG:HD3  | 1.99                     | 0.44              |
| 1:A:4115:ASN:O    | 1:A:4119:ARG:HG2  | 2.18                     | 0.44              |
| 1:A:639:ALA:HB2   | 1:A:676:ASN:HB2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1090:ARG:NH2  | 1:A:1091:GLU:OE2  | 2.51                     | 0.44              |
| 1:A:1102:GLU:HG2  | 1:A:1106:ILE:HD12 | 2.00                     | 0.44              |
| 1:A:1770:GLN:HA   | 1:A:1822:ARG:HH22 | 1.83                     | 0.44              |
| 1:A:2123:PRO:HB2  | 1:A:2125:TRP:HD1  | 1.83                     | 0.44              |
| 1:A:2511:ILE:HD13 | 1:A:2550:ILE:HG22 | 1.99                     | 0.44              |
| 1:A:2589:TYR:HB2  | 1:A:2777:HIS:ND1  | 2.33                     | 0.44              |
| 1:A:2592:ASP:OD1  | 1:A:2593:SER:N    | 2.51                     | 0.44              |
| 1:A:3347:CYS:HA   | 1:A:3350:GLU:HB2  | 2.00                     | 0.44              |
| 1:A:614:PRO:HB3   | 1:A:620:PHE:CE1   | 2.53                     | 0.43              |
| 1:A:1421:GLU:OE2  | 1:A:1422:LYS:HG2  | 2.17                     | 0.43              |
| 1:A:1693:VAL:HG21 | 1:A:1746:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:2140:LEU:HB3  | 1:A:2143:ARG:HH21 | 1.83                     | 0.43              |
| 1:A:2589:TYR:HB3  | 1:A:2775:TYR:O    | 2.17                     | 0.43              |
| 1:A:3065:ILE:HG22 | 1:A:3069:MET:HG2  | 2.00                     | 0.43              |
| 1:A:3405:PRO:HA   | 1:A:3406:ALA:HA   | 1.52                     | 0.43              |
| 1:A:4084:SER:OG   | 1:A:4087:HIS:N    | 2.49                     | 0.43              |
| 1:A:334:HIS:O     | 1:A:337:LYS:HG2   | 2.18                     | 0.43              |
| 1:A:726:LEU:O     | 1:A:730:LEU:HD23  | 2.17                     | 0.43              |
| 1:A:759:GLY:HA3   | 1:A:799:TYR:OH    | 2.18                     | 0.43              |
| 1:A:1238:GLN:OE1  | 1:A:1243:TYR:HB2  | 2.19                     | 0.43              |
| 1:A:1395:LEU:HB3  | 1:A:1396:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:1866:GLN:OE1  | 1:A:1866:GLN:N    | 2.51                     | 0.43              |
| 1:A:2220:MET:HA   | 1:A:2223:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:3601:VAL:HG23 | 1:A:3656:LEU:HD11 | 1.99                     | 0.43              |
| 1:A:4065:LEU:HA   | 1:A:4074:PHE:HE1  | 1.83                     | 0.43              |
| 1:A:1585:SER:OG   | 1:A:1588:ASP:OD1  | 2.34                     | 0.43              |
| 1:A:3530:VAL:HG21 | 1:A:3568:ILE:HG13 | 1.99                     | 0.43              |
| 1:A:667:TYR:O     | 1:A:671:SER:N     | 2.50                     | 0.43              |
| 1:A:1805:PHE:O    | 1:A:1816:ARG:HD3  | 2.18                     | 0.43              |
| 1:A:2447:LYS:HB2  | 1:A:2450:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:3548:GLY:O    | 1:A:3552:LYS:N    | 2.41                     | 0.43              |
| 1:A:1491:ILE:HG13 | 1:A:1492:ALA:H    | 1.84                     | 0.43              |
| 1:A:1976:LEU:HD12 | 1:A:1976:LEU:HA   | 1.73                     | 0.43              |
| 1:A:2085:MET:SD   | 1:A:2090:ARG:NH1  | 2.92                     | 0.43              |
| 1:A:2474:TYR:HE2  | 1:A:2517:LEU:HD13 | 1.83                     | 0.43              |
| 1:A:3325:ASP:HA   | 1:A:3328:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:3655:LYS:HD3  | 1:A:3658:ASP:OD2  | 2.18                     | 0.43              |
| 1:A:4090:ARG:HH12 | 1:A:4110:GLN:HA   | 1.83                     | 0.43              |
| 1:A:193:ALA:HB1   | 1:A:197:PHE:HE2   | 1.83                     | 0.43              |
| 1:A:197:PHE:HA    | 1:A:200:PHE:HB3   | 1.99                     | 0.43              |
| 1:A:714:VAL:HG11  | 1:A:732:PHE:HE2   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:753:GLN:NE2   | 1:A:791:ASP:O     | 2.34                     | 0.43              |
| 1:A:880:MET:SD    | 1:A:883:TYR:HB2   | 2.58                     | 0.43              |
| 1:A:2501:LEU:O    | 1:A:2505:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:2508:GLN:NE2  | 1:A:2549:LYS:HG3  | 2.33                     | 0.43              |
| 1:A:4020:MET:HG2  | 1:A:4027:TRP:NE1  | 2.33                     | 0.43              |
| 1:A:178:LEU:HD23  | 1:A:178:LEU:H     | 1.84                     | 0.43              |
| 1:A:298:LEU:HD22  | 1:A:316:LEU:HD11  | 2.01                     | 0.43              |
| 1:A:338:LEU:O     | 1:A:342:MET:HG2   | 2.19                     | 0.43              |
| 1:A:468:LEU:HB3   | 1:A:478:CYS:SG    | 2.59                     | 0.43              |
| 1:A:733:LEU:HD11  | 1:A:748:TYR:CE1   | 2.53                     | 0.43              |
| 1:A:1260:LEU:O    | 1:A:1264:LEU:HD23 | 2.18                     | 0.43              |
| 1:A:1852:LYS:HD2  | 1:A:1918:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:2298:GLU:HA   | 1:A:2301:GLN:OE1  | 2.19                     | 0.43              |
| 1:A:3100:LYS:O    | 1:A:3103:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:3155:VAL:O    | 1:A:3158:LYS:HG2  | 2.18                     | 0.43              |
| 1:A:3168:TYR:HD2  | 1:A:3241:LYS:HZ2  | 1.65                     | 0.43              |
| 1:A:3946:PHE:HE2  | 1:A:4005:PHE:HE2  | 1.65                     | 0.43              |
| 1:A:736:LEU:HD23  | 1:A:736:LEU:HA    | 1.87                     | 0.43              |
| 1:A:1910:GLU:N    | 1:A:1910:GLU:OE2  | 2.52                     | 0.43              |
| 1:A:1977:ILE:HG12 | 1:A:1979:GLU:H    | 1.84                     | 0.43              |
| 1:A:3386:SER:O    | 1:A:3389:VAL:HG12 | 2.18                     | 0.43              |
| 1:A:3508:LYS:HA   | 1:A:3508:LYS:HD3  | 1.83                     | 0.43              |
| 1:A:63:PHE:HA     | 1:A:66:LEU:HG     | 2.01                     | 0.43              |
| 1:A:764:PRO:O     | 1:A:767:GLU:HG2   | 2.18                     | 0.43              |
| 1:A:946:THR:O     | 1:A:946:THR:OG1   | 2.34                     | 0.43              |
| 1:A:2352:HIS:CE1  | 1:A:2359:LYS:HB2  | 2.54                     | 0.43              |
| 1:A:2356:MET:HG2  | 1:A:2358:ASP:H    | 1.83                     | 0.43              |
| 1:A:2296:SER:HA   | 1:A:2299:TYR:CD2  | 2.54                     | 0.43              |
| 1:A:244:THR:HG23  | 1:A:285:CYS:SG    | 2.58                     | 0.42              |
| 1:A:737:PRO:HD2   | 1:A:740:ILE:HD12  | 2.01                     | 0.42              |
| 1:A:924:ARG:HA    | 1:A:924:ARG:HD2   | 1.80                     | 0.42              |
| 1:A:999:LYS:HE2   | 1:A:999:LYS:HB2   | 1.83                     | 0.42              |
| 1:A:1743:MET:O    | 1:A:1747:LEU:HD23 | 2.19                     | 0.42              |
| 1:A:1851:LEU:HD21 | 1:A:1870:LYS:HA   | 2.01                     | 0.42              |
| 1:A:2213:ASN:OD1  | 1:A:2214:ARG:N    | 2.51                     | 0.42              |
| 1:A:2405:VAL:HG11 | 1:A:2441:LYS:HB2  | 2.01                     | 0.42              |
| 1:A:3281:CYS:HA   | 1:A:3301:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:3332:THR:O    | 1:A:3335:ARG:HG2  | 2.19                     | 0.42              |
| 1:A:425:ASP:OD1   | 1:A:426:THR:N     | 2.52                     | 0.42              |
| 1:A:1250:LEU:O    | 1:A:1253:THR:HG22 | 2.19                     | 0.42              |
| 1:A:2294:ILE:HG13 | 1:A:2295:GLN:H    | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3150:ASN:N    | 1:A:3150:ASN:OD1  | 2.53                     | 0.42              |
| 1:A:111:CYS:HA    | 1:A:114:VAL:HG12  | 2.01                     | 0.42              |
| 1:A:1766:LEU:HB2  | 1:A:1778:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:2195:SER:O    | 1:A:5009:UNK:N    | 2.52                     | 0.42              |
| 1:A:3575:LEU:HD23 | 1:A:3575:LEU:HA   | 1.90                     | 0.42              |
| 1:A:54:GLN:O      | 1:A:58:VAL:HG13   | 2.19                     | 0.42              |
| 1:A:911:LEU:HD23  | 1:A:911:LEU:HA    | 1.90                     | 0.42              |
| 1:A:2482:ASP:OD1  | 1:A:2530:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:2788:SER:O    | 1:A:2792:THR:HG22 | 2.19                     | 0.42              |
| 1:A:3359:ILE:O    | 1:A:3362:LEU:HB3  | 2.19                     | 0.42              |
| 1:A:3507:ASP:HA   | 1:A:3542:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:3609:MET:HB2  | 1:A:3612:ARG:HH21 | 1.84                     | 0.42              |
| 1:A:3916:TRP:CE2  | 1:A:4050:LYS:HE2  | 2.55                     | 0.42              |
| 1:A:57:LEU:HD23   | 1:A:57:LEU:HA     | 1.92                     | 0.42              |
| 1:A:195:ASN:HA    | 1:A:198:ARG:NE    | 2.34                     | 0.42              |
| 1:A:376:ILE:HG23  | 1:A:377:ASN:N     | 2.34                     | 0.42              |
| 1:A:1302:ALA:HA   | 1:A:1382:ILE:HG22 | 2.02                     | 0.42              |
| 1:A:2793:PRO:O    | 1:A:2796:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:3881:ASP:OD1  | 1:A:3881:ASP:N    | 2.52                     | 0.42              |
| 1:A:4084:SER:HB3  | 1:A:4088:ASN:H    | 1.84                     | 0.42              |
| 1:A:1797:LEU:O    | 1:A:1801:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:2891:ARG:O    | 1:A:2895:GLU:OE1  | 2.38                     | 0.42              |
| 1:A:3183:ILE:HD13 | 1:A:3183:ILE:HA   | 1.85                     | 0.42              |
| 1:A:3496:ILE:O    | 1:A:3499:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:3809:THR:HG22 | 1:A:3931:ALA:HA   | 2.00                     | 0.42              |
| 1:A:83:GLU:HG2    | 1:A:87:LYS:NZ     | 2.35                     | 0.42              |
| 1:A:132:ILE:HG22  | 1:A:173:LYS:NZ    | 2.35                     | 0.42              |
| 1:A:236:LYS:HG3   | 1:A:243:GLN:HE21  | 1.85                     | 0.42              |
| 1:A:1442:GLN:HA   | 1:A:1445:ARG:HD3  | 2.02                     | 0.42              |
| 1:A:1793:THR:O    | 1:A:1797:LEU:HG   | 2.19                     | 0.42              |
| 1:A:2352:HIS:NE2  | 1:A:2359:LYS:HB2  | 2.35                     | 0.42              |
| 1:A:3675:LYS:N    | 1:A:3676:PRO:HD3  | 2.34                     | 0.42              |
| 1:A:54:GLN:HA     | 1:A:57:LEU:HB2    | 2.01                     | 0.42              |
| 1:A:567:GLU:OE2   | 1:A:570:LYS:HD3   | 2.20                     | 0.42              |
| 1:A:1206:LEU:HA   | 1:A:1209:LYS:HD3  | 2.01                     | 0.42              |
| 1:A:185:HIS:O     | 1:A:188:GLU:HG2   | 2.19                     | 0.42              |
| 1:A:586:GLN:HB2   | 1:A:613:HIS:HD2   | 1.84                     | 0.42              |
| 1:A:2411:LEU:HA   | 1:A:2411:LEU:HD12 | 1.79                     | 0.42              |
| 1:A:3706:ASP:OD1  | 1:A:3706:ASP:N    | 2.48                     | 0.42              |
| 1:A:3883:LEU:HD12 | 1:A:3883:LEU:HA   | 1.94                     | 0.42              |
| 1:A:3946:PHE:CE2  | 1:A:4005:PHE:HE2  | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1225:GLU:HG3  | 1:A:1236:LEU:HB2  | 2.01                     | 0.42              |
| 1:A:1575:LEU:H    | 1:A:1575:LEU:HD23 | 1.85                     | 0.42              |
| 1:A:1709:GLU:HA   | 1:A:1712:ARG:NE   | 2.35                     | 0.42              |
| 1:A:2485:ARG:HA   | 1:A:2499:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:3694:PHE:O    | 1:A:3696:ARG:HD3  | 2.19                     | 0.42              |
| 1:A:22:ALA:HB3    | 1:A:34:LEU:HD21   | 2.01                     | 0.41              |
| 1:A:1392:MET:HA   | 1:A:1396:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:2085:MET:HA   | 1:A:2088:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:2339:GLU:H    | 1:A:2339:GLU:CD   | 2.22                     | 0.41              |
| 1:A:4025:GLY:HA2  | 1:A:4028:ILE:HD11 | 2.01                     | 0.41              |
| 1:A:21:ALA:HA     | 1:A:24:ARG:CZ     | 2.50                     | 0.41              |
| 1:A:1261:LEU:HD11 | 1:A:1340:ARG:HG3  | 2.01                     | 0.41              |
| 1:A:2210:VAL:O    | 1:A:2214:ARG:HG3  | 2.19                     | 0.41              |
| 1:A:3681:LYS:O    | 1:A:3685:PRO:HD2  | 2.19                     | 0.41              |
| 1:A:3839:TYR:HD1  | 1:A:3874:ARG:NH1  | 2.19                     | 0.41              |
| 1:A:4054:ALA:O    | 1:A:4103:GLN:NE2  | 2.53                     | 0.41              |
| 1:A:470:ALA:C     | 1:A:471:LYS:HD2   | 2.40                     | 0.41              |
| 1:A:766:ALA:O     | 1:A:770:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:1783:ARG:HB3  | 1:A:1787:ARG:HH21 | 1.84                     | 0.41              |
| 1:A:1906:THR:OG1  | 1:A:1908:GLY:O    | 2.30                     | 0.41              |
| 1:A:2247:ASP:OD1  | 1:A:2247:ASP:N    | 2.53                     | 0.41              |
| 1:A:3413:TYR:HD1  | 1:A:3449:LYS:HD3  | 1.85                     | 0.41              |
| 1:A:3455:LYS:NZ   | 1:A:3489:SER:O    | 2.54                     | 0.41              |
| 1:A:3896:ALA:O    | 1:A:3900:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:470:ALA:HB1   | 1:A:553:VAL:HG11  | 2.01                     | 0.41              |
| 1:A:1149:LYS:HE2  | 1:A:1149:LYS:HB2  | 1.89                     | 0.41              |
| 1:A:1320:ASN:N    | 1:A:1320:ASN:OD1  | 2.53                     | 0.41              |
| 1:A:1532:LEU:HD12 | 1:A:1532:LEU:HA   | 1.91                     | 0.41              |
| 1:A:1930:GLU:H    | 1:A:1934:LEU:HD21 | 1.85                     | 0.41              |
| 1:A:2380:ASN:O    | 1:A:2384:PHE:N    | 2.49                     | 0.41              |
| 1:A:2492:ASP:H    | 1:A:2496:GLN:HE22 | 1.67                     | 0.41              |
| 1:A:3360:LEU:O    | 1:A:3364:GLY:N    | 2.51                     | 0.41              |
| 1:A:3671:ASN:OD1  | 1:A:3672:LYS:N    | 2.54                     | 0.41              |
| 1:A:183:GLU:OE2   | 1:A:183:GLU:N     | 2.54                     | 0.41              |
| 1:A:497:LEU:HA    | 1:A:498:PRO:HD3   | 1.93                     | 0.41              |
| 1:A:923:ASP:C     | 1:A:925:GLN:H     | 2.22                     | 0.41              |
| 1:A:2251:ILE:HD12 | 1:A:2251:ILE:H    | 1.85                     | 0.41              |
| 1:A:2368:THR:HG21 | 1:A:2375:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:3051:LEU:O    | 1:A:3056:GLU:HB3  | 2.20                     | 0.41              |
| 1:A:3320:ILE:HG13 | 1:A:3320:ILE:O    | 2.19                     | 0.41              |
| 1:A:3462:ARG:HH22 | 1:A:3708:ARG:HG2  | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:670:LEU:O     | 1:A:673:THR:HB    | 2.21                     | 0.41              |
| 1:A:2147:ALA:O    | 1:A:2151:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:2218:PHE:O    | 1:A:2222:HIS:ND1  | 2.51                     | 0.41              |
| 1:A:2421:VAL:HG23 | 1:A:2457:PRO:HG3  | 2.02                     | 0.41              |
| 1:A:2441:LYS:O    | 1:A:2444:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:3571:PHE:CD2  | 1:A:3699:LEU:HD21 | 2.55                     | 0.41              |
| 1:A:539:GLN:O     | 1:A:541:MET:N     | 2.54                     | 0.41              |
| 1:A:1231:GLN:O    | 1:A:1233:SER:N    | 2.53                     | 0.41              |
| 1:A:1300:SER:HA   | 1:A:1304:HIS:HB2  | 2.02                     | 0.41              |
| 1:A:2554:PHE:O    | 1:A:2555:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:3640:PHE:HA   | 1:A:3643:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:3779:SER:O    | 1:A:3782:SER:N    | 2.49                     | 0.41              |
| 1:A:3881:ASP:HA   | 1:A:3966:GLN:HE22 | 1.86                     | 0.41              |
| 1:A:762:TYR:HD2   | 1:A:765:LEU:HG    | 1.86                     | 0.41              |
| 1:A:1022:ASP:OD1  | 1:A:1022:ASP:N    | 2.54                     | 0.41              |
| 1:A:1445:ARG:HG2  | 1:A:1507:CYS:SG   | 2.61                     | 0.41              |
| 1:A:1572:LEU:HD23 | 1:A:1572:LEU:HA   | 1.96                     | 0.41              |
| 1:A:2258:GLU:OE2  | 1:A:2259:LYS:NZ   | 2.41                     | 0.41              |
| 1:A:2289:ASP:HB3  | 1:A:2290:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:3107:ILE:HD13 | 1:A:3107:ILE:HA   | 1.92                     | 0.41              |
| 1:A:3324:ARG:NH2  | 1:A:3325:ASP:OD1  | 2.44                     | 0.41              |
| 1:A:3564:GLN:HG2  | 1:A:3565:GLY:N    | 2.36                     | 0.41              |
| 1:A:3959:MET:SD   | 1:A:3959:MET:N    | 2.94                     | 0.41              |
| 1:A:104:SER:O     | 1:A:107:ILE:HB    | 2.21                     | 0.41              |
| 1:A:294:PHE:O     | 1:A:298:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:340:TYR:O     | 1:A:344:GLN:HG2   | 2.21                     | 0.41              |
| 1:A:540:MET:SD    | 1:A:540:MET:N     | 2.94                     | 0.41              |
| 1:A:800:LEU:O     | 1:A:852:ARG:NH2   | 2.53                     | 0.41              |
| 1:A:933:LEU:HD21  | 1:A:937:MET:HE3   | 2.02                     | 0.41              |
| 1:A:1000:LYS:HA   | 1:A:1000:LYS:HD2  | 1.88                     | 0.41              |
| 1:A:1071:ASN:OD1  | 1:A:1072:ALA:N    | 2.54                     | 0.41              |
| 1:A:1358:LEU:HA   | 1:A:1411:TYR:OH   | 2.21                     | 0.41              |
| 1:A:1906:THR:HG23 | 1:A:1908:GLY:H    | 1.86                     | 0.41              |
| 1:A:1933:LEU:HD21 | 1:A:1936:ARG:HB3  | 2.03                     | 0.41              |
| 1:A:2340:SER:HA   | 1:A:2343:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:2341:LEU:O    | 1:A:2345:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:2412:TYR:HA   | 1:A:2415:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:257:ARG:HG3   | 1:A:260:ILE:HD12  | 2.02                     | 0.41              |
| 1:A:789:TYR:CD1   | 1:A:792:ILE:HD11  | 2.56                     | 0.41              |
| 1:A:894:PHE:HB3   | 1:A:905:ILE:HG23  | 2.03                     | 0.41              |
| 1:A:899:ARG:HG2   | 1:A:2569:SER:HA   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1388:ASP:H    | 1:A:1391:VAL:HG22 | 1.86                     | 0.41              |
| 1:A:1422:LYS:HD3  | 1:A:1422:LYS:HA   | 1.81                     | 0.41              |
| 1:A:2409:THR:OG1  | 1:A:2410:GLU:N    | 2.54                     | 0.41              |
| 1:A:2517:LEU:HD23 | 1:A:2517:LEU:HA   | 1.85                     | 0.41              |
| 1:A:2773:ARG:NH2  | 1:A:2785:ILE:HD11 | 2.36                     | 0.41              |
| 1:A:300:TRP:CZ3   | 1:A:308:LEU:HD21  | 2.56                     | 0.40              |
| 1:A:1691:GLN:O    | 1:A:1694:THR:HG22 | 2.20                     | 0.40              |
| 1:A:2522:ARG:HG2  | 1:A:2561:PHE:HE1  | 1.86                     | 0.40              |
| 1:A:2917:PRO:HB2  | 1:A:2919:ASP:OD1  | 2.21                     | 0.40              |
| 1:A:3240:MET:HE3  | 1:A:3240:MET:O    | 2.21                     | 0.40              |
| 1:A:3605:ASN:O    | 1:A:3608:LYS:HG3  | 2.21                     | 0.40              |
| 1:A:1378:GLU:OE2  | 1:A:1380:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:1935:GLU:HG2  | 1:A:1936:ARG:N    | 2.36                     | 0.40              |
| 1:A:3114:TYR:OH   | 1:A:3125:ARG:NH2  | 2.55                     | 0.40              |
| 1:A:353:ASP:N     | 1:A:353:ASP:OD1   | 2.53                     | 0.40              |
| 1:A:770:LEU:HD11  | 1:A:855:VAL:HG22  | 2.03                     | 0.40              |
| 1:A:789:TYR:HD1   | 1:A:792:ILE:HD11  | 1.86                     | 0.40              |
| 1:A:872:THR:O     | 1:A:872:THR:HG22  | 2.22                     | 0.40              |
| 1:A:1667:SER:O    | 1:A:1670:GLU:HG2  | 2.22                     | 0.40              |
| 1:A:1916:ILE:HD13 | 1:A:1916:ILE:HA   | 1.93                     | 0.40              |
| 1:A:2572:TYR:CE2  | 1:A:2788:SER:HB2  | 2.56                     | 0.40              |
| 1:A:3838:GLU:OE1  | 1:A:3874:ARG:NH1  | 2.54                     | 0.40              |
| 1:A:491:CYS:SG    | 1:A:626:LEU:HB2   | 2.61                     | 0.40              |
| 1:A:1247:PRO:HB2  | 1:A:1250:LEU:HB2  | 2.02                     | 0.40              |
| 1:A:1362:ASP:N    | 1:A:1362:ASP:OD1  | 2.53                     | 0.40              |
| 1:A:1914:THR:O    | 1:A:1918:LEU:HG   | 2.21                     | 0.40              |
| 1:A:2943:PHE:CE1  | 1:A:2947:ILE:HD12 | 2.56                     | 0.40              |
| 1:A:3355:LYS:HG3  | 1:A:3358:ARG:HH22 | 1.86                     | 0.40              |
| 1:A:3582:GLU:HG2  | 1:A:3583:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:995:PHE:HB3   | 1:A:1005:ASP:OD1  | 2.22                     | 0.40              |
| 1:A:1292:LYS:H    | 1:A:1292:LYS:HG2  | 1.70                     | 0.40              |
| 1:A:1541:ALA:HA   | 1:A:1550:VAL:HG12 | 2.02                     | 0.40              |
| 1:A:2270:ASN:O    | 1:A:2274:ILE:HG12 | 2.22                     | 0.40              |
| 1:A:2869:LEU:HD23 | 1:A:2869:LEU:HA   | 1.89                     | 0.40              |
| 1:A:3062:LEU:HG   | 1:A:3089:LEU:HD11 | 2.04                     | 0.40              |
| 1:A:3465:PHE:O    | 1:A:3468:LEU:HB2  | 2.22                     | 0.40              |
| 1:A:3493:TRP:NE1  | 1:A:3711:PRO:HG3  | 2.37                     | 0.40              |
| 1:A:3913:ILE:HD12 | 1:A:3913:ILE:HA   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 3640/4156 (88%) | 3354 (92%) | 284 (8%) | 2 (0%)   | 51          | 83 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3480 | LEU  |
| 1   | A     | 2787 | HIS  |

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-----------------|-------------|----------|-------------|----|
| 1   | A     | 3203/3671 (87%) | 3190 (100%) | 13 (0%)  | 91          | 94 |

All (13) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 117  | LYS  |
| 1   | A     | 299  | LYS  |
| 1   | A     | 379  | LYS  |
| 1   | A     | 1412 | LYS  |
| 1   | A     | 1497 | ARG  |
| 1   | A     | 1612 | LYS  |
| 1   | A     | 2239 | LYS  |
| 1   | A     | 2283 | ASN  |
| 1   | A     | 2356 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3098 | ARG  |
| 1   | A     | 3478 | GLU  |
| 1   | A     | 3638 | LYS  |
| 1   | A     | 3696 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 334  | HIS  |
| 1   | A     | 356  | ASN  |
| 1   | A     | 1367 | HIS  |
| 1   | A     | 1611 | GLN  |
| 1   | A     | 3139 | GLN  |
| 1   | A     | 4092 | GLN  |

### 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 ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 4128:MET  | C      | 5009:UNK  | N      | 93.18        |
| 1     | A     | 5016:UNK  | C      | 6001:UNK  | N      | 48.96        |

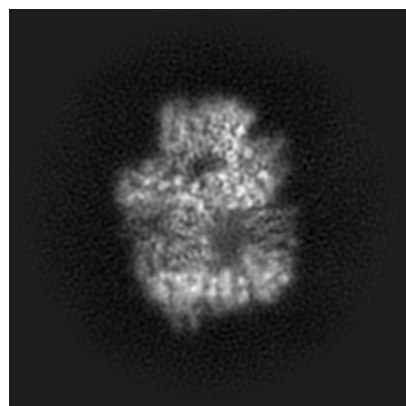
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11211. These allow visual inspection of the internal detail of the map and identification of artifacts.

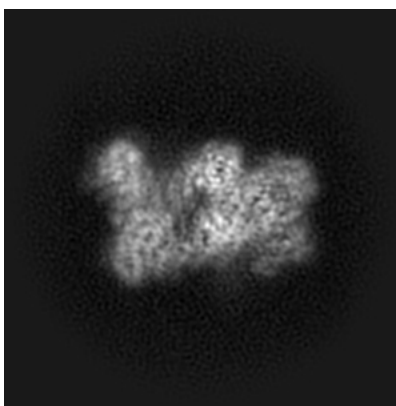
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

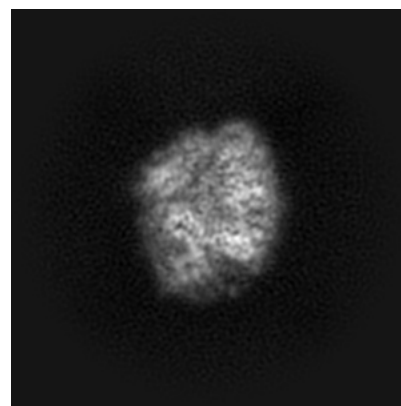
#### 6.1.1 Primary map



X

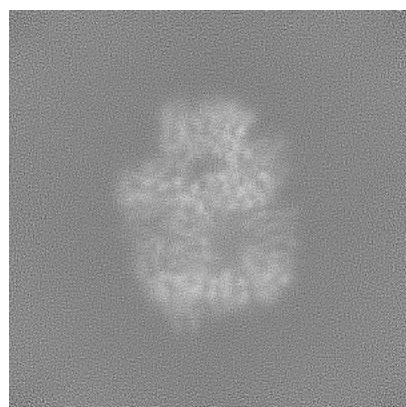


Y

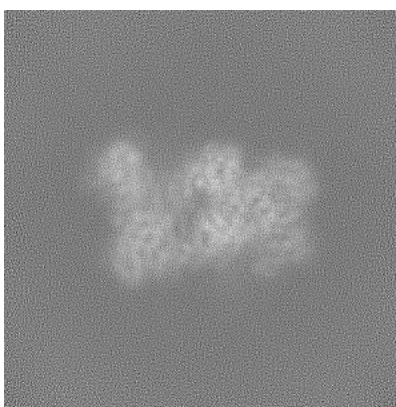


Z

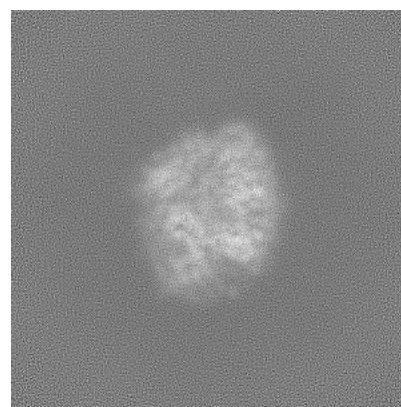
#### 6.1.2 Raw map



X



Y

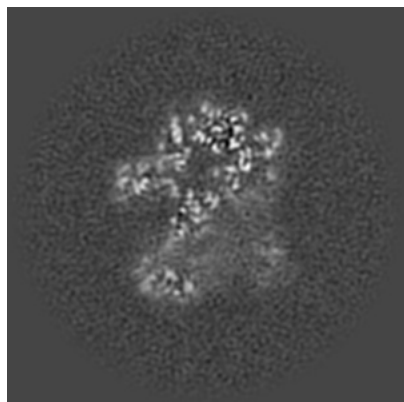


Z

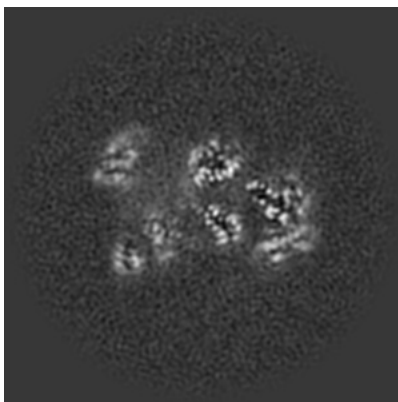
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

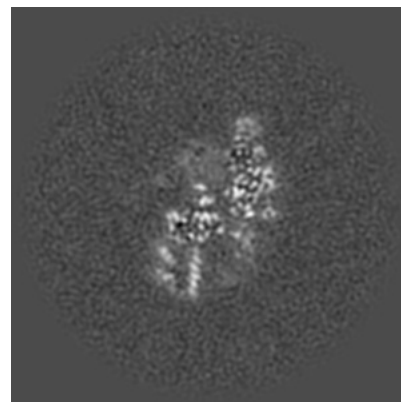
### 6.2.1 Primary map



X Index: 215

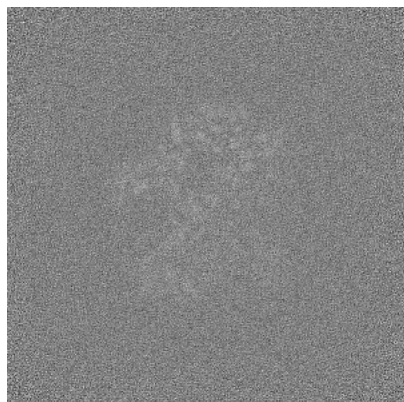


Y Index: 215

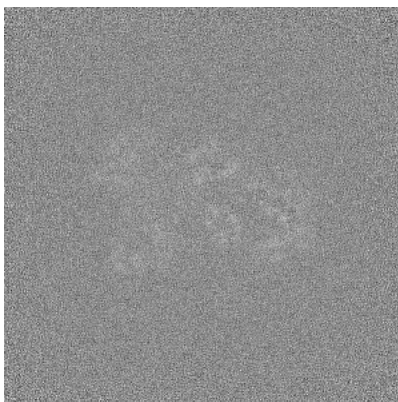


Z Index: 215

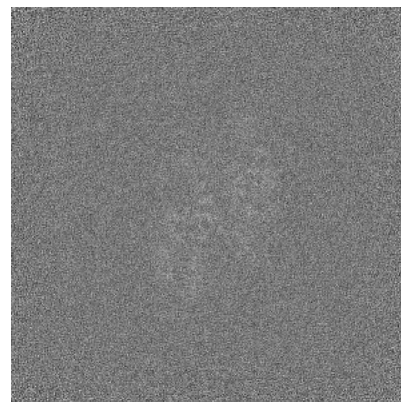
### 6.2.2 Raw map



X Index: 215



Y Index: 215

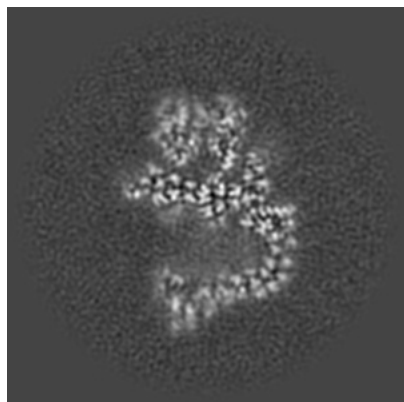


Z Index: 215

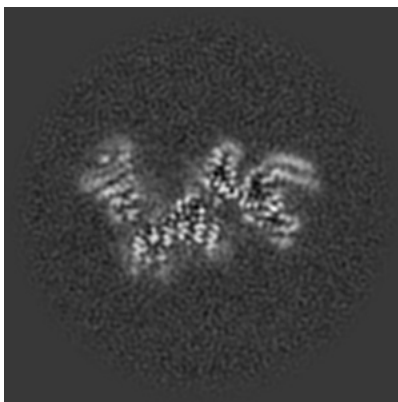
The images above show central slices of the map in three orthogonal directions.

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

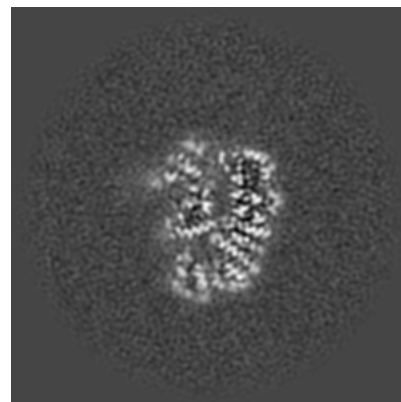
### 6.3.1 Primary map



X Index: 246

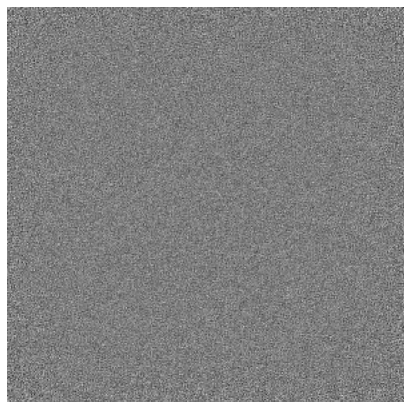


Y Index: 185

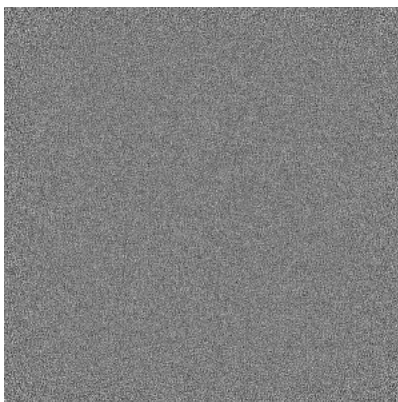


Z Index: 228

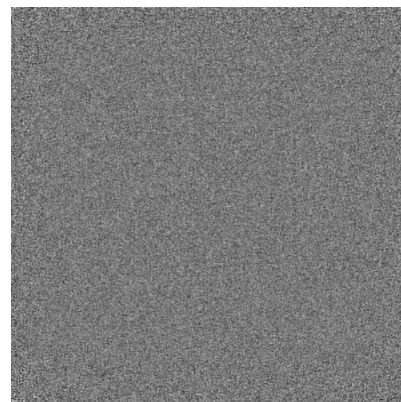
### 6.3.2 Raw map



X Index: 0



Y Index: 0



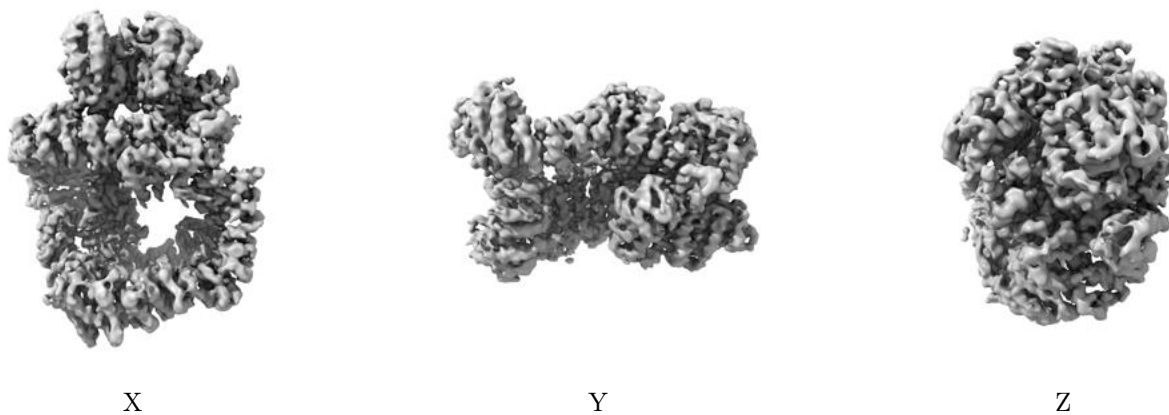
Z Index: 0

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



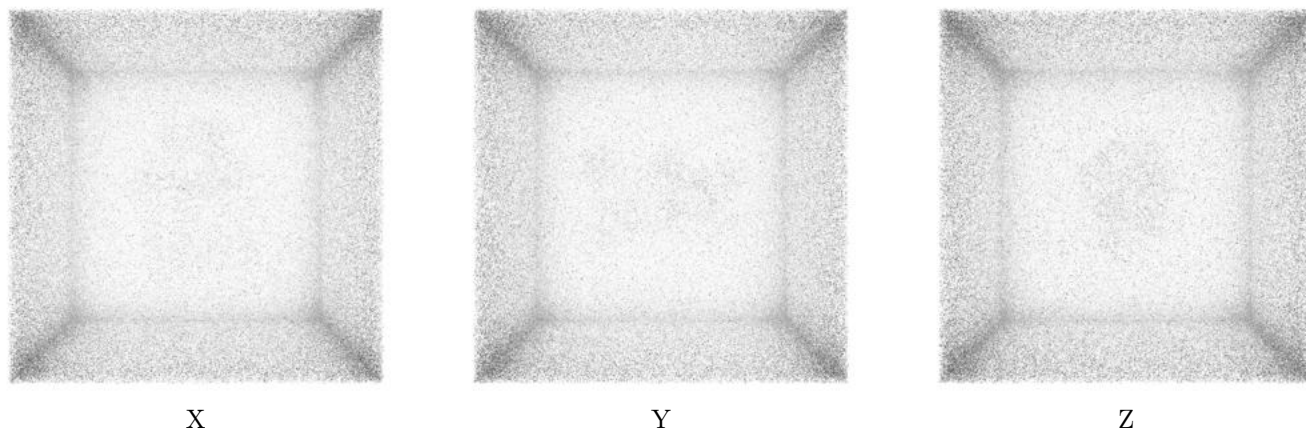
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

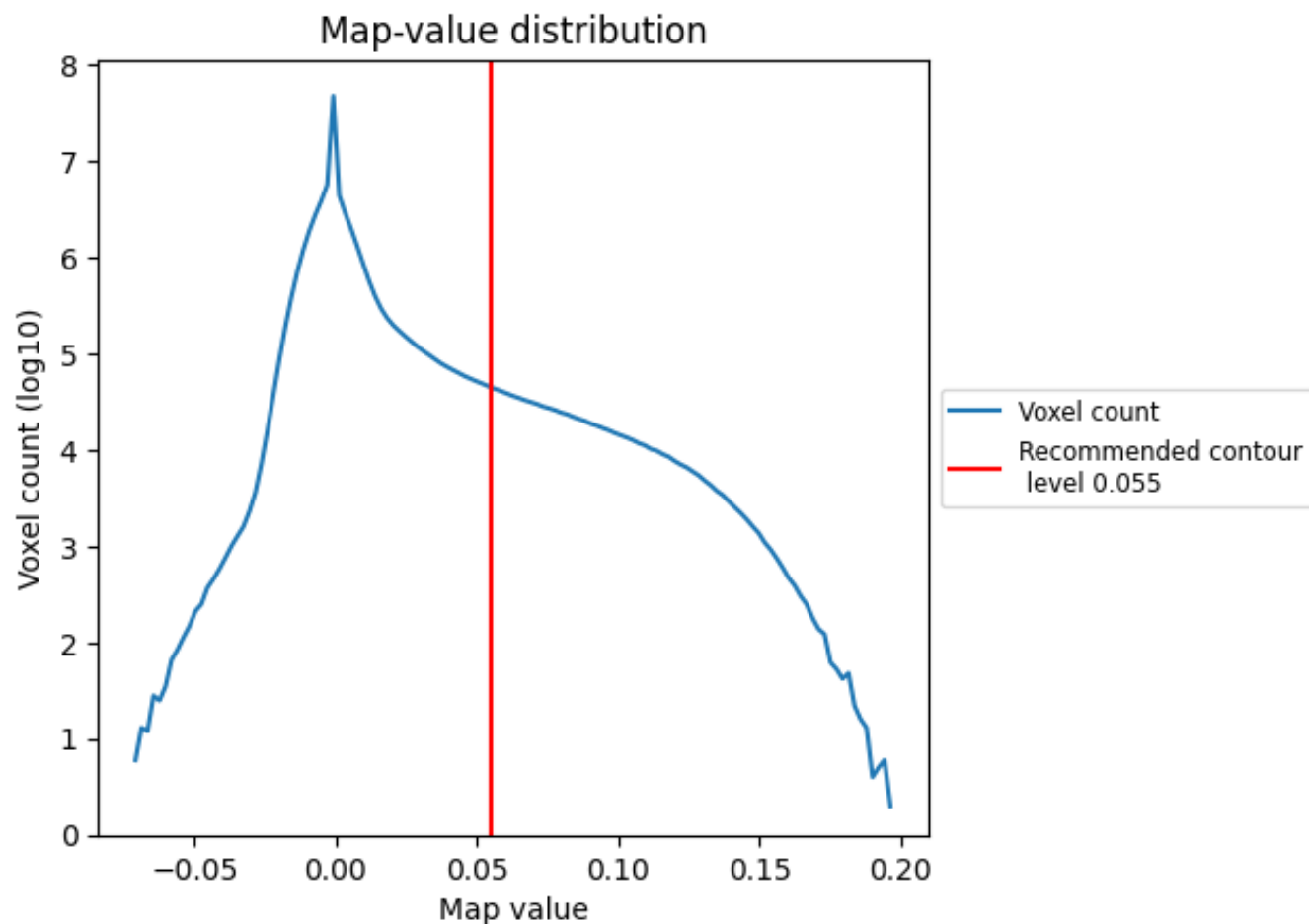
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

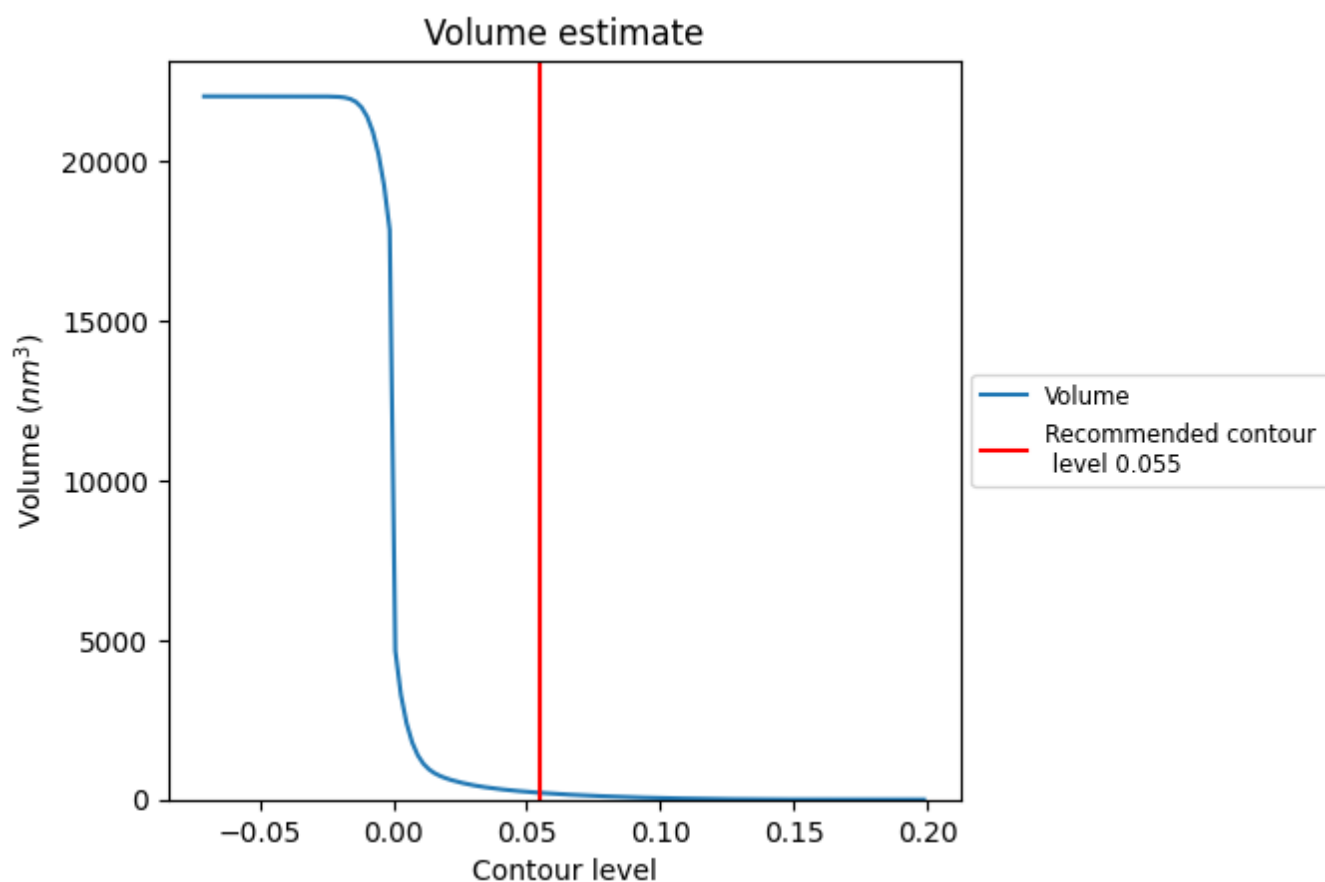
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

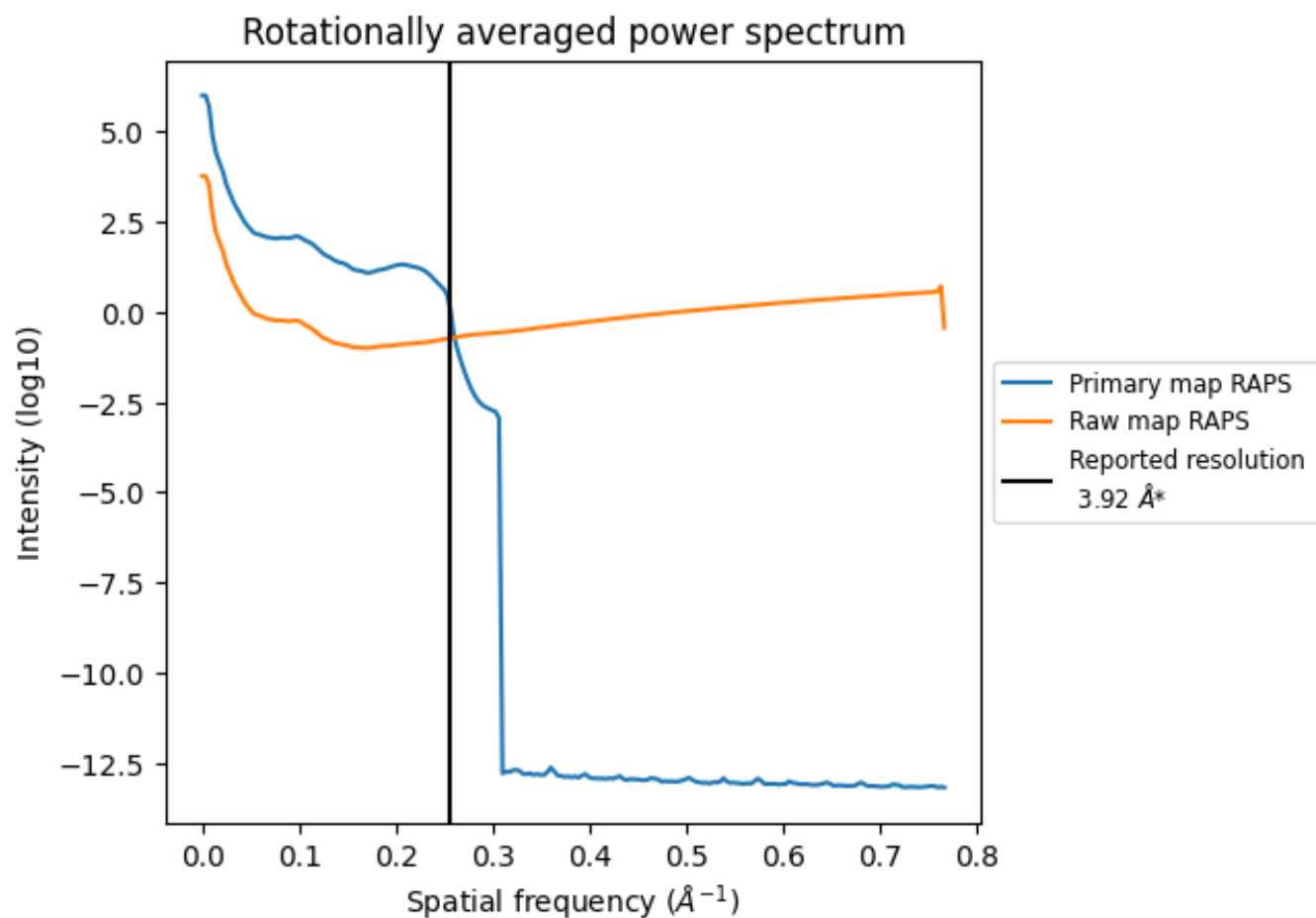


The volume at the recommended contour level is 212 nm<sup>3</sup>; this corresponds to an approximate mass of 191 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

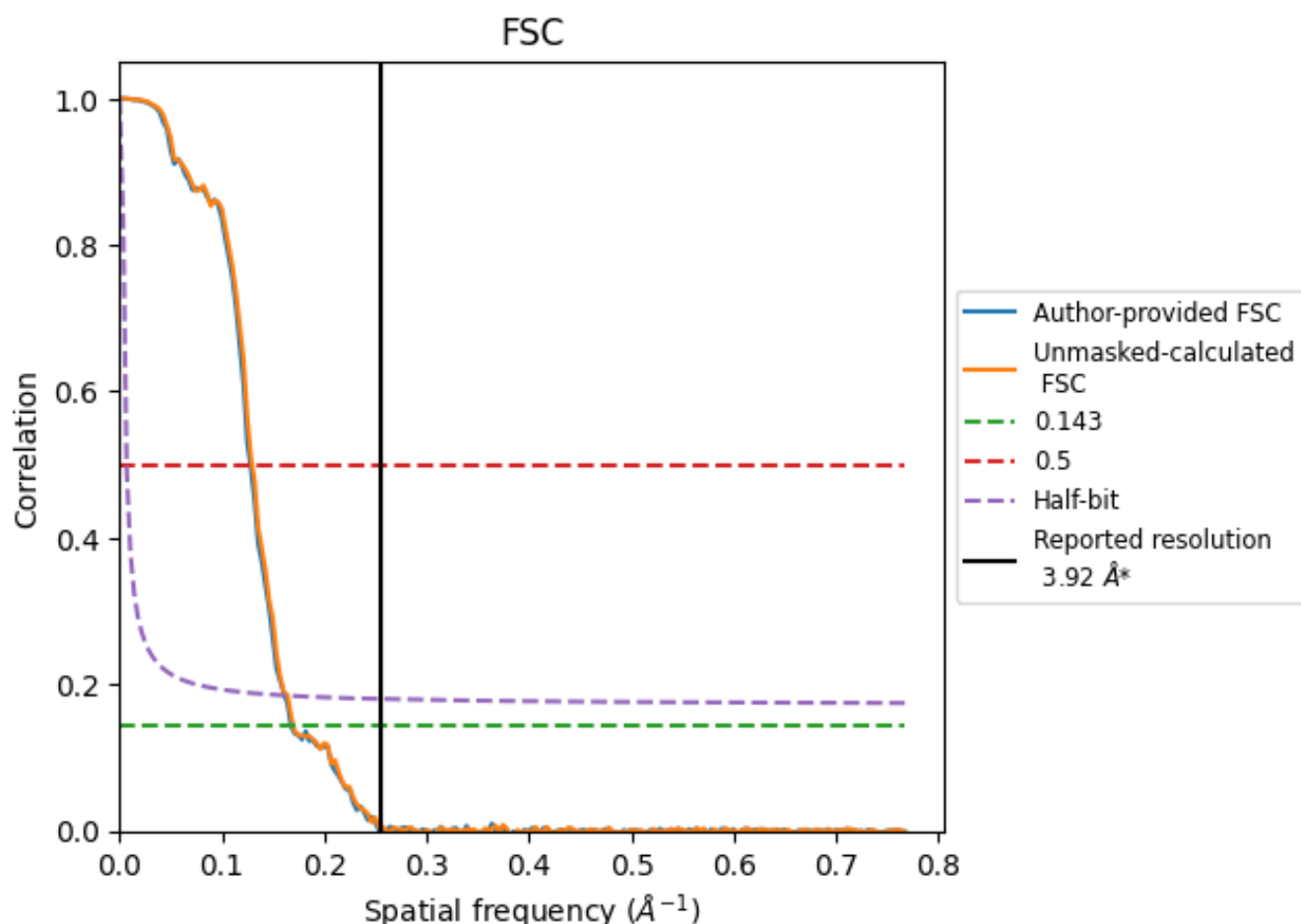


\*Reported resolution corresponds to spatial frequency of 0.255 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.255 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.92                               | -    | -        |
| Author-provided FSC curve | 5.97                               | 7.82 | 6.20     |
| Unmasked-calculated*      | 5.88                               | 7.72 | 6.09     |

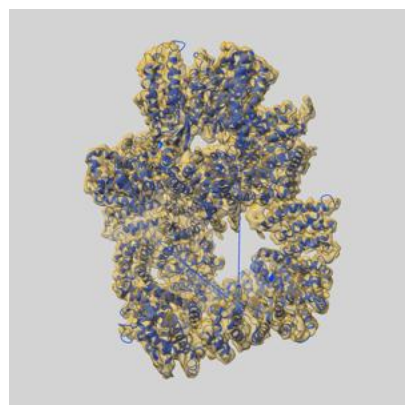
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.97 differs from the reported value 3.92 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.88 differs from the reported value 3.92 by more than 10 %

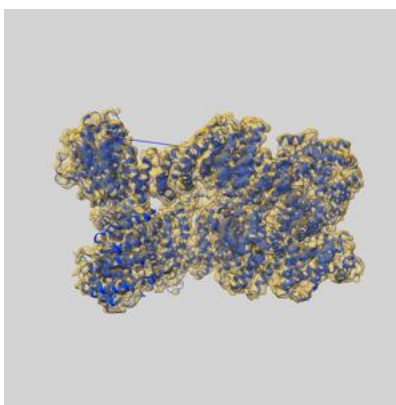
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11211 and PDB model 6ZH2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

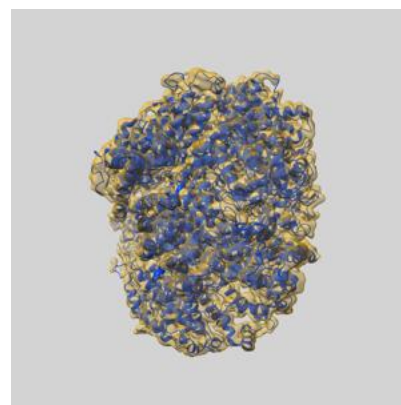
### 9.1 Map-model overlay [i](#)



X



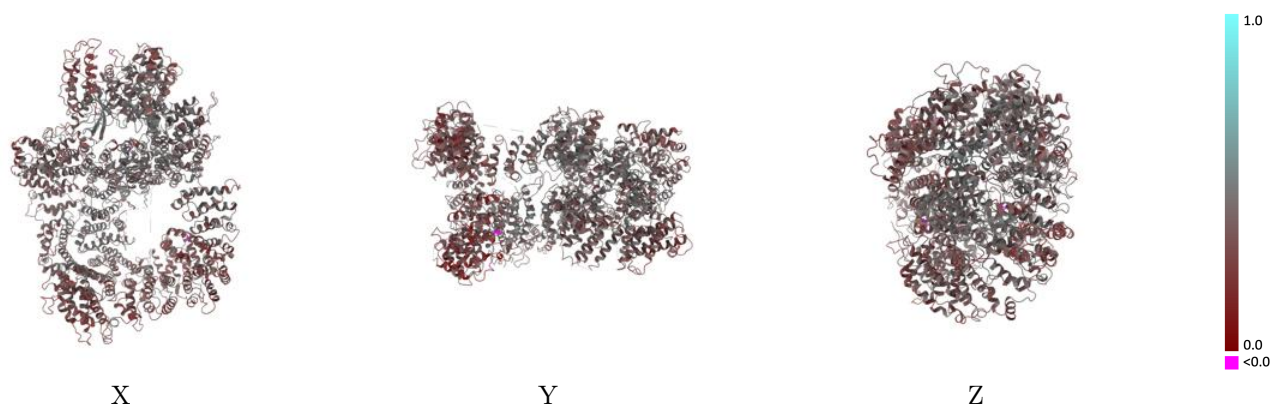
Y



Z

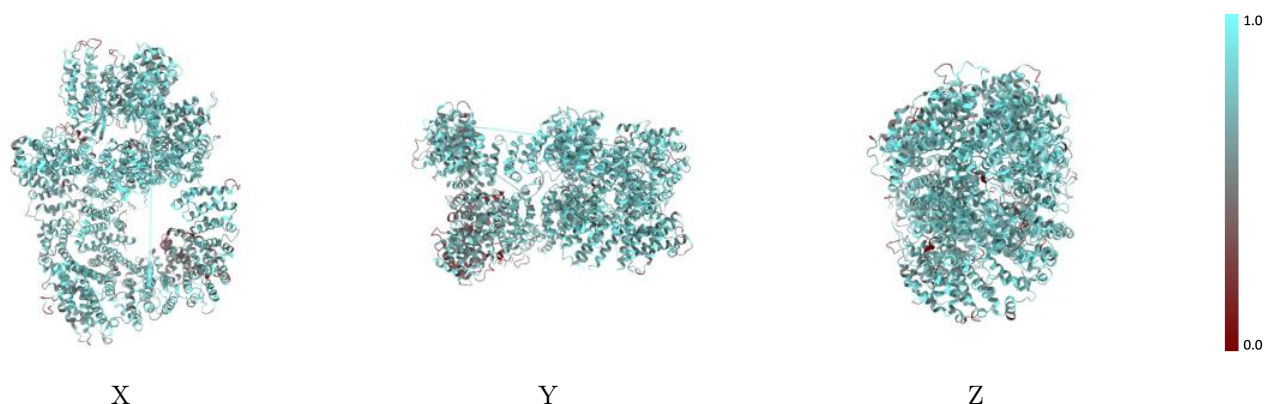
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



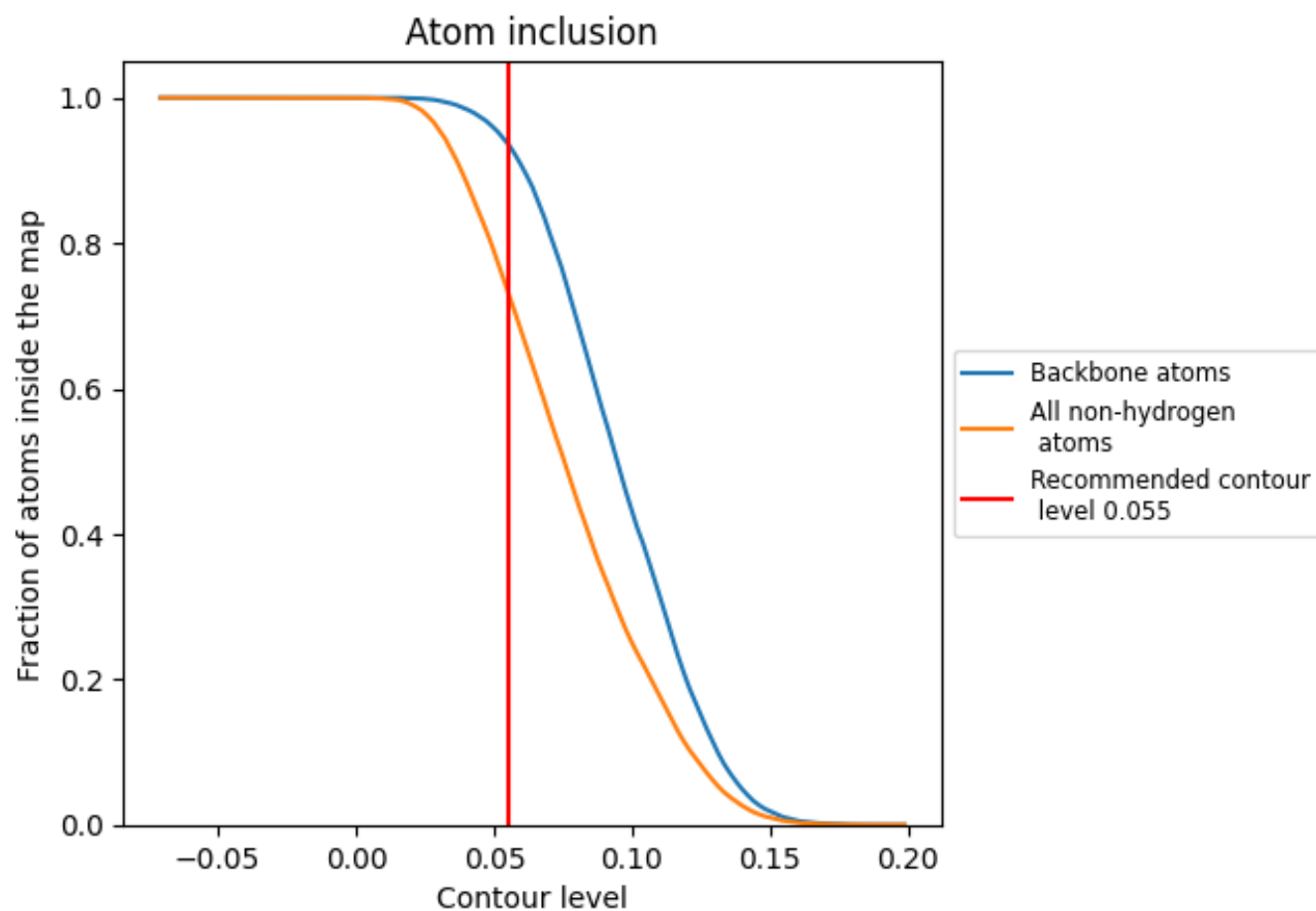
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7346 | <div></div> 0.3790 |
| A     | <div></div> 0.7346 | <div></div> 0.3790 |

