



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:39 PM EDT

PDB ID : 3M4O / pdb\_00003m4o  
Title : RNA polymerase II elongation complex B  
Authors : Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.  
Deposited on : 2010-03-11  
Resolution : 3.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

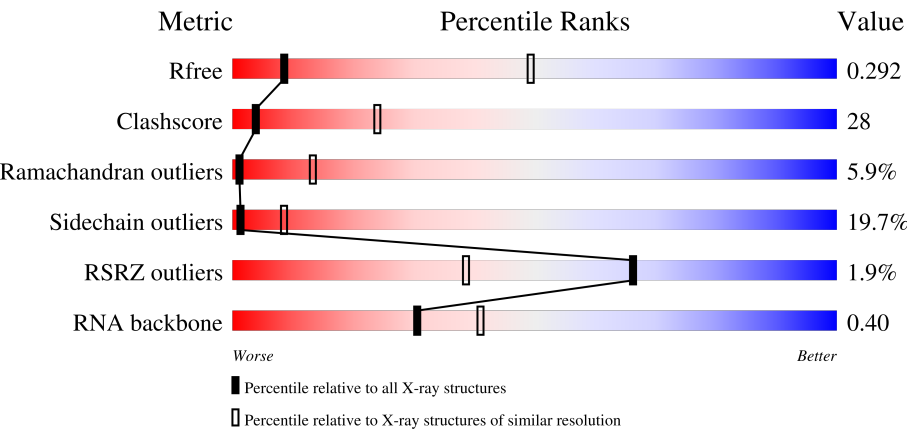
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.57 Å.

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



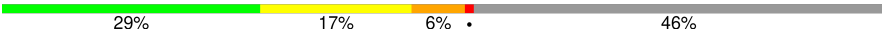
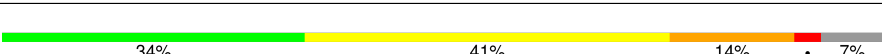
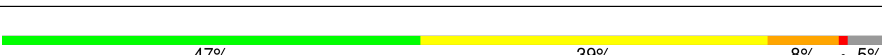
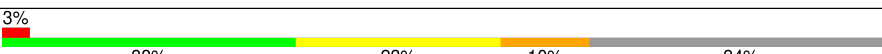
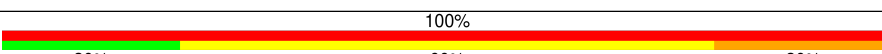
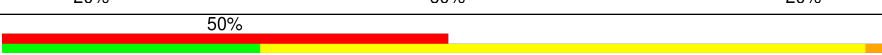
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1521 (3.66-3.50)                                      |
| Clashscore            | 190562                      | 1595 (3.66-3.50)                                      |
| Ramachandran outliers | 187476                      | 1551 (3.66-3.50)                                      |
| Sidechain outliers    | 187428                      | 1551 (3.66-3.50)                                      |
| RSRZ outliers         | 180081                      | 1520 (3.66-3.50)                                      |
| RNA backbone          | 3983                        | 1013 (4.10-3.06)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                      |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------|
| 1   | A     | 1733   | <div><div></div><div><div>35%</div><div>35%</div><div>10%</div><div>•</div><div>20%</div></div></div> |
| 2   | B     | 1224   | <div><div>39%</div><div>39%</div><div>11%</div><div>•</div><div>10%</div></div>                       |
| 3   | C     | 318    | <div><div>36%</div><div>34%</div><div>13%</div><div>•</div><div>16%</div></div>                       |
| 4   | E     | 215    | <div><div>52%</div><div>39%</div><div>9%</div></div>                                                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 5   | F     | 155    |  |
| 6   | H     | 146    |  |
| 7   | I     | 122    |  |
| 8   | J     | 70     |  |
| 9   | K     | 120    |  |
| 10  | L     | 70     |  |
| 11  | R     | 10     |  |
| 12  | T     | 28     |  |
| 13  | N     | 14     |  |

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1395     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10969 | 6917 | 1923 | 2068 | 61 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1106     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8792  | 5568 | 1538 | 1631 | 55 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | F     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 679   | 434 | 115 | 127 | 3 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | H     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1068  | 673 | 180 | 211 | 4 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | I     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 363   | 224 | 72 | 63 | 4 |         |         |       |

- Molecule 11 is a RNA chain called RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 11  | R     | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 220   | 99 | 47 | 65 | 9 |         |         |       |

- Molecule 12 is a DNA chain called DNA (28-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 12  | T     | 28       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 553   | 265 | 92 | 168 | 28 |         |         |       |

- Molecule 13 is a DNA chain called DNA (5'-D(P\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 13  | N     | 14       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 296   | 140 | 55 | 87 | 14 |         |         |       |

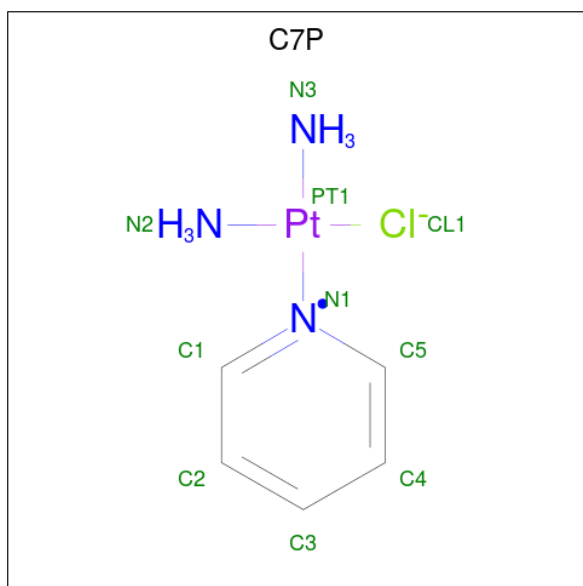
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | A     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 14  | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | I     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 14  | J     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | L     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (CCD ID: C7P) (formula: C<sub>5</sub>H<sub>11</sub>ClN<sub>3</sub>Pt).

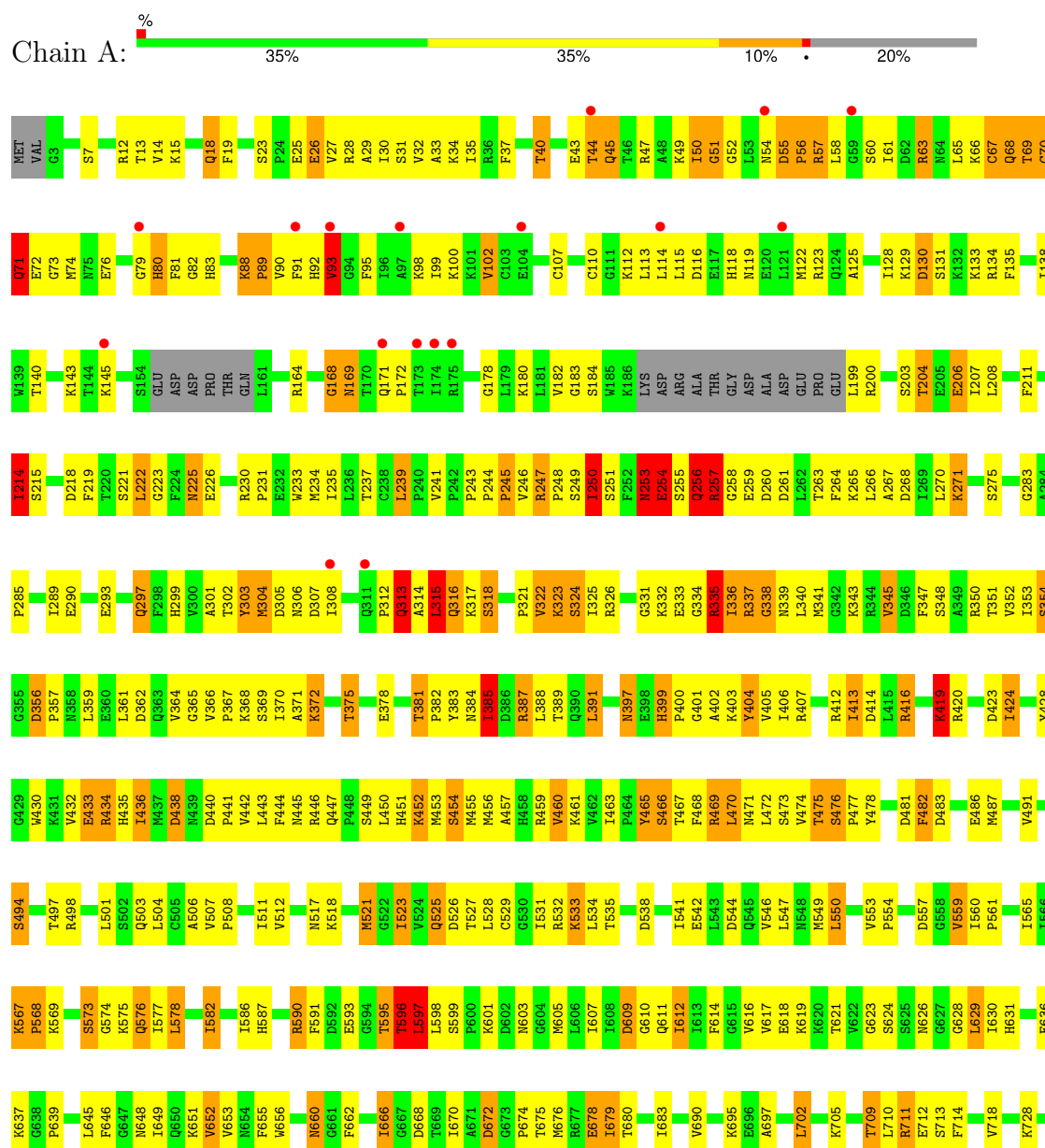


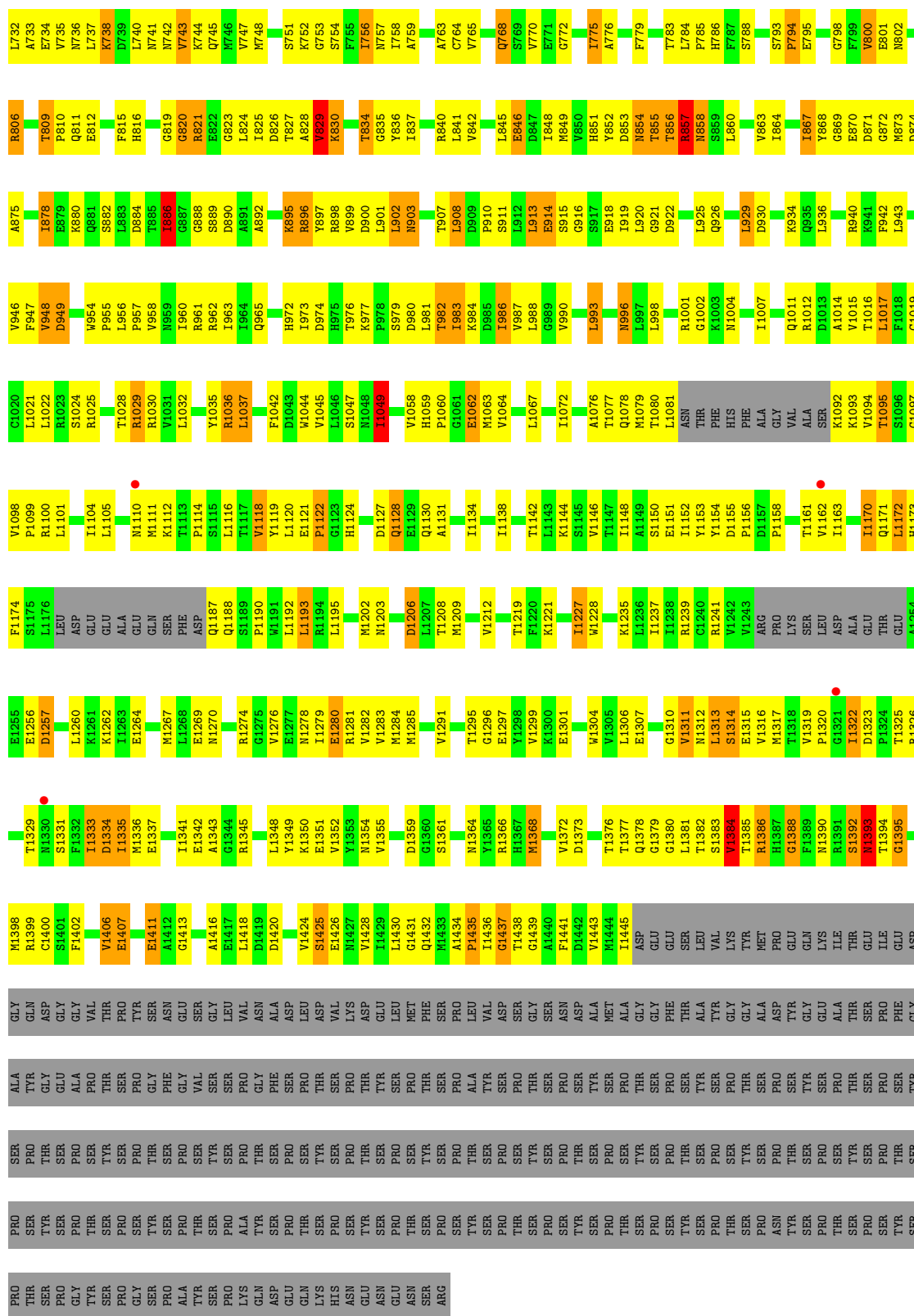
| Mol | Chain | Residues | Atoms |   |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|----|---------|---------|
| 16  | T     | 1        | Total | C | N | Pt | 0       | 0       |
|     |       |          | 9     | 5 | 3 | 1  |         |         |

### 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

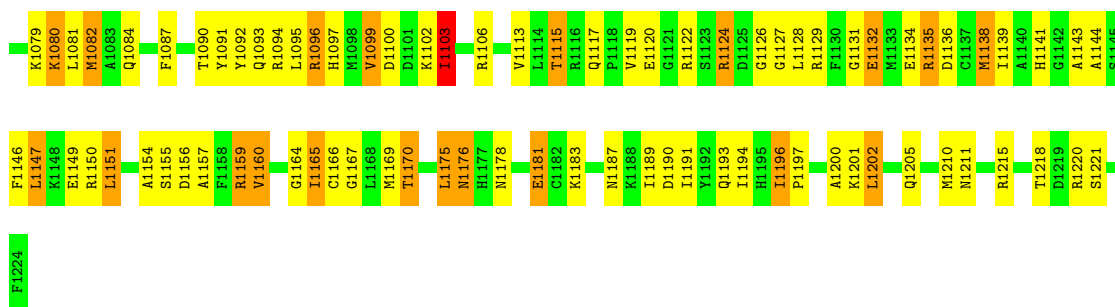
#### • Molecule 1: DNA-directed RNA polymerase II subunit RPB1



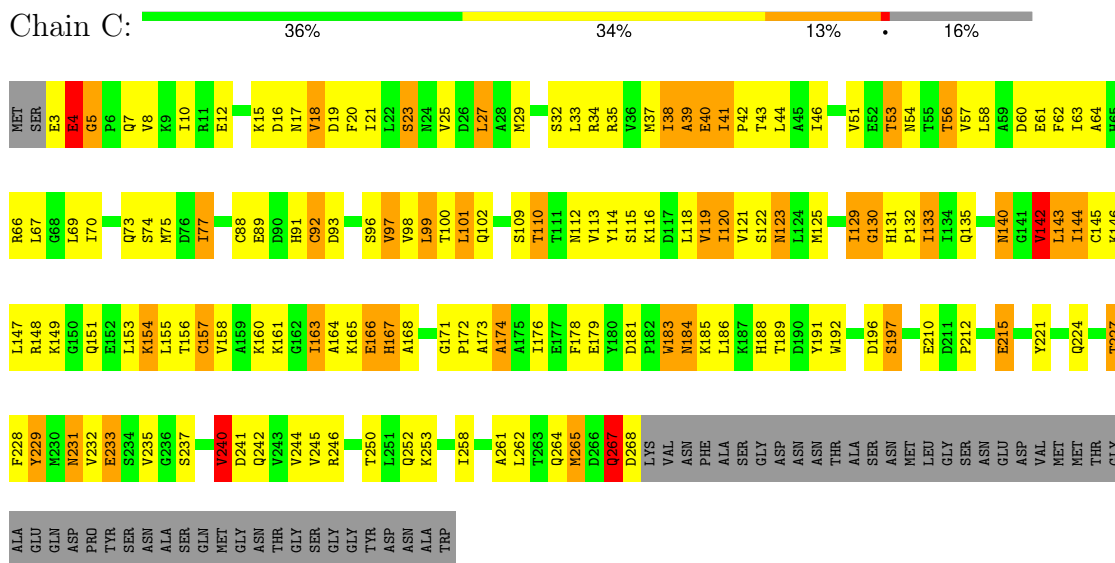




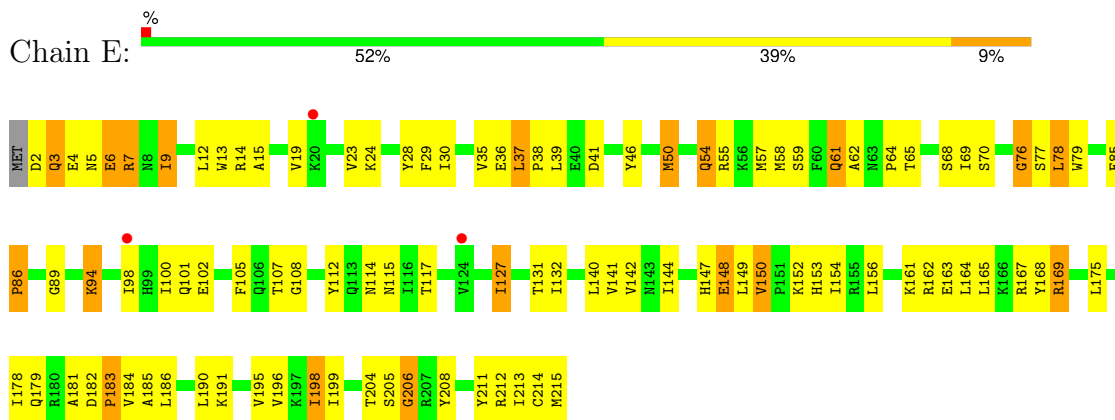
|       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |     |     |     |     |     |     |      |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-----|-----|-----|-----|-----|-----|------|
| ALA   | GLN   | HIS   | THR   | THR   | ALA   | GLU   | ASN  | SER  | GLU  | LYS  | ASN  | ILE  | TYR  | GLY  | PRO  | ASP  | GLY  | PHE  | GLU  | D20  | E21  | S22  | I25  | T26  | A27  | E28  | I34  | F37  | F38  | R39  | E40  | V44  | S45  | Q46  | F54  | V55  | D56  | Y57  | T58  | L59  | Q60  | D61  | I62  | I63  | C64  | E65  | D66  | S67  | T68  | L69  | I70  | LEU  | GLU  | ALA  | ILE   | ASP   |       |     |     |     |     |     |     |      |
| VAL   | PRO   | GLY   | ARG   | THR   | LEU   | LYS   | SER  | ASP  | TYR  | GLU  | ASN  | ILE  | TYR  | GLY  | SER  | ASP  | ASP  | ASP  | GLY  | GLU  | S235 | S236 | V237 | K164 | K99  | P100 | M101 | V102 | M103 | E104 | R159 | I172 | G247 | M173 | G107 | V108 | T109 | H110 | A111 | L112 | Y113 | P114 | Q115 | E116 | T185 | D188 | L189 | Y190 | L191 | L192 | S126 | G127 | E194 | D198 | M199  | K133  | K134  | ARG | THR | TYR | GLU | ALA | ILE | S208 |
| V211  | A214  | E216  | R217  | S218  | A219  | G220  | N221 | V223 | Q224 | V225 | K228 | I234 | S235 | S236 | V237 | K164 | K99  | P100 | M101 | V102 | M103 | E104 | R159 | I172 | G247 | M173 | G107 | V108 | T109 | H110 | A111 | L112 | Y113 | P114 | Q115 | E116 | T185 | D188 | L189 | Y190 | L191 | L192 | S126 | G127 | E194 | D198 | M199 | K133 | K134 | ARG  | THR  | TYR  | GLU  | ALA  | ILE   | S208  |       |     |     |     |     |     |     |      |
| I282  | V283  | I284  | I285  | I286  | R287  | A288  | I291 | I292 | P293 | D294 | E295 | E296 | I297 | H300 | V305 | N306 | W308 | Q309 | N310 | L311 | E312 | N313 | L314 | K315 | P316 | C317 | V318 | G321 | S322 | S325 | T323 | B326 | R327 | L331 | G335 | ARG  | ARG  | GLY  | THR  | ALA  | LEU  | GLY  | ILE  | LYS  | K345 | E346 | K347 | L348 | I349 | Q357 | K358 |      |      |      |       |       |       |     |     |     |     |     |     |      |
| E359  | F360  | L361  | P362  | H363  | F364  | T365  | Q366 | L367 | E368 | R373 | K374 | L378 | G379 | Y380 | K381 | I382 | N383 | R384 | L385 | L386 | L387 | C388 | A389 | D391 | D394 | D399 | H400 | F401 | G402 | S403 | K404 | R405 | L406 | D407 | G410 | P411 | L412 | L413 | A414 | Q415 | L416 | F417 | K418 | K422 | K423 | L424 | T425 | Y431 | V436 |      |      |      |      |      |       |       |       |     |     |     |     |     |     |      |
| E437  | GLU   | ALA   | HIS   | ASP   | PHE   | ASN   | MET  | LYS  | A446 | A447 | A450 | K451 | T452 | L453 | T454 | L457 | K458 | Y459 | A460 | L461 | A462 | T463 | G464 | G467 | E468 | Q469 | K470 | K471 | A472 | F473 | S474 | S475 | R476 | A477 | G478 | V479 | S480 | Q481 | V482 | L483 | N484 | R485 | Y486 | T487 | Y488 | S489 | T491 | L492 | S493 | R496 | R497 | N499 |      |      |       |       |       |     |     |     |     |     |     |      |
| I502  | GLY   | ARG   | ASP   | GLY   | LYS   | LEU   | A509 | Q513 | L514 | H515 | N516 | T517 | H518 | W519 | G520 | C523 | T527 | P528 | E529 | G530 | Q531 | K537 | L541 | M542 | S543 | C544 | I545 | S546 | N547 | G548 | T549 | D550 | P551 | M552 | I554 | I555 | T556 | F557 | W561 | G562 | M563 | L566 | Y569 | V570 | K573 | S574 | P575 | D576 | A577 |      |      |      |      |      |       |       |       |     |     |     |     |     |     |      |
| T578  | R579  | V585  | V589  | H590  | R591  | N592  | P593 | L596 | L603 | R604 | K606 | E612 | V613 | M615 | I616 | I619 | R620 | E621 | K625 | I626 | F627 | S628 | C644 | D629 | A630 | G631 | R632 | G633 | Y634 | R635 | P636 | L637 | F638 | I639 | V640 | E641 | D642 | E644 | G647 | H648 | L651 | K652 | V653 | R654 | I658 | L661 |      |      |      |      |      |      |      |      |       |       |       |     |     |     |     |     |     |      |
| E665  | D668  | ILE   | GLU   | GLY   | GLY   | PHE   | GLU  | VAL  | E678 | W681 | S682 | S683 | L684 | L685 | N686 | L689 | V690 | E691 | Y692 | A695 | E698 | I701 | L702 | I703 | A704 | M705 | Q706 | P707 | E708 | D709 | L710 | E711 | P712 | A715 | ASN  | GLU  | ASN  | ASP  | LEU  | D722 | V723 | R724 | P725 | T726 | K727 | R728 | I729 | R730 |      |      |      |      |      |      |       |       |       |     |     |     |     |     |     |      |
| V731  | S732  | H733  | H734  | A735  | T736  | F738  | T739 | H740 | C741 | T742 | E743 | A744 | P745 | S746 | R747 | I748 | L749 | G750 | V751 | A752 | K753 | S754 | I755 | V756 | P759 | D760 | S761 | R762 | S763 | P764 | R765 | R766 | Y769 | Q770 | S771 | G774 | K775 | A776 | M777 | V780 | T783 | N784 | Y785 | R788 | M789 | D790 | T791 | K792 | A793 | N794 | I795 |      |      |      |       |       |       |     |     |     |     |     |     |      |
| L796  | Y797  | Y798  | P799  | Q800  | K801  | P802  | L803 | G804 | T805 | T806 | A807 | A808 | M809 | L812 | R815 | A819 | G820 | N821 | K822 | V825 | A826 | I827 | S831 | G832 | Y833 | N834 | Q835 | E836 | D837 | S838 | M839 | I840 | R841 | N842 | Q843 | S844 | S845 | I846 | D847 | R848 | G849 | F851 | R852 | S853 | L854 | R857 | S858 | Y859 | M860 | D861 | Q862 |      |      |      |       |       |       |     |     |     |     |     |     |      |
| E863  | K864  | K865  | Y866  | C867  | M868  | S869  | I870 | T871 | E872 | T873 | F874 | E875 | K876 | P877 | Q878 | R879 | T880 | N881 | T882 | L883 | R884 | M885 | K886 | Y890 | L893 | D894 | I899 | A900 | P901 | G902 | I911 | I912 | G913 | K914 | T915 | P916 | P917 | G918 | S919 | PRO  | ASP  | GLU  | GLU  | LEU  | GLY  | GLN  | THR  | ALA  | TYR  | HIS  | S933 | K934 | R935 |      |       |       |       |     |     |     |     |     |     |      |
| D936  | A937  | S938  | T939  | P940  | P1007 | P1008 | R942 | S943 | T944 | E945 | V952 | L953 | V954 | T955 | T956 | N957 | Q958 | D959 | G960 | L961 | K962 | F963 | V964 | K965 | V966 | T970 | T971 | I973 | P974 | Q975 | I976 | R977 | D978 | K979 | F980 | A981 | S982 | R983 | H984 | G985 | C986 | K987 | G988 | T989 | I990 | G991 | I992 | T993 | Y994 | R995 | O996 | E997 | D998 | M999 | P1000 | F1001 | N1002 |     |     |     |     |     |     |      |
| A1003 | E1004 | G1005 | T1006 | P1007 | P1008 | R1009 | R942 | S943 | T944 | E945 | V952 | L953 | V954 | T955 | T956 | N957 | Q958 | D959 | G960 | L961 | K962 | F963 | V964 | K965 | V966 | T970 | T971 | I973 | P974 | Q975 | I976 | R977 | D978 | K979 | F980 | A981 | S982 | R983 | H984 | G985 | C986 | K987 | G988 | T989 | I990 | G991 | I992 | T993 | Y994 | R995 | O996 | E997 | D998 | M999 | P1000 | F1001 | N1002 |     |     |     |     |     |     |      |



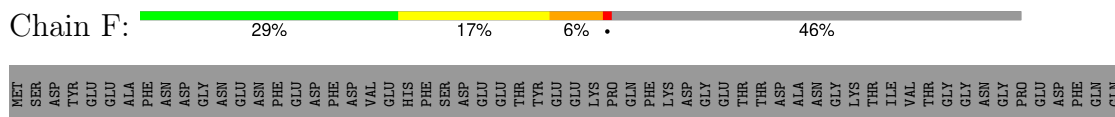
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

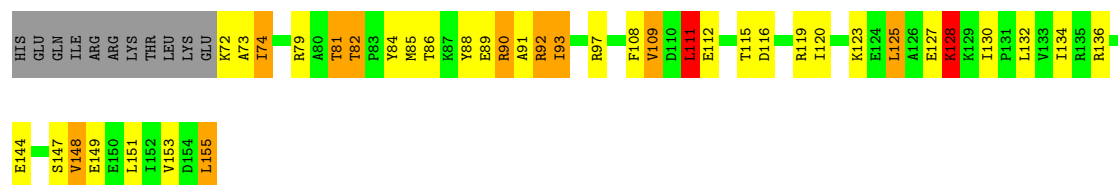


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

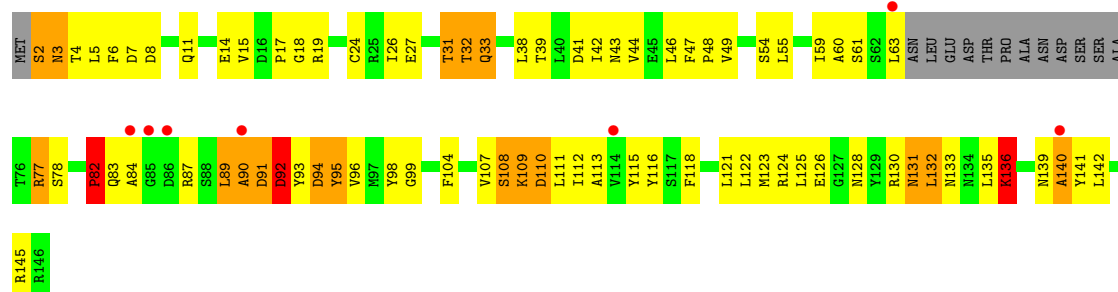


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

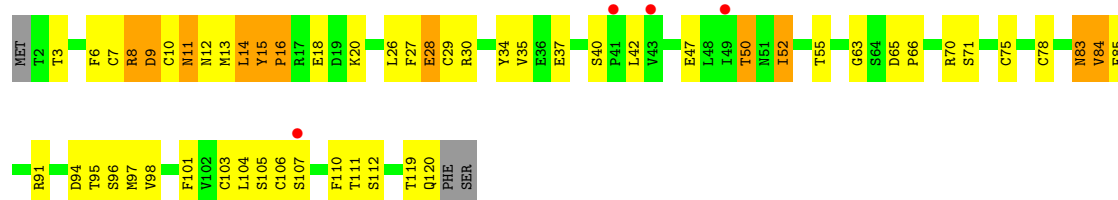




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



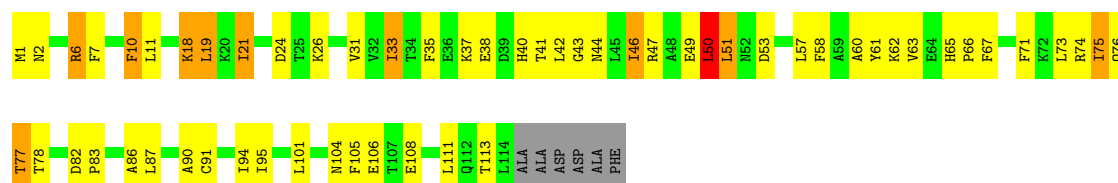
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



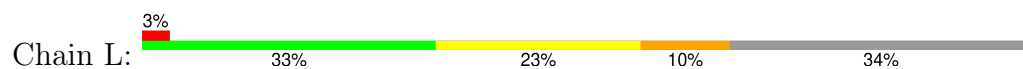
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



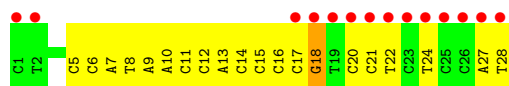
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3')



- Molecule 12: DNA (28-MER)



- Molecule 13: DNA (5'-D(P\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 168.11Å 222.13Å 191.78Å<br>90.00° 100.99° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 40.00 – 3.57<br>40.00 – 3.57                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.5 (40.00-3.57)<br>90.4 (40.00-3.57)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.17                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.94 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0102                                             | Depositor        |
| R, $R_{free}$                                                           | 0.241 , 0.292<br>0.248 , 0.292                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3681 reflections (4.50%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.269                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 111.1                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 29227                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 130.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, C7P

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     | 0.74         | 2/11163 (0.0%) | 1.09        | 38/15091 (0.3%)  |
| 2   | B     | 0.79         | 0/8963         | 1.09        | 38/12086 (0.3%)  |
| 3   | C     | 0.71         | 0/2133         | 1.06        | 9/2891 (0.3%)    |
| 4   | E     | 0.66         | 0/1788         | 0.98        | 2/2406 (0.1%)    |
| 5   | F     | 0.69         | 0/691          | 1.06        | 4/933 (0.4%)     |
| 6   | H     | 0.64         | 0/1086         | 0.98        | 4/1470 (0.3%)    |
| 7   | I     | 0.70         | 0/989          | 1.02        | 2/1331 (0.2%)    |
| 8   | J     | 0.82         | 0/541          | 1.19        | 5/727 (0.7%)     |
| 9   | K     | 0.71         | 0/937          | 0.98        | 1/1265 (0.1%)    |
| 10  | L     | 0.85         | 0/365          | 1.09        | 1/485 (0.2%)     |
| 11  | R     | 0.51         | 0/248          | 0.98        | 1/387 (0.3%)     |
| 12  | T     | 0.43         | 0/615          | 1.11        | 3/941 (0.3%)     |
| 13  | N     | 0.27         | 0/332          | 0.83        | 0/513            |
| All | All   | 0.73         | 2/29851 (0.0%) | 1.07        | 108/40526 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 6   | H     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 250 | ILE  | CA-CB | 6.34 | 1.60        | 1.54     |
| 1   | A     | 483 | ASP  | N-CA  | 5.46 | 1.53        | 1.46     |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | J     | 5    | VAL  | N-CA-C   | -8.86 | 98.15       | 109.58   |
| 1   | A     | 452  | LYS  | N-CA-C   | -8.73 | 101.71      | 111.14   |
| 1   | A     | 313  | GLN  | N-CA-C   | 8.16  | 117.87      | 108.49   |
| 1   | A     | 596  | THR  | CB-CA-C  | -8.11 | 100.63      | 111.82   |
| 2   | B     | 99   | LYS  | CA-C-N   | 7.92  | 129.75      | 119.84   |
| 2   | B     | 99   | LYS  | C-N-CA   | 7.92  | 129.75      | 119.84   |
| 2   | B     | 37   | PHE  | N-CA-C   | -7.75 | 99.81       | 110.35   |
| 1   | A     | 81   | PHE  | N-CA-C   | 7.61  | 119.77      | 110.41   |
| 1   | A     | 250  | ILE  | N-CA-C   | 7.61  | 121.50      | 110.09   |
| 6   | H     | 92   | ASP  | N-CA-C   | -7.42 | 103.54      | 112.59   |
| 2   | B     | 1017 | ILE  | CA-C-N   | -7.05 | 111.02      | 119.84   |
| 2   | B     | 1017 | ILE  | C-N-CA   | -7.05 | 111.02      | 119.84   |
| 2   | B     | 734  | HIS  | N-CA-C   | 6.96  | 120.10      | 110.35   |
| 2   | B     | 476  | ARG  | CB-CA-C  | -6.96 | 96.57       | 110.42   |
| 1   | A     | 253  | ASN  | N-CA-C   | 6.94  | 125.58      | 110.80   |
| 2   | B     | 296  | GLU  | N-CA-C   | -6.91 | 103.85      | 112.90   |
| 1   | A     | 239  | LEU  | CA-C-N   | 6.79  | 127.16      | 119.83   |
| 1   | A     | 239  | LEU  | C-N-CA   | 6.79  | 127.16      | 119.83   |
| 3   | C     | 4    | GLU  | N-CA-C   | 6.71  | 118.48      | 111.03   |
| 2   | B     | 476  | ARG  | N-CA-C   | 6.68  | 125.02      | 110.80   |
| 1   | A     | 1393 | ASN  | N-CA-C   | 6.67  | 125.00      | 110.80   |
| 1   | A     | 88   | LYS  | CA-C-N   | 6.66  | 128.16      | 119.84   |
| 1   | A     | 88   | LYS  | C-N-CA   | 6.66  | 128.16      | 119.84   |
| 8   | J     | 3    | VAL  | CA-C-N   | -6.64 | 112.92      | 119.90   |
| 8   | J     | 3    | VAL  | C-N-CA   | -6.64 | 112.92      | 119.90   |
| 1   | A     | 466  | SER  | N-CA-C   | 6.63  | 120.96      | 113.01   |
| 2   | B     | 273  | LEU  | CA-C-N   | 6.53  | 128.00      | 119.84   |
| 2   | B     | 273  | LEU  | C-N-CA   | 6.53  | 128.00      | 119.84   |
| 1   | A     | 776  | ALA  | N-CA-C   | 6.51  | 118.73      | 110.33   |
| 1   | A     | 886  | ILE  | N-CA-C   | 6.46  | 116.57      | 110.30   |
| 1   | A     | 857  | ARG  | N-CA-C   | 6.41  | 118.69      | 109.14   |
| 2   | B     | 838  | SER  | N-CA-C   | -6.40 | 99.34       | 109.07   |
| 6   | H     | 109  | LYS  | CA-C-N   | 6.39  | 133.21      | 121.70   |
| 6   | H     | 109  | LYS  | C-N-CA   | 6.39  | 133.21      | 121.70   |
| 1   | A     | 973  | ILE  | N-CA-C   | 6.34  | 117.00      | 107.75   |
| 12  | T     | 18   | DG   | N3-C4-C5 | -6.19 | 119.12      | 128.40   |
| 2   | B     | 475  | SER  | N-CA-C   | -6.16 | 105.61      | 113.01   |
| 3   | C     | 181  | ASP  | CA-C-N   | 6.12  | 125.33      | 118.97   |
| 3   | C     | 181  | ASP  | C-N-CA   | 6.12  | 125.33      | 118.97   |
| 2   | B     | 861  | ASP  | N-CA-C   | 6.09  | 116.60      | 108.38   |
| 8   | J     | 3    | VAL  | CB-CA-C  | -6.06 | 104.94      | 110.88   |
| 1   | A     | 247  | ARG  | CA-C-N   | 5.96  | 127.29      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 247  | ARG  | C-N-CA      | 5.96  | 127.29      | 119.84   |
| 1   | A     | 595  | THR  | N-CA-C      | 5.95  | 118.43      | 108.73   |
| 1   | A     | 356  | ASP  | N-CA-C      | 5.92  | 119.14      | 108.55   |
| 1   | A     | 829  | VAL  | CB-CA-C     | 5.91  | 120.15      | 112.24   |
| 4   | E     | 182  | ASP  | CA-C-N      | 5.88  | 127.19      | 119.84   |
| 4   | E     | 182  | ASP  | C-N-CA      | 5.88  | 127.19      | 119.84   |
| 1   | A     | 652  | VAL  | CB-CA-C     | -5.88 | 104.37      | 112.24   |
| 1   | A     | 993  | LEU  | N-CA-C      | -5.86 | 102.60      | 111.56   |
| 2   | B     | 69   | LEU  | N-CA-C      | 5.85  | 118.76      | 109.81   |
| 3   | C     | 39   | ALA  | N-CA-C      | 5.84  | 117.30      | 110.41   |
| 2   | B     | 1157 | ALA  | N-CA-C      | -5.80 | 101.62      | 110.14   |
| 1   | A     | 482  | PHE  | N-CA-C      | 5.78  | 120.02      | 111.87   |
| 1   | A     | 345  | VAL  | N-CA-C      | 5.78  | 118.18      | 108.81   |
| 2   | B     | 644  | GLU  | N-CA-C      | 5.78  | 117.83      | 108.41   |
| 2   | B     | 762  | ASN  | N-CA-C      | 5.78  | 118.52      | 108.76   |
| 2   | B     | 323  | VAL  | N-CA-C      | -5.77 | 104.90      | 113.39   |
| 1   | A     | 356  | ASP  | CA-C-N      | 5.75  | 127.03      | 119.84   |
| 1   | A     | 356  | ASP  | C-N-CA      | 5.75  | 127.03      | 119.84   |
| 2   | B     | 740  | HIS  | N-CA-C      | 5.74  | 118.00      | 108.13   |
| 2   | B     | 916  | THR  | CA-C-N      | 5.74  | 125.75      | 119.90   |
| 2   | B     | 916  | THR  | C-N-CA      | 5.74  | 125.75      | 119.90   |
| 3   | C     | 20   | PHE  | N-CA-C      | 5.72  | 118.82      | 108.69   |
| 8   | J     | 5    | VAL  | CB-CA-C     | -5.69 | 102.61      | 111.26   |
| 2   | B     | 769  | TYR  | N-CA-C      | -5.67 | 104.73      | 111.03   |
| 5   | F     | 116  | ASP  | CA-C-N      | 5.64  | 126.89      | 119.84   |
| 5   | F     | 116  | ASP  | C-N-CA      | 5.64  | 126.89      | 119.84   |
| 1   | A     | 366  | VAL  | N-CA-C      | 5.52  | 113.02      | 107.55   |
| 2   | B     | 21   | GLU  | N-CA-C      | 5.51  | 120.07      | 113.23   |
| 1   | A     | 794  | PRO  | CA-C-N      | 5.46  | 127.91      | 120.54   |
| 1   | A     | 794  | PRO  | C-N-CA      | 5.46  | 127.91      | 120.54   |
| 2   | B     | 326  | ASP  | N-CA-C      | 5.46  | 117.69      | 109.23   |
| 12  | T     | 18   | DG   | C2-N3-C4    | 5.43  | 119.94      | 111.80   |
| 2   | B     | 228  | LYS  | N-CA-C      | 5.42  | 119.00      | 107.67   |
| 1   | A     | 61   | ILE  | N-CA-C      | 5.35  | 116.24      | 111.90   |
| 1   | A     | 481  | ASP  | N-CA-C      | -5.33 | 101.35      | 108.86   |
| 1   | A     | 247  | ARG  | N-CA-C      | 5.28  | 116.36      | 108.76   |
| 2   | B     | 201  | GLY  | N-CA-C      | -5.28 | 107.40      | 115.00   |
| 1   | A     | 646  | PHE  | N-CA-C      | -5.26 | 105.46      | 111.14   |
| 7   | I     | 28   | GLU  | N-CA-C      | 5.26  | 117.94      | 108.48   |
| 5   | F     | 74   | ILE  | CA-C-N      | 5.25  | 125.99      | 120.11   |
| 5   | F     | 74   | ILE  | C-N-CA      | 5.25  | 125.99      | 120.11   |
| 11  | R     | 8    | G    | C4'-C3'-C2' | -5.25 | 97.35       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 971  | THR  | N-CA-C   | -5.23 | 100.72      | 109.24   |
| 2   | B     | 1075 | GLY  | N-CA-C   | 5.21  | 118.94      | 112.64   |
| 1   | A     | 200  | ARG  | N-CA-C   | 5.21  | 117.44      | 110.35   |
| 2   | B     | 616  | ILE  | CB-CA-C  | -5.16 | 104.08      | 111.31   |
| 1   | A     | 1377 | THR  | N-CA-C   | 5.16  | 119.44      | 113.20   |
| 3   | C     | 5    | GLY  | CA-C-N   | 5.16  | 126.29      | 119.84   |
| 3   | C     | 5    | GLY  | C-N-CA   | 5.16  | 126.29      | 119.84   |
| 2   | B     | 759  | PRO  | N-CA-C   | -5.15 | 107.91      | 114.35   |
| 3   | C     | 135  | GLN  | N-CA-C   | -5.15 | 107.00      | 113.28   |
| 1   | A     | 1311 | VAL  | N-CA-C   | 5.14  | 115.87      | 107.24   |
| 2   | B     | 552  | MET  | CA-C-N   | -5.14 | 114.37      | 119.56   |
| 2   | B     | 552  | MET  | C-N-CA   | -5.14 | 114.37      | 119.56   |
| 7   | I     | 85   | PHE  | N-CA-C   | 5.13  | 116.61      | 108.96   |
| 12  | T     | 18   | DG   | N3-C4-N9 | 5.10  | 133.65      | 126.00   |
| 2   | B     | 606  | LYS  | N-CA-C   | -5.08 | 107.74      | 114.04   |
| 2   | B     | 1154 | ALA  | N-CA-C   | -5.08 | 103.90      | 110.19   |
| 3   | C     | 60   | ASP  | N-CA-C   | 5.07  | 117.20      | 111.11   |
| 6   | H     | 91   | ASP  | N-CA-C   | 5.07  | 116.90      | 108.02   |
| 2   | B     | 621  | GLU  | N-CA-C   | -5.07 | 106.51      | 113.30   |
| 9   | K     | 62   | LYS  | N-CA-C   | 5.05  | 116.27      | 107.93   |
| 10  | L     | 67   | PHE  | N-CA-C   | 5.02  | 116.57      | 108.34   |
| 2   | B     | 636  | PRO  | CA-C-N   | 5.02  | 130.73      | 121.70   |
| 2   | B     | 636  | PRO  | C-N-CA   | 5.02  | 130.73      | 121.70   |
| 1   | A     | 1313 | LEU  | N-CA-C   | -5.00 | 106.86      | 113.12   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1172 | LEU  | Peptide |
| 6   | H     | 136  | LYS  | Peptide |
| 6   | H     | 82   | PRO  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10969 | 0        | 11071    | 705     | 0            |
| 2   | B     | 8792  | 0        | 8824     | 582     | 0            |
| 3   | C     | 2095  | 0        | 2052     | 160     | 0            |
| 4   | E     | 1752  | 0        | 1776     | 74      | 0            |
| 5   | F     | 679   | 0        | 701      | 32      | 0            |
| 6   | H     | 1068  | 0        | 1040     | 67      | 0            |
| 7   | I     | 971   | 0        | 929      | 35      | 0            |
| 8   | J     | 532   | 0        | 543      | 64      | 0            |
| 9   | K     | 919   | 0        | 929      | 57      | 0            |
| 10  | L     | 363   | 0        | 387      | 18      | 0            |
| 11  | R     | 220   | 0        | 110      | 12      | 0            |
| 12  | T     | 553   | 0        | 315      | 24      | 0            |
| 13  | N     | 296   | 0        | 160      | 3       | 0            |
| 14  | A     | 2     | 0        | 0        | 0       | 0            |
| 14  | B     | 1     | 0        | 0        | 0       | 0            |
| 14  | C     | 1     | 0        | 0        | 0       | 0            |
| 14  | I     | 2     | 0        | 0        | 0       | 0            |
| 14  | J     | 1     | 0        | 0        | 0       | 0            |
| 14  | L     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 16  | T     | 9     | 0        | 5        | 5       | 0            |
| All | All   | 29227 | 0        | 28842    | 1646    | 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 28.

All (1646) 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:30:ILE:HG12   | 2:B:1170:THR:HG21 | 1.31                     | 1.13              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:HD2   | 1.79                     | 1.10              |
| 1:A:401:GLY:C     | 1:A:435:HIS:HD2   | 1.59                     | 1.09              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:CD    | 1.82                     | 1.09              |
| 1:A:315:LEU:HB2   | 1:A:316:GLN:HA    | 1.18                     | 1.08              |
| 5:F:93:ILE:HD11   | 5:F:134:ILE:HD11  | 1.14                     | 1.07              |
| 7:I:7:CYS:SG      | 7:I:10:CYS:SG     | 2.52                     | 1.07              |
| 2:B:635:ARG:HB2   | 2:B:636:PRO:CD    | 1.82                     | 1.07              |
| 1:A:1323:ASP:OD1  | 1:A:1325:THR:HG22 | 1.53                     | 1.06              |
| 2:B:635:ARG:HB2   | 2:B:636:PRO:HD3   | 1.09                     | 1.05              |
| 2:B:636:PRO:HB2   | 2:B:637:LEU:HA    | 1.39                     | 1.05              |
| 2:B:956:THR:HB    | 10:L:46:VAL:HG21  | 1.37                     | 1.05              |
| 1:A:1118:VAL:HG23 | 1:A:1306:LEU:HB2  | 1.39                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:868:TYR:HE1   | 1:A:1064:VAL:HG11 | 1.21                     | 1.03              |
| 3:C:56:THR:HG23   | 3:C:147:LEU:HD23  | 1.39                     | 1.03              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:HD2   | 1.06                     | 1.02              |
| 2:B:778:MET:HE1   | 2:B:1094:ARG:HH11 | 1.21                     | 1.01              |
| 1:A:256:GLN:HA    | 1:A:257:ARG:HB3   | 1.35                     | 1.01              |
| 2:B:1006:ILE:HD11 | 8:J:43:ARG:HB2    | 1.41                     | 0.98              |
| 2:B:65:GLU:HG3    | 2:B:66:ASP:H      | 1.29                     | 0.97              |
| 1:A:1342:GLU:HG2  | 4:E:212:ARG:NH1   | 1.80                     | 0.97              |
| 1:A:899:VAL:HB    | 1:A:929:LEU:HD12  | 1.48                     | 0.96              |
| 1:A:868:TYR:CE2   | 1:A:1366:ARG:HD3  | 2.00                     | 0.96              |
| 6:H:47:PHE:HB3    | 6:H:95:TYR:HD1    | 1.29                     | 0.95              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:CG    | 1.79                     | 0.94              |
| 1:A:869:GLY:O     | 4:E:204:THR:HG21  | 1.66                     | 0.94              |
| 2:B:485:ARG:HG2   | 2:B:485:ARG:HH11  | 1.29                     | 0.94              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.47                     | 0.94              |
| 1:A:567:LYS:HB3   | 6:H:96:VAL:H      | 1.32                     | 0.94              |
| 2:B:636:PRO:HB2   | 2:B:637:LEU:CA    | 1.96                     | 0.93              |
| 1:A:351:THR:HG23  | 2:B:1103:ILE:HD12 | 1.49                     | 0.93              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:OG    | 1.53                     | 0.92              |
| 5:F:111:LEU:HD12  | 5:F:111:LEU:H     | 1.33                     | 0.91              |
| 1:A:261:ASP:HB3   | 1:A:323:LYS:HD2   | 1.49                     | 0.91              |
| 1:A:407:ARG:HD3   | 1:A:413:ILE:HD11  | 1.50                     | 0.91              |
| 1:A:1342:GLU:HG2  | 4:E:212:ARG:HH12  | 1.33                     | 0.91              |
| 2:B:726:ALA:HB1   | 2:B:1051:THR:HG21 | 1.51                     | 0.91              |
| 1:A:1364:ASN:ND2  | 1:A:1366:ARG:HG2  | 1.84                     | 0.91              |
| 1:A:401:GLY:C     | 1:A:435:HIS:CD2   | 2.49                     | 0.91              |
| 1:A:335:ARG:HH11  | 2:B:1202:LEU:HD12 | 1.36                     | 0.91              |
| 3:C:56:THR:HG23   | 3:C:147:LEU:CD2   | 2.01                     | 0.91              |
| 1:A:851:HIS:CD2   | 1:A:857:ARG:HG3   | 2.06                     | 0.90              |
| 1:A:315:LEU:CB    | 1:A:316:GLN:HA    | 2.00                     | 0.90              |
| 1:A:899:VAL:HB    | 1:A:929:LEU:CD1   | 2.00                     | 0.90              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:HG11 | 2.06                     | 0.89              |
| 1:A:404:TYR:HB2   | 1:A:433:GLU:HG3   | 1.54                     | 0.89              |
| 2:B:800:GLN:HB3   | 8:J:52:THR:CG2    | 2.03                     | 0.88              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:NE2   | 1.89                     | 0.88              |
| 2:B:479:VAL:O     | 2:B:480:SER:HB3   | 1.72                     | 0.88              |
| 1:A:1156:PRO:HA   | 1:A:1190:PRO:HB3  | 1.54                     | 0.87              |
| 2:B:474:SER:HA    | 2:B:476:ARG:HG3   | 1.55                     | 0.87              |
| 3:C:231:ASN:HD22  | 3:C:231:ASN:C     | 1.82                     | 0.86              |
| 1:A:873:MET:HG2   | 1:A:957:PRO:HG3   | 1.57                     | 0.86              |
| 2:B:981:ALA:O     | 2:B:982:SER:O     | 1.93                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1065:GLN:HG2  | 2:B:1069:PHE:HB2  | 1.54                     | 0.85              |
| 8:J:10:CYS:SG     | 8:J:43:ARG:HD2    | 2.16                     | 0.85              |
| 5:F:93:ILE:CD1    | 5:F:134:ILE:HD11  | 2.04                     | 0.85              |
| 1:A:131:SER:HB3   | 1:A:223:GLY:HA2   | 1.58                     | 0.85              |
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:H     | 1.25                     | 0.85              |
| 1:A:353:ILE:HG22  | 1:A:468:PHE:HB2   | 1.56                     | 0.85              |
| 1:A:836:TYR:CZ    | 1:A:840:ARG:HD2   | 2.12                     | 0.85              |
| 2:B:986:GLN:NE2   | 2:B:1020:ARG:HD2  | 1.92                     | 0.85              |
| 6:H:38:LEU:HD11   | 6:H:123:MET:HE2   | 1.57                     | 0.85              |
| 2:B:796:LEU:HB3   | 2:B:799:PRO:HD3   | 1.58                     | 0.84              |
| 1:A:575:LYS:HB3   | 1:A:612:ILE:HD11  | 1.58                     | 0.84              |
| 1:A:1017:LEU:HB2  | 4:E:206:GLY:H     | 1.40                     | 0.84              |
| 2:B:485:ARG:HH11  | 2:B:485:ARG:CG    | 1.90                     | 0.84              |
| 2:B:614:SER:H     | 2:B:632:ARG:HH12  | 1.26                     | 0.84              |
| 2:B:114:PRO:HG2   | 2:B:181:LEU:HD11  | 1.59                     | 0.84              |
| 2:B:639:ILE:HD11  | 2:B:691:GLU:HB2   | 1.57                     | 0.84              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:ND1   | 1.93                     | 0.83              |
| 2:B:176:SER:O     | 2:B:182:SER:HB3   | 1.78                     | 0.83              |
| 1:A:1134:ILE:O    | 1:A:1138:ILE:HG12 | 1.79                     | 0.83              |
| 2:B:40:GLU:OE1    | 2:B:682:SER:HB2   | 1.78                     | 0.83              |
| 7:I:71:SER:H      | 7:I:83:ASN:HD21   | 1.26                     | 0.82              |
| 1:A:901:LEU:H     | 1:A:926:GLN:HE21  | 1.26                     | 0.82              |
| 6:H:47:PHE:HB3    | 6:H:95:TYR:CD1    | 2.12                     | 0.82              |
| 1:A:738:LYS:HB3   | 6:H:19:ARG:HH22   | 1.44                     | 0.82              |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG   | 2.19                     | 0.82              |
| 2:B:542:MET:HG3   | 2:B:747:MET:HE2   | 1.61                     | 0.82              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HH11 | 1.27                     | 0.81              |
| 3:C:56:THR:HG21   | 3:C:145:CYS:SG    | 2.20                     | 0.81              |
| 1:A:1004:ASN:ND2  | 4:E:167:ARG:HD2   | 1.96                     | 0.81              |
| 2:B:744:HIS:CD2   | 2:B:746:SER:OG    | 2.34                     | 0.81              |
| 2:B:126:SER:OG    | 2:B:172:ILE:HD11  | 1.79                     | 0.81              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:CE2   | 2.16                     | 0.80              |
| 1:A:851:HIS:HD2   | 1:A:857:ARG:HG3   | 1.43                     | 0.80              |
| 2:B:273:LEU:HD21  | 2:B:360:PHE:HD1   | 1.45                     | 0.80              |
| 1:A:134:ARG:HD2   | 1:A:221:SER:O     | 1.81                     | 0.80              |
| 1:A:765:VAL:CG2   | 1:A:800:VAL:HB    | 2.12                     | 0.80              |
| 1:A:590:ARG:HG3   | 1:A:590:ARG:HH11  | 1.47                     | 0.80              |
| 2:B:778:MET:HE1   | 2:B:1094:ARG:NH1  | 1.97                     | 0.79              |
| 1:A:913:LEU:HD12  | 1:A:915:SER:H     | 1.47                     | 0.79              |
| 2:B:843:GLN:HB2   | 2:B:993:THR:HB    | 1.64                     | 0.79              |
| 8:J:25:LEU:O      | 8:J:29:GLU:HA     | 1.82                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:NH1  | 1.80                     | 0.79              |
| 3:C:74:SER:O      | 3:C:77:ILE:HB     | 1.83                     | 0.79              |
| 3:C:91:HIS:CE1    | 3:C:158:VAL:HG21  | 2.18                     | 0.78              |
| 1:A:49:LYS:O      | 1:A:50:ILE:HG12   | 1.82                     | 0.78              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:HG3   | 1.48                     | 0.78              |
| 2:B:459:TYR:HD2   | 2:B:459:TYR:C     | 1.92                     | 0.78              |
| 2:B:783:THR:HG21  | 8:J:59:LYS:HB3    | 1.65                     | 0.78              |
| 2:B:976:ILE:HG23  | 2:B:977:GLY:N     | 1.99                     | 0.78              |
| 1:A:23:SER:O      | 1:A:27:VAL:HG23   | 1.82                     | 0.78              |
| 2:B:474:SER:CA    | 2:B:476:ARG:HG3   | 2.12                     | 0.78              |
| 3:C:73:GLN:HA     | 3:C:133:ILE:HD11  | 1.66                     | 0.78              |
| 1:A:436:ILE:HD11  | 1:A:491:VAL:HG11  | 1.63                     | 0.78              |
| 2:B:639:ILE:HA    | 2:B:740:HIS:HB3   | 1.65                     | 0.78              |
| 6:H:104:PHE:CZ    | 6:H:136:LYS:HA    | 2.19                     | 0.78              |
| 1:A:541:ILE:HG21  | 1:A:549:MET:HE3   | 1.66                     | 0.78              |
| 1:A:351:THR:HG23  | 2:B:1103:ILE:CD1  | 2.13                     | 0.77              |
| 2:B:1138:MET:HE3  | 2:B:1138:MET:HA   | 1.64                     | 0.77              |
| 1:A:1101:LEU:O    | 1:A:1105:LEU:HD12 | 1.83                     | 0.77              |
| 2:B:638:PHE:O     | 2:B:740:HIS:HB2   | 1.84                     | 0.77              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:HE3   | 1.66                     | 0.77              |
| 2:B:459:TYR:C     | 2:B:459:TYR:CD2   | 2.63                     | 0.77              |
| 2:B:706:GLN:O     | 2:B:710:LEU:HB2   | 1.83                     | 0.77              |
| 8:J:56:LEU:HB3    | 8:J:60:PHE:HE2    | 1.49                     | 0.77              |
| 2:B:384:ARG:HH12  | 2:B:579:ARG:HH21  | 1.32                     | 0.77              |
| 2:B:955:THR:HG22  | 2:B:956:THR:N     | 1.98                     | 0.77              |
| 1:A:752:LYS:HD2   | 2:B:1015:HIS:O    | 1.85                     | 0.76              |
| 2:B:249:ARG:HG3   | 2:B:251:ILE:HD11  | 1.66                     | 0.76              |
| 1:A:14:VAL:H      | 1:A:1432:GLN:HE22 | 1.30                     | 0.76              |
| 4:E:12:LEU:HD11   | 4:E:58:MET:HE1    | 1.67                     | 0.76              |
| 1:A:351:THR:CG2   | 2:B:1103:ILE:HD12 | 2.15                     | 0.76              |
| 2:B:698:GLU:O     | 2:B:701:ILE:HD13  | 1.86                     | 0.76              |
| 2:B:416:LEU:HD11  | 2:B:460:ALA:CB    | 2.15                     | 0.76              |
| 3:C:186:LEU:HB3   | 3:C:188:HIS:HD2   | 1.50                     | 0.76              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:HE21  | 1.49                     | 0.76              |
| 2:B:847:ASP:HB3   | 3:C:167:HIS:CD2   | 2.20                     | 0.76              |
| 2:B:120:ARG:HB3   | 2:B:955:THR:HG21  | 1.66                     | 0.76              |
| 3:C:46:ILE:HD12   | 3:C:157:CYS:HB2   | 1.67                     | 0.76              |
| 2:B:701:ILE:HG13  | 2:B:740:HIS:CE1   | 2.20                     | 0.76              |
| 2:B:986:GLN:NE2   | 2:B:1016:ALA:HB1  | 2.00                     | 0.76              |
| 2:B:884:ARG:O     | 2:B:936:ASP:HB3   | 1.85                     | 0.75              |
| 11:R:9:G:C2       | 12:T:21:DC:O2     | 2.39                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:589:VAL:HG12  | 2:B:590:HIS:H     | 1.50                     | 0.75              |
| 1:A:315:LEU:HB2   | 1:A:316:GLN:CA    | 2.09                     | 0.75              |
| 1:A:1077:THR:HB   | 1:A:1078:GLN:HE21 | 1.50                     | 0.75              |
| 1:A:1011:GLN:NE2  | 1:A:1015:VAL:HG21 | 2.01                     | 0.75              |
| 3:C:165:LYS:O     | 9:K:6:ARG:NH1     | 2.20                     | 0.74              |
| 1:A:559:VAL:HG12  | 1:A:559:VAL:O     | 1.87                     | 0.74              |
| 3:C:56:THR:CG2    | 3:C:147:LEU:HD23  | 2.14                     | 0.74              |
| 2:B:640:VAL:HG12  | 2:B:640:VAL:O     | 1.87                     | 0.74              |
| 3:C:101:LEU:HD21  | 3:C:113:VAL:HG11  | 1.69                     | 0.74              |
| 2:B:408:LEU:HD22  | 2:B:545:ILE:HD12  | 1.67                     | 0.74              |
| 2:B:422:LYS:HA    | 2:B:425:THR:HG22  | 1.69                     | 0.74              |
| 1:A:553:VAL:HG22  | 1:A:652:VAL:CG2   | 2.17                     | 0.74              |
| 1:A:1118:VAL:CG2  | 1:A:1306:LEU:HB2  | 2.15                     | 0.73              |
| 1:A:304:MET:HG2   | 2:B:1210:MET:HG3  | 1.70                     | 0.73              |
| 2:B:578:THR:OG1   | 2:B:593:PRO:HG3   | 1.88                     | 0.73              |
| 2:B:916:THR:HG23  | 2:B:916:THR:O     | 1.88                     | 0.73              |
| 3:C:133:ILE:HD12  | 3:C:237:SER:HA    | 1.69                     | 0.73              |
| 2:B:800:GLN:HB3   | 8:J:52:THR:HG22   | 1.70                     | 0.73              |
| 3:C:3:GLU:HG3     | 3:C:4:GLU:H       | 1.53                     | 0.73              |
| 1:A:886:ILE:HD11  | 1:A:943:LEU:HB3   | 1.71                     | 0.73              |
| 1:A:347:PHE:HB2   | 2:B:1150:ARG:HH22 | 1.53                     | 0.73              |
| 2:B:1164:GLY:HA3  | 2:B:1190:ASP:HB3  | 1.71                     | 0.73              |
| 2:B:102:VAL:HG11  | 2:B:122:LEU:HD13  | 1.71                     | 0.73              |
| 2:B:640:VAL:HG23  | 2:B:740:HIS:HA    | 1.71                     | 0.73              |
| 11:R:4:G:H2'      | 11:R:5:A:H8       | 1.54                     | 0.73              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:HA    | 1.70                     | 0.72              |
| 1:A:69:THR:O      | 1:A:71:GLN:HG3    | 1.88                     | 0.72              |
| 4:E:15:ALA:O      | 4:E:19:VAL:HG23   | 1.89                     | 0.72              |
| 6:H:89:LEU:O      | 6:H:91:ASP:N      | 2.20                     | 0.72              |
| 1:A:759:ALA:O     | 1:A:763:ALA:HB3   | 1.90                     | 0.72              |
| 1:A:351:THR:HG22  | 1:A:352:VAL:O     | 1.89                     | 0.72              |
| 2:B:957:ASN:O     | 2:B:959:ASP:N     | 2.23                     | 0.72              |
| 1:A:1364:ASN:ND2  | 1:A:1366:ARG:HH11 | 1.87                     | 0.72              |
| 2:B:1135:ARG:NH2  | 2:B:1136:ASP:OD1  | 2.16                     | 0.72              |
| 1:A:367:PRO:HG2   | 1:A:370:ILE:HD12  | 1.72                     | 0.72              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:HD2   | 2.20                     | 0.72              |
| 4:E:28:TYR:CE1    | 4:E:78:LEU:HD13   | 2.24                     | 0.72              |
| 2:B:1002:THR:CG2  | 2:B:1006:ILE:HB   | 2.19                     | 0.71              |
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:N     | 1.88                     | 0.71              |
| 1:A:218:ASP:O     | 1:A:222:LEU:HD11  | 1.90                     | 0.71              |
| 1:A:532:ARG:HH12  | 1:A:745:GLN:HE21  | 1.36                     | 0.71              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:34:ILE:HG23   | 2:B:542:MET:HE3  | 1.71                     | 0.71              |
| 2:B:1106:ARG:HD2  | 2:B:1126:GLY:O   | 1.90                     | 0.71              |
| 1:A:809:THR:HG21  | 2:B:730:ARG:HG3  | 1.71                     | 0.71              |
| 1:A:840:ARG:HG2   | 1:A:1402:PHE:HZ  | 1.55                     | 0.71              |
| 1:A:858:ASN:C     | 1:A:858:ASN:HD22 | 1.97                     | 0.71              |
| 4:E:100:ILE:HG23  | 4:E:105:PHE:HB2  | 1.73                     | 0.71              |
| 3:C:43:THR:HG22   | 3:C:44:LEU:H     | 1.55                     | 0.71              |
| 3:C:66:ARG:NH2    | 8:J:3:VAL:O      | 2.23                     | 0.71              |
| 1:A:826:ASP:O     | 1:A:830:LYS:N    | 2.20                     | 0.71              |
| 2:B:590:HIS:CD2   | 2:B:596:LEU:HD22 | 2.26                     | 0.71              |
| 2:B:1008:PRO:HB3  | 2:B:1087:PHE:HE1 | 1.56                     | 0.71              |
| 6:H:47:PHE:CB     | 6:H:95:TYR:HD1   | 2.03                     | 0.71              |
| 1:A:271:LYS:O     | 1:A:275:SER:HB2  | 1.91                     | 0.70              |
| 1:A:443:LEU:HD21  | 1:A:455:MET:HB3  | 1.72                     | 0.70              |
| 2:B:65:GLU:HG3    | 2:B:66:ASP:N     | 2.06                     | 0.70              |
| 4:E:77:SER:HB3    | 4:E:105:PHE:HD2  | 1.57                     | 0.70              |
| 1:A:568:PRO:HD3   | 6:H:94:ASP:O     | 1.89                     | 0.70              |
| 1:A:793:SER:HB2   | 1:A:794:PRO:HD2  | 1.73                     | 0.70              |
| 6:H:109:LYS:HB3   | 6:H:110:ASP:CG   | 2.16                     | 0.70              |
| 1:A:457:ALA:O     | 1:A:507:VAL:HG23 | 1.92                     | 0.70              |
| 1:A:573:SER:O     | 1:A:576:GLN:HB2  | 1.92                     | 0.70              |
| 1:A:626:ASN:O     | 1:A:631:HIS:CD2  | 2.45                     | 0.70              |
| 1:A:1436:ILE:O    | 1:A:1437:GLY:C   | 2.35                     | 0.70              |
| 2:B:1082:MET:HA   | 3:C:189:THR:HA   | 1.73                     | 0.70              |
| 16:T:29:C7P:H6    | 16:T:29:C7P:N3   | 2.05                     | 0.70              |
| 1:A:55:ASP:O      | 1:A:57:ARG:N     | 2.24                     | 0.70              |
| 1:A:261:ASP:HB3   | 1:A:323:LYS:CD   | 2.22                     | 0.70              |
| 1:A:596:THR:O     | 1:A:598:LEU:N    | 2.24                     | 0.70              |
| 2:B:175:ARG:HG3   | 2:B:175:ARG:NH1  | 2.05                     | 0.70              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:HG2  | 1.53                     | 0.70              |
| 1:A:399:HIS:O     | 1:A:401:GLY:N    | 2.24                     | 0.70              |
| 2:B:955:THR:HG23  | 10:L:54:ARG:O    | 1.92                     | 0.70              |
| 6:H:82:PRO:C      | 6:H:84:ALA:H     | 2.00                     | 0.70              |
| 1:A:565:ILE:HG23  | 1:A:567:LYS:HG2  | 1.73                     | 0.69              |
| 2:B:1084:GLN:NE2  | 3:C:191:TYR:HA   | 2.06                     | 0.69              |
| 7:I:101:PHE:HE1   | 7:I:112:SER:HB3  | 1.57                     | 0.69              |
| 1:A:1319:VAL:HG12 | 1:A:1320:PRO:O   | 1.92                     | 0.69              |
| 2:B:986:GLN:HE22  | 2:B:1016:ALA:HB1 | 1.57                     | 0.69              |
| 1:A:351:THR:CG2   | 1:A:352:VAL:N    | 2.55                     | 0.69              |
| 1:A:901:LEU:HA    | 1:A:907:THR:HG23 | 1.75                     | 0.69              |
| 2:B:912:ILE:O     | 2:B:938:SER:HB3  | 1.92                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:10:CYS:SG     | 8:J:43:ARG:CD     | 2.80                     | 0.69              |
| 1:A:335:ARG:NH1   | 2:B:1202:LEU:HD12 | 2.07                     | 0.69              |
| 1:A:49:LYS:NZ     | 1:A:60:SER:HA     | 2.07                     | 0.69              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD    | 2.53                     | 0.69              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:HE2   | 1.55                     | 0.69              |
| 1:A:1059:HIS:ND1  | 5:F:86:THR:HA     | 2.08                     | 0.69              |
| 7:I:71:SER:H      | 7:I:83:ASN:ND2    | 1.91                     | 0.69              |
| 1:A:942:PHE:C     | 1:A:942:PHE:CD2   | 2.69                     | 0.69              |
| 2:B:292:ILE:HD11  | 2:B:327:ARG:HG2   | 1.73                     | 0.69              |
| 1:A:129:LYS:O     | 1:A:130:ASP:HB2   | 1.91                     | 0.68              |
| 1:A:365:GLY:O     | 1:A:468:PHE:HA    | 1.93                     | 0.68              |
| 1:A:896:ARG:HH11  | 1:A:897:TYR:HE1   | 1.39                     | 0.68              |
| 2:B:849:GLY:HA2   | 2:B:852:ARG:HD2   | 1.75                     | 0.68              |
| 2:B:1081:LEU:O    | 3:C:189:THR:HG23  | 1.93                     | 0.68              |
| 2:B:310:MET:O     | 2:B:313:MET:HB2   | 1.92                     | 0.68              |
| 5:F:132:LEU:O     | 5:F:148:VAL:HG23  | 1.94                     | 0.68              |
| 9:K:21:ILE:HG13   | 9:K:33:ILE:HG23   | 1.75                     | 0.68              |
| 3:C:242:GLN:O     | 3:C:246:ARG:HB2   | 1.94                     | 0.68              |
| 1:A:404:TYR:HA    | 1:A:413:ILE:O     | 1.93                     | 0.68              |
| 1:A:806:ARG:NH2   | 2:B:729:ILE:HD11  | 2.08                     | 0.68              |
| 2:B:976:ILE:HG23  | 2:B:977:GLY:H     | 1.56                     | 0.68              |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:HG2  | 1.58                     | 0.68              |
| 1:A:630:ILE:HD12  | 1:A:630:ILE:H     | 1.59                     | 0.68              |
| 4:E:19:VAL:O      | 4:E:23:VAL:HG23   | 1.94                     | 0.68              |
| 1:A:335:ARG:HH11  | 2:B:1202:LEU:CD1  | 2.06                     | 0.68              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:HD3   | 1.76                     | 0.68              |
| 2:B:174:LEU:HD13  | 2:B:204:ILE:HD12  | 1.74                     | 0.68              |
| 9:K:7:PHE:O       | 9:K:11:LEU:HB2    | 1.94                     | 0.68              |
| 2:B:986:GLN:HE21  | 2:B:1020:ARG:HD2  | 1.59                     | 0.68              |
| 3:C:27:LEU:HD12   | 3:C:228:PHE:HE2   | 1.59                     | 0.68              |
| 1:A:107:CYS:HB2   | 1:A:114:LEU:HD21  | 1.76                     | 0.67              |
| 1:A:353:ILE:CD1   | 1:A:487:MET:HE3   | 2.24                     | 0.67              |
| 1:A:662:PHE:O     | 2:B:828:ALA:HA    | 1.94                     | 0.67              |
| 2:B:807:ARG:CG    | 2:B:807:ARG:HH11  | 2.08                     | 0.67              |
| 3:C:34:ARG:HA     | 3:C:37:MET:HE3    | 1.76                     | 0.67              |
| 3:C:123:ASN:HD22  | 3:C:125:MET:H     | 1.43                     | 0.67              |
| 1:A:438:ASP:HA    | 1:A:460:VAL:O     | 1.95                     | 0.67              |
| 2:B:58:THR:O      | 2:B:62:ILE:HG12   | 1.93                     | 0.67              |
| 2:B:834:ASN:O     | 2:B:1013:ASN:HB2  | 1.94                     | 0.67              |
| 6:H:89:LEU:HD13   | 6:H:91:ASP:OD1    | 1.95                     | 0.67              |
| 1:A:351:THR:HG22  | 1:A:352:VAL:N     | 2.08                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1138:ILE:HG22 | 1:A:1279:ILE:HG21 | 1.75                     | 0.67              |
| 1:A:1279:ILE:HG22 | 1:A:1279:ILE:O    | 1.94                     | 0.67              |
| 4:E:144:ILE:O     | 4:E:150:VAL:HG21  | 1.93                     | 0.67              |
| 1:A:553:VAL:HG22  | 1:A:652:VAL:HG22  | 1.75                     | 0.67              |
| 7:I:71:SER:N      | 7:I:83:ASN:HD21   | 1.92                     | 0.67              |
| 2:B:642:ASP:O     | 2:B:644:GLU:N     | 2.28                     | 0.67              |
| 1:A:19:PHE:O      | 1:A:1416:ALA:HA   | 1.94                     | 0.67              |
| 1:A:436:ILE:HD11  | 1:A:491:VAL:CG1   | 2.25                     | 0.67              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:H     | 1.60                     | 0.67              |
| 1:A:868:TYR:CZ    | 1:A:1366:ARG:HD3  | 2.29                     | 0.67              |
| 2:B:879:ARG:HH22  | 2:B:885:MET:HE2   | 1.58                     | 0.67              |
| 2:B:635:ARG:CB    | 2:B:636:PRO:CD    | 2.67                     | 0.66              |
| 1:A:436:ILE:CD1   | 1:A:491:VAL:HG11  | 2.25                     | 0.66              |
| 1:A:645:LEU:HD11  | 1:A:649:ILE:HD11  | 1.77                     | 0.66              |
| 2:B:211:VAL:CG2   | 2:B:483:LEU:HG    | 2.25                     | 0.66              |
| 7:I:83:ASN:C      | 7:I:83:ASN:HD22   | 2.04                     | 0.66              |
| 1:A:1017:LEU:HB2  | 4:E:206:GLY:N     | 2.09                     | 0.66              |
| 1:A:826:ASP:HA    | 1:A:829:VAL:HG12  | 1.78                     | 0.66              |
| 2:B:1084:GLN:HE22 | 3:C:191:TYR:HA    | 1.59                     | 0.66              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H    | 1.60                     | 0.66              |
| 2:B:684:LEU:HD23  | 2:B:689:LEU:HD12  | 1.77                     | 0.66              |
| 1:A:1025:ARG:HG3  | 1:A:1030:ARG:NH1  | 2.11                     | 0.66              |
| 1:A:1206:ASP:HB2  | 1:A:1274:ARG:HH22 | 1.61                     | 0.66              |
| 6:H:31:THR:O      | 6:H:32:THR:OG1    | 2.14                     | 0.66              |
| 1:A:783:THR:CG2   | 1:A:815:PHE:HE2   | 2.09                     | 0.65              |
| 2:B:955:THR:HG22  | 2:B:956:THR:H     | 1.59                     | 0.65              |
| 2:B:37:PHE:O      | 2:B:38:PHE:HB2    | 1.94                     | 0.65              |
| 3:C:33:LEU:HG     | 3:C:37:MET:HE2    | 1.77                     | 0.65              |
| 1:A:37:PHE:HB2    | 1:A:52:GLY:HA3    | 1.78                     | 0.65              |
| 1:A:354:SER:O     | 1:A:469:ARG:HA    | 1.96                     | 0.65              |
| 1:A:852:TYR:CE2   | 1:A:1060:PRO:HB2  | 2.32                     | 0.65              |
| 2:B:168:GLY:N     | 2:B:450:ALA:HB1   | 2.12                     | 0.65              |
| 1:A:575:LYS:HB3   | 1:A:612:ILE:CD1   | 2.26                     | 0.65              |
| 3:C:142:VAL:HG21  | 8:J:5:VAL:HG13    | 1.79                     | 0.65              |
| 2:B:705:MET:H     | 2:B:710:LEU:HD12  | 1.61                     | 0.65              |
| 1:A:1385:THR:HG22 | 1:A:1386:ARG:H    | 1.62                     | 0.65              |
| 2:B:791:THR:O     | 2:B:792:MET:HB2   | 1.96                     | 0.65              |
| 3:C:8:VAL:HG11    | 9:K:105:PHE:HD1   | 1.61                     | 0.65              |
| 1:A:765:VAL:HG22  | 1:A:800:VAL:HB    | 1.79                     | 0.65              |
| 2:B:169:ARG:H     | 2:B:454:THR:HG23  | 1.60                     | 0.65              |
| 3:C:38:ILE:HG12   | 3:C:176:ILE:HD12  | 1.77                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:199:ILE:O    | 4:E:199:ILE:HG22  | 1.96                     | 0.65              |
| 11:R:4:G:H2'     | 11:R:5:A:C8       | 2.32                     | 0.65              |
| 1:A:541:ILE:HG21 | 1:A:549:MET:CE    | 2.26                     | 0.65              |
| 1:A:913:LEU:HD11 | 1:A:981:LEU:O     | 1.96                     | 0.65              |
| 2:B:863:GLU:O    | 2:B:864:LYS:HG2   | 1.97                     | 0.65              |
| 4:E:77:SER:HB3   | 4:E:105:PHE:CD2   | 2.32                     | 0.65              |
| 1:A:744:LYS:O    | 1:A:748:MET:HG3   | 1.97                     | 0.65              |
| 1:A:573:SER:H    | 1:A:576:GLN:HG3   | 1.60                     | 0.65              |
| 8:J:1:MET:H1     | 8:J:56:LEU:HB2    | 1.62                     | 0.65              |
| 1:A:413:ILE:CD1  | 1:A:413:ILE:H     | 2.10                     | 0.64              |
| 1:A:837:ILE:HG22 | 1:A:841:LEU:HD12  | 1.79                     | 0.64              |
| 2:B:641:GLU:HG2  | 2:B:643:ASP:OD2   | 1.96                     | 0.64              |
| 3:C:7:GLN:HB2    | 3:C:23:SER:HB2    | 1.79                     | 0.64              |
| 3:C:43:THR:HG22  | 3:C:44:LEU:N      | 2.11                     | 0.64              |
| 3:C:133:ILE:CD1  | 3:C:237:SER:HA    | 2.26                     | 0.64              |
| 2:B:999:MET:HE2  | 2:B:1011:ILE:HD11 | 1.79                     | 0.64              |
| 1:A:343:LYS:HD2  | 2:B:1151:LEU:HG   | 1.80                     | 0.64              |
| 1:A:465:TYR:HB3  | 2:B:976:ILE:HG21  | 1.79                     | 0.64              |
| 1:A:1206:ASP:C   | 1:A:1274:ARG:HH12 | 2.04                     | 0.64              |
| 8:J:1:MET:N      | 8:J:56:LEU:HB2    | 2.13                     | 0.64              |
| 3:C:186:LEU:CB   | 3:C:188:HIS:HD2   | 2.11                     | 0.64              |
| 9:K:44:ASN:HA    | 9:K:61:TYR:CE2    | 2.31                     | 0.64              |
| 2:B:541:LEU:HB2  | 2:B:747:MET:HE3   | 1.79                     | 0.64              |
| 2:B:701:ILE:HG13 | 2:B:740:HIS:HE1   | 1.60                     | 0.64              |
| 2:B:809:MET:HE1  | 2:B:983:ARG:HH21  | 1.63                     | 0.64              |
| 1:A:550:LEU:HD21 | 1:A:561:PRO:HD2   | 1.79                     | 0.64              |
| 4:E:86:PRO:HB3   | 4:E:114:ASN:HD22  | 1.63                     | 0.64              |
| 2:B:976:ILE:O    | 2:B:990:ILE:HB    | 1.97                     | 0.64              |
| 5:F:93:ILE:HD11  | 5:F:134:ILE:CD1   | 2.08                     | 0.64              |
| 2:B:702:LEU:HD23 | 2:B:737:THR:HG22  | 1.79                     | 0.64              |
| 3:C:15:LYS:O     | 3:C:240:VAL:HG22  | 1.97                     | 0.63              |
| 1:A:942:PHE:CD2  | 1:A:942:PHE:O     | 2.50                     | 0.63              |
| 1:A:1348:LEU:HG  | 1:A:1372:VAL:HG22 | 1.80                     | 0.63              |
| 2:B:493:SER:OG   | 2:B:497:ARG:NH2   | 2.31                     | 0.63              |
| 2:B:766:ARG:HH21 | 2:B:1020:ARG:HB3  | 1.62                     | 0.63              |
| 6:H:139:ASN:O    | 6:H:140:ALA:HB2   | 1.98                     | 0.63              |
| 3:C:54:ASN:CG    | 3:C:54:ASN:O      | 2.41                     | 0.63              |
| 1:A:889:SER:HB2  | 1:A:892:ALA:H     | 1.63                     | 0.63              |
| 2:B:255:GLN:HB2  | 2:B:272:THR:OG1   | 1.98                     | 0.63              |
| 2:B:1084:GLN:OE1 | 2:B:1084:GLN:N    | 2.31                     | 0.63              |
| 3:C:39:ALA:HA    | 3:C:164:ALA:HB3   | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:401:GLY:O     | 1:A:435:HIS:HD2   | 1.80                     | 0.63              |
| 2:B:485:ARG:HG2   | 2:B:485:ARG:NH1   | 2.04                     | 0.63              |
| 2:B:479:VAL:O     | 2:B:480:SER:CB    | 2.46                     | 0.63              |
| 1:A:131:SER:HB3   | 1:A:223:GLY:CA    | 2.28                     | 0.63              |
| 1:A:630:ILE:HD12  | 1:A:630:ILE:N     | 2.13                     | 0.63              |
| 8:J:43:ARG:HG2    | 8:J:46:CYS:HB2    | 1.81                     | 0.63              |
| 1:A:244:PRO:HB2   | 1:A:245:PRO:HD3   | 1.81                     | 0.63              |
| 1:A:590:ARG:HH11  | 1:A:590:ARG:CG    | 2.12                     | 0.63              |
| 2:B:64:CYS:O      | 2:B:65:GLU:HB3    | 1.98                     | 0.63              |
| 1:A:265:LYS:C     | 1:A:267:ALA:H     | 2.06                     | 0.62              |
| 1:A:547:LEU:HD22  | 9:K:58:PHE:HD1    | 1.63                     | 0.62              |
| 2:B:992:ILE:HD12  | 9:K:67:PHE:HE2    | 1.64                     | 0.62              |
| 9:K:19:LEU:HD22   | 9:K:35:PHE:CE2    | 2.34                     | 0.62              |
| 6:H:89:LEU:C      | 6:H:91:ASP:H      | 2.07                     | 0.62              |
| 8:J:9:SER:OG      | 8:J:48:ARG:NH2    | 2.33                     | 0.62              |
| 1:A:871:ASP:HB3   | 4:E:204:THR:HG23  | 1.80                     | 0.62              |
| 2:B:273:LEU:HB3   | 2:B:276:ILE:HD12  | 1.81                     | 0.62              |
| 2:B:976:ILE:CG2   | 2:B:977:GLY:H     | 2.12                     | 0.62              |
| 1:A:542:GLU:OE1   | 1:A:569:LYS:NZ    | 2.29                     | 0.62              |
| 7:I:50:THR:HG22   | 7:I:52:ILE:HG22   | 1.82                     | 0.62              |
| 1:A:1155:ASP:OD1  | 1:A:1162:VAL:HG23 | 1.99                     | 0.62              |
| 1:A:1436:ILE:O    | 1:A:1439:GLY:N    | 2.28                     | 0.62              |
| 1:A:1342:GLU:HG3  | 4:E:198:ILE:HG21  | 1.82                     | 0.62              |
| 1:A:1077:THR:HB   | 1:A:1078:GLN:NE2  | 2.15                     | 0.62              |
| 2:B:749:LEU:HD22  | 2:B:753:ALA:HB1   | 1.80                     | 0.62              |
| 2:B:801:LYS:O     | 2:B:801:LYS:HG3   | 2.00                     | 0.62              |
| 2:B:864:LYS:HB3   | 2:B:871:THR:HA    | 1.81                     | 0.62              |
| 1:A:649:ILE:O     | 1:A:653:VAL:HG23  | 2.00                     | 0.61              |
| 2:B:1066:SER:O    | 2:B:1067:ARG:HD3  | 2.00                     | 0.61              |
| 10:L:46:VAL:HG12  | 10:L:47:ARG:H     | 1.65                     | 0.61              |
| 1:A:457:ALA:HB3   | 1:A:506:ALA:HA    | 1.81                     | 0.61              |
| 1:A:886:ILE:HD11  | 1:A:943:LEU:CB    | 2.31                     | 0.61              |
| 1:A:1011:GLN:HE22 | 1:A:1015:VAL:HG21 | 1.61                     | 0.61              |
| 6:H:2:SER:O       | 6:H:3:ASN:HB2     | 1.98                     | 0.61              |
| 7:I:8:ARG:O       | 7:I:9:ASP:HB2     | 2.00                     | 0.61              |
| 1:A:67:CYS:O      | 1:A:70:CYS:HB3    | 2.00                     | 0.61              |
| 1:A:293:GLU:O     | 1:A:297:GLN:HB3   | 2.00                     | 0.61              |
| 1:A:1390:ASN:O    | 1:A:1399:ARG:HD2  | 2.01                     | 0.61              |
| 3:C:142:VAL:CG2   | 8:J:5:VAL:HG13    | 2.30                     | 0.61              |
| 2:B:614:SER:H     | 2:B:632:ARG:NH1   | 1.98                     | 0.61              |
| 5:F:125:LEU:HB2   | 5:F:130:ILE:HD11  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1435:PRO:C    | 1:A:1436:ILE:HD12 | 2.25                     | 0.61              |
| 2:B:628:THR:O     | 2:B:628:THR:CG2   | 2.48                     | 0.61              |
| 3:C:186:LEU:HB3   | 3:C:188:HIS:CD2   | 2.32                     | 0.61              |
| 2:B:726:ALA:CB    | 2:B:1051:THR:HG21 | 2.26                     | 0.61              |
| 1:A:214:ILE:HG23  | 1:A:215:SER:H     | 1.65                     | 0.61              |
| 1:A:1119:TYR:HD1  | 1:A:1326:ARG:HB3  | 1.65                     | 0.61              |
| 2:B:215:GLN:HE22  | 2:B:499:ASN:HD22  | 1.48                     | 0.61              |
| 2:B:708:GLU:HG3   | 2:B:709:ASP:H     | 1.65                     | 0.61              |
| 2:B:976:ILE:CG2   | 2:B:977:GLY:N     | 2.63                     | 0.61              |
| 8:J:43:ARG:CG     | 8:J:46:CYS:HB2    | 2.31                     | 0.61              |
| 1:A:44:THR:O      | 1:A:45:GLN:HB2    | 2.01                     | 0.61              |
| 3:C:69:LEU:O      | 8:J:6:ARG:HD2     | 2.01                     | 0.61              |
| 1:A:259:GLU:HG2   | 1:A:260:ASP:H     | 1.66                     | 0.61              |
| 1:A:413:ILE:N     | 1:A:413:ILE:HD12  | 2.15                     | 0.61              |
| 1:A:899:VAL:CB    | 1:A:929:LEU:HD12  | 2.25                     | 0.61              |
| 2:B:65:GLU:CG     | 2:B:66:ASP:H      | 2.03                     | 0.61              |
| 2:B:464:GLY:HA2   | 2:B:479:VAL:O     | 2.01                     | 0.61              |
| 2:B:1020:ARG:HG3  | 2:B:1022:THR:HG22 | 1.81                     | 0.61              |
| 3:C:142:VAL:H     | 8:J:16:ASP:HB3    | 1.65                     | 0.61              |
| 1:A:413:ILE:CD1   | 1:A:413:ILE:N     | 2.64                     | 0.61              |
| 2:B:826:ALA:O     | 2:B:1011:ILE:HA   | 2.01                     | 0.61              |
| 3:C:51:VAL:HG22   | 3:C:155:LEU:CD2   | 2.30                     | 0.61              |
| 3:C:144:ILE:HG22  | 3:C:145:CYS:HB3   | 1.83                     | 0.60              |
| 6:H:109:LYS:HB3   | 6:H:110:ASP:OD2   | 2.00                     | 0.60              |
| 2:B:635:ARG:NH2   | 2:B:742:GLU:OE2   | 2.34                     | 0.60              |
| 2:B:636:PRO:CB    | 2:B:637:LEU:HA    | 2.23                     | 0.60              |
| 2:B:899:ILE:HD11  | 2:B:911:ILE:HA    | 1.82                     | 0.60              |
| 2:B:981:ALA:HB2   | 2:B:987:LYS:HA    | 1.83                     | 0.60              |
| 2:B:840:ILE:HG12  | 2:B:992:ILE:HG22  | 1.83                     | 0.60              |
| 2:B:918:ILE:HG13  | 2:B:935:ARG:HH11  | 1.64                     | 0.60              |
| 1:A:1120:LEU:O    | 1:A:1323:ASP:HB2  | 2.01                     | 0.60              |
| 2:B:983:ARG:NH1   | 2:B:1091:TYR:HB3  | 2.16                     | 0.60              |
| 1:A:256:GLN:CA    | 1:A:257:ARG:HB3   | 2.20                     | 0.60              |
| 1:A:381:THR:HG23  | 1:A:383:TYR:CD1   | 2.36                     | 0.60              |
| 1:A:19:PHE:HB3    | 1:A:1413:GLY:HA2  | 1.84                     | 0.60              |
| 1:A:974:ASP:OD2   | 1:A:977:LYS:HB2   | 2.01                     | 0.60              |
| 1:A:1155:ASP:OD2  | 1:A:1161:THR:HA   | 2.01                     | 0.60              |
| 2:B:273:LEU:CB    | 2:B:276:ILE:HD12  | 2.32                     | 0.60              |
| 2:B:800:GLN:CB    | 8:J:52:THR:HG22   | 2.31                     | 0.60              |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:HB   | 1.82                     | 0.60              |
| 3:C:258:ILE:HD11  | 9:K:42:LEU:CD2    | 2.32                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:8:PHE:H       | 8:J:49:MET:HE3    | 1.66                     | 0.60              |
| 8:J:36:LEU:HD11   | 8:J:51:LEU:HB2    | 1.82                     | 0.60              |
| 1:A:444:PHE:HE2   | 1:A:470:LEU:HD23  | 1.66                     | 0.60              |
| 2:B:115:GLN:HE21  | 2:B:119:LEU:CD1   | 2.15                     | 0.60              |
| 2:B:378:LEU:O     | 2:B:382:ILE:HG12  | 2.02                     | 0.60              |
| 2:B:589:VAL:HG12  | 2:B:590:HIS:N     | 2.17                     | 0.60              |
| 2:B:704:ALA:HB3   | 2:B:741:CYS:HB2   | 1.83                     | 0.60              |
| 8:J:56:LEU:HB3    | 8:J:60:PHE:CE2    | 2.35                     | 0.60              |
| 2:B:174:LEU:O     | 2:B:175:ARG:CB    | 2.50                     | 0.60              |
| 2:B:520:GLY:HA2   | 2:B:748:ILE:HA    | 1.83                     | 0.60              |
| 1:A:423:ASP:CG    | 1:A:424:ILE:H     | 2.09                     | 0.59              |
| 1:A:565:ILE:HG23  | 1:A:567:LYS:HE3   | 1.83                     | 0.59              |
| 1:A:711:ARG:HG3   | 7:I:97:MET:HE3    | 1.83                     | 0.59              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.84                     | 0.59              |
| 2:B:638:PHE:O     | 2:B:740:HIS:CB    | 2.50                     | 0.59              |
| 3:C:184:ASN:HD21  | 3:C:189:THR:H     | 1.49                     | 0.59              |
| 1:A:1017:LEU:HB2  | 4:E:205:SER:HA    | 1.84                     | 0.59              |
| 2:B:174:LEU:O     | 2:B:175:ARG:HB2   | 2.02                     | 0.59              |
| 3:C:123:ASN:HD22  | 3:C:125:MET:N     | 2.00                     | 0.59              |
| 1:A:452:LYS:O     | 2:B:1141:HIS:HE1  | 1.85                     | 0.59              |
| 1:A:482:PHE:O     | 2:B:989:THR:HG23  | 2.02                     | 0.59              |
| 1:A:407:ARG:HD3   | 1:A:413:ILE:CD1   | 2.29                     | 0.59              |
| 1:A:472:LEU:HD11  | 2:B:835:GLN:NE2   | 2.17                     | 0.59              |
| 1:A:821:ARG:O     | 1:A:825:ILE:HG12  | 2.02                     | 0.59              |
| 1:A:1029:ARG:HG3  | 1:A:1029:ARG:HH11 | 1.66                     | 0.59              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HG2  | 1.67                     | 0.59              |
| 2:B:681:TRP:CH2   | 2:B:690:VAL:HG11  | 2.38                     | 0.59              |
| 2:B:737:THR:HG23  | 7:I:66:PRO:HB3    | 1.84                     | 0.59              |
| 5:F:128:LYS:NZ    | 5:F:148:VAL:O     | 2.27                     | 0.59              |
| 11:R:3:G:H22      | 12:T:27:DA:H1'    | 1.67                     | 0.59              |
| 2:B:546:SER:OG    | 2:B:631:GLY:N     | 2.24                     | 0.59              |
| 2:B:872:GLU:HG2   | 2:B:916:THR:OG1   | 2.01                     | 0.59              |
| 2:B:1115:THR:HB   | 2:B:1117:GLN:HG3  | 1.83                     | 0.59              |
| 1:A:908:LEU:HD11  | 1:A:983:ILE:HD11  | 1.82                     | 0.59              |
| 1:A:18:GLN:HE21   | 1:A:1418:LEU:HD12 | 1.66                     | 0.59              |
| 2:B:749:LEU:HD22  | 2:B:753:ALA:CB    | 2.33                     | 0.59              |
| 2:B:803:LEU:N     | 2:B:822:ASN:HD21  | 1.99                     | 0.59              |
| 9:K:58:PHE:HE2    | 9:K:74:ARG:HE     | 1.49                     | 0.59              |
| 10:L:48:CYS:SG    | 10:L:49:LYS:N     | 2.74                     | 0.59              |
| 1:A:40:THR:HG21   | 1:A:259:GLU:OE1   | 2.03                     | 0.59              |
| 1:A:533:LYS:HD3   | 1:A:745:GLN:NE2   | 2.18                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:955:THR:CG2  | 2:B:956:THR:N     | 2.66                     | 0.59              |
| 1:A:447:GLN:NE2  | 12:T:20:DC:H4'    | 2.18                     | 0.59              |
| 1:A:567:LYS:HB3  | 6:H:96:VAL:N      | 2.10                     | 0.59              |
| 1:A:1111:MET:O   | 1:A:1114:PRO:HD3  | 2.03                     | 0.59              |
| 1:A:1392:SER:O   | 1:A:1394:THR:N    | 2.33                     | 0.59              |
| 2:B:737:THR:HG21 | 7:I:66:PRO:O      | 2.03                     | 0.59              |
| 1:A:49:LYS:HZ2   | 1:A:60:SER:HA     | 1.66                     | 0.59              |
| 1:A:332:LYS:H    | 1:A:337:ARG:HB3   | 1.68                     | 0.59              |
| 2:B:550:ASP:OD1  | 2:B:551:PRO:HD2   | 2.03                     | 0.58              |
| 1:A:683:ILE:HG21 | 1:A:801:GLU:HG3   | 1.85                     | 0.58              |
| 2:B:198:ASP:OD1  | 2:B:485:ARG:NH2   | 2.36                     | 0.58              |
| 6:H:93:TYR:CD2   | 6:H:145:ARG:HB3   | 2.39                     | 0.58              |
| 2:B:211:VAL:HG23 | 2:B:483:LEU:HG    | 1.86                     | 0.58              |
| 2:B:373:ARG:HA   | 2:B:566:LEU:HD23  | 1.85                     | 0.58              |
| 1:A:535:THR:HG21 | 1:A:617:VAL:HG23  | 1.85                     | 0.58              |
| 1:A:768:GLN:HG2  | 1:A:816:HIS:HA    | 1.85                     | 0.58              |
| 1:A:840:ARG:HG2  | 1:A:1402:PHE:CZ   | 2.36                     | 0.58              |
| 2:B:590:HIS:HD2  | 2:B:596:LEU:HD22  | 1.68                     | 0.58              |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA    | 1.85                     | 0.58              |
| 4:E:3:GLN:HG3    | 4:E:5:ASN:H       | 1.67                     | 0.58              |
| 1:A:741:ASN:HD21 | 1:A:743:VAL:HG23  | 1.68                     | 0.58              |
| 1:A:1032:LEU:O   | 1:A:1036:ARG:HG2  | 2.04                     | 0.58              |
| 2:B:108:VAL:HG12 | 2:B:109:THR:H     | 1.67                     | 0.58              |
| 2:B:706:GLN:HB3  | 2:B:708:GLU:HG3   | 1.84                     | 0.58              |
| 2:B:839:MET:CE   | 2:B:1010:LEU:HD21 | 2.32                     | 0.58              |
| 4:E:29:PHE:HD1   | 4:E:65:THR:HG22   | 1.69                     | 0.58              |
| 1:A:402:ALA:N    | 1:A:435:HIS:HD2   | 1.99                     | 0.58              |
| 1:A:508:PRO:HA   | 1:A:511:ILE:HG13  | 1.84                     | 0.58              |
| 1:A:868:TYR:HE2  | 1:A:1366:ARG:HD3  | 1.64                     | 0.58              |
| 2:B:25:ILE:HD11  | 2:B:651:LEU:HD12  | 1.85                     | 0.58              |
| 8:J:7:CYS:HA     | 8:J:49:MET:HG2    | 1.84                     | 0.58              |
| 1:A:362:ASP:OD2  | 1:A:459:ARG:NH1   | 2.36                     | 0.58              |
| 1:A:626:ASN:O    | 1:A:631:HIS:HD2   | 1.85                     | 0.58              |
| 2:B:701:ILE:CG1  | 2:B:740:HIS:HE1   | 2.16                     | 0.58              |
| 9:K:24:ASP:CG    | 9:K:74:ARG:HH11   | 2.12                     | 0.58              |
| 1:A:929:LEU:HD21 | 1:A:983:ILE:HG23  | 1.86                     | 0.58              |
| 1:A:1119:TYR:CD1 | 1:A:1326:ARG:HB3  | 2.38                     | 0.58              |
| 2:B:408:LEU:HG   | 2:B:409:ALA:H     | 1.69                     | 0.58              |
| 3:C:3:GLU:HB3    | 9:K:104:ASN:OD1   | 2.03                     | 0.58              |
| 1:A:93:VAL:CG2   | 1:A:301:ALA:HA    | 2.34                     | 0.57              |
| 1:A:896:ARG:NH1  | 1:A:897:TYR:HE1   | 2.01                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1114:PRO:HB2  | 1:A:1311:VAL:HG23 | 1.86                     | 0.57              |
| 2:B:288:ALA:HB1   | 2:B:331:LEU:HD12  | 1.85                     | 0.57              |
| 2:B:846:ILE:HG23  | 2:B:974:PRO:HG2   | 1.84                     | 0.57              |
| 4:E:127:ILE:O     | 4:E:127:ILE:HG12  | 2.04                     | 0.57              |
| 1:A:1349:TYR:O    | 1:A:1351:GLU:N    | 2.37                     | 0.57              |
| 2:B:841:MET:CE    | 2:B:990:ILE:HD11  | 2.34                     | 0.57              |
| 3:C:166:GLU:O     | 3:C:167:HIS:CB    | 2.52                     | 0.57              |
| 1:A:494:SER:O     | 1:A:498:ARG:HG3   | 2.05                     | 0.57              |
| 1:A:1349:TYR:O    | 1:A:1350:LYS:C    | 2.45                     | 0.57              |
| 3:C:115:SER:HB3   | 3:C:142:VAL:HG12  | 1.85                     | 0.57              |
| 6:H:41:ASP:HB2    | 6:H:121:LEU:HB3   | 1.85                     | 0.57              |
| 1:A:350:ARG:HD2   | 2:B:1128:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:775:ILE:HG13  | 1:A:798:GLY:HA3   | 1.85                     | 0.57              |
| 2:B:1155:SER:OG   | 2:B:1156:ASP:N    | 2.36                     | 0.57              |
| 1:A:214:ILE:CG2   | 1:A:215:SER:N     | 2.67                     | 0.57              |
| 1:A:1239:ARG:HH22 | 1:A:1241:ARG:HH22 | 1.53                     | 0.57              |
| 1:A:65:LEU:O      | 1:A:71:GLN:HA     | 2.03                     | 0.57              |
| 6:H:128:ASN:O     | 6:H:131:ASN:ND2   | 2.38                     | 0.57              |
| 1:A:960:ILE:HG12  | 1:A:1049:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:1343:ALA:HB1  | 4:E:149:LEU:HB2   | 1.87                     | 0.57              |
| 2:B:778:MET:O     | 2:B:819:ALA:HB1   | 2.05                     | 0.57              |
| 2:B:1006:ILE:HG22 | 2:B:1007:VAL:N    | 2.18                     | 0.57              |
| 4:E:94:LYS:HE2    | 4:E:94:LYS:HA     | 1.86                     | 0.57              |
| 1:A:99:ILE:HG12   | 1:A:234:MET:SD    | 2.45                     | 0.57              |
| 1:A:407:ARG:HH11  | 1:A:413:ILE:HD11  | 1.69                     | 0.57              |
| 1:A:508:PRO:O     | 1:A:511:ILE:HG13  | 2.05                     | 0.57              |
| 1:A:1012:ARG:O    | 1:A:1016:THR:OG1  | 2.21                     | 0.57              |
| 2:B:701:ILE:CB    | 2:B:740:HIS:HE1   | 2.18                     | 0.57              |
| 2:B:849:GLY:HA2   | 2:B:852:ARG:CD    | 2.35                     | 0.57              |
| 2:B:879:ARG:CZ    | 2:B:879:ARG:H     | 2.17                     | 0.57              |
| 8:J:1:MET:H1      | 8:J:57:ILE:H      | 1.53                     | 0.57              |
| 2:B:879:ARG:H     | 2:B:879:ARG:NE    | 2.02                     | 0.57              |
| 5:F:111:LEU:HD12  | 5:F:111:LEU:N     | 2.12                     | 0.57              |
| 1:A:690:VAL:HG22  | 1:A:718:VAL:HG22  | 1.86                     | 0.57              |
| 2:B:636:PRO:HB2   | 2:B:637:LEU:CB    | 2.35                     | 0.57              |
| 2:B:785:TYR:CE2   | 8:J:60:PHE:HE1    | 2.23                     | 0.57              |
| 2:B:942:ARG:CB    | 2:B:945:GLU:HB2   | 2.35                     | 0.57              |
| 3:C:67:LEU:HD23   | 3:C:144:ILE:HD11  | 1.86                     | 0.57              |
| 4:E:15:ALA:HA     | 4:E:140:LEU:O     | 2.05                     | 0.57              |
| 1:A:507:VAL:HG13  | 1:A:521:MET:HE1   | 1.86                     | 0.56              |
| 1:A:619:LYS:O     | 1:A:623:GLY:N     | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:516:ASN:H     | 2:B:516:ASN:HD22  | 1.51                     | 0.56              |
| 6:H:116:TYR:O     | 6:H:122:LEU:HA    | 2.05                     | 0.56              |
| 2:B:661:LEU:HD11  | 2:B:684:LEU:HD11  | 1.86                     | 0.56              |
| 4:E:178:ILE:HB    | 4:E:212:ARG:HD3   | 1.87                     | 0.56              |
| 1:A:79:GLY:H      | 2:B:1205:GLN:HE22 | 1.54                     | 0.56              |
| 1:A:264:PHE:CZ    | 1:A:317:LYS:HB2   | 2.39                     | 0.56              |
| 1:A:535:THR:HG22  | 1:A:616:VAL:HA    | 1.86                     | 0.56              |
| 1:A:1101:LEU:O    | 1:A:1105:LEU:CD1  | 2.53                     | 0.56              |
| 2:B:590:HIS:HD2   | 2:B:596:LEU:CD2   | 2.18                     | 0.56              |
| 3:C:40:GLU:HA     | 3:C:163:ILE:CG2   | 2.35                     | 0.56              |
| 5:F:155:LEU:HD23  | 5:F:155:LEU:H     | 1.69                     | 0.56              |
| 9:K:37:LYS:O      | 9:K:38:GLU:HG2    | 2.05                     | 0.56              |
| 1:A:57:ARG:O      | 1:A:68:GLN:HG2    | 2.05                     | 0.56              |
| 1:A:533:LYS:HD3   | 1:A:745:GLN:HE22  | 1.69                     | 0.56              |
| 1:A:666:ILE:HG23  | 2:B:1026:LEU:HB2  | 1.87                     | 0.56              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:CE1   | 2.39                     | 0.56              |
| 1:A:413:ILE:HG21  | 1:A:424:ILE:HD11  | 1.87                     | 0.56              |
| 2:B:487:THR:HG22  | 2:B:488:TYR:N     | 2.20                     | 0.56              |
| 2:B:569:TYR:CE1   | 2:B:589:VAL:HG21  | 2.40                     | 0.56              |
| 1:A:1095:THR:HB   | 1:A:1100:ARG:HD3  | 1.87                     | 0.56              |
| 2:B:487:THR:OG1   | 2:B:777:ALA:O     | 2.23                     | 0.56              |
| 2:B:766:ARG:NH2   | 2:B:1020:ARG:HB3  | 2.21                     | 0.56              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:HD21 | 1.88                     | 0.56              |
| 2:B:1187:ASN:HD21 | 2:B:1190:ASP:H    | 1.54                     | 0.56              |
| 1:A:99:ILE:HA     | 1:A:102:VAL:HG23  | 1.87                     | 0.56              |
| 1:A:336:ILE:H     | 1:A:336:ILE:HD12  | 1.71                     | 0.56              |
| 1:A:382:PRO:HA    | 1:A:428:TYR:HE2   | 1.70                     | 0.56              |
| 1:A:471:ASN:O     | 1:A:474:VAL:HG12  | 2.06                     | 0.56              |
| 1:A:1325:THR:HG23 | 1:A:1326:ARG:HG3  | 1.87                     | 0.56              |
| 2:B:486:TYR:OH    | 2:B:1096:ARG:HB3  | 2.06                     | 0.56              |
| 2:B:882:THR:HG22  | 2:B:883:LEU:N     | 2.21                     | 0.56              |
| 3:C:231:ASN:HD22  | 3:C:232:VAL:N     | 2.03                     | 0.56              |
| 1:A:56:PRO:O      | 1:A:57:ARG:HB2    | 2.05                     | 0.56              |
| 2:B:640:VAL:HG22  | 2:B:651:LEU:HD22  | 1.88                     | 0.56              |
| 5:F:81:THR:HG21   | 5:F:136:ARG:HD3   | 1.88                     | 0.56              |
| 1:A:508:PRO:HA    | 1:A:511:ILE:CG1   | 2.36                     | 0.56              |
| 1:A:586:ILE:HD11  | 1:A:637:LYS:CG    | 2.36                     | 0.56              |
| 1:A:1334:ASP:O    | 1:A:1335:ILE:C    | 2.49                     | 0.56              |
| 2:B:1155:SER:OG   | 2:B:1156:ASP:OD2  | 2.24                     | 0.56              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:H     | 2.04                     | 0.56              |
| 1:A:466:SER:HB3   | 2:B:1103:ILE:HG13 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:636:PRO:HB2   | 2:B:637:LEU:HB3   | 1.88                     | 0.56              |
| 2:B:185:THR:OG1   | 2:B:188:ASP:HB2   | 2.05                     | 0.55              |
| 5:F:108:PHE:O     | 5:F:109:VAL:HG13  | 2.06                     | 0.55              |
| 8:J:53:HIS:HE1    | 8:J:55:ASP:OD1    | 1.89                     | 0.55              |
| 6:H:17:PRO:O      | 6:H:19:ARG:N      | 2.39                     | 0.55              |
| 1:A:590:ARG:HH22  | 1:A:621:THR:HA    | 1.70                     | 0.55              |
| 11:R:5:A:H2'      | 11:R:6:G:C8       | 2.42                     | 0.55              |
| 1:A:102:VAL:HB    | 1:A:211:PHE:HZ    | 1.70                     | 0.55              |
| 1:A:497:THR:CG2   | 2:B:1146:PHE:HD1  | 2.19                     | 0.55              |
| 1:A:858:ASN:ND2   | 1:A:860:LEU:H     | 2.03                     | 0.55              |
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 2.06                     | 0.55              |
| 2:B:879:ARG:NH2   | 2:B:885:MET:HE2   | 2.20                     | 0.55              |
| 1:A:595:THR:OG1   | 1:A:603:ASN:HB3   | 2.07                     | 0.55              |
| 1:A:1063:MET:SD   | 1:A:1436:ILE:HG13 | 2.45                     | 0.55              |
| 2:B:113:TYR:O     | 2:B:114:PRO:C     | 2.47                     | 0.55              |
| 2:B:380:TYR:HE1   | 2:B:579:ARG:HE    | 1.55                     | 0.55              |
| 4:E:64:PRO:HD3    | 4:E:76:GLY:O      | 2.06                     | 0.55              |
| 9:K:91:CYS:O      | 9:K:95:ILE:HG13   | 2.07                     | 0.55              |
| 11:R:5:A:H2'      | 11:R:6:G:H8       | 1.71                     | 0.55              |
| 12:T:6:DC:H2''    | 12:T:7:DA:OP2     | 2.07                     | 0.55              |
| 1:A:33:ALA:HB1    | 1:A:35:ILE:HG12   | 1.87                     | 0.55              |
| 1:A:214:ILE:HG23  | 1:A:215:SER:N     | 2.21                     | 0.55              |
| 3:C:18:VAL:O      | 3:C:231:ASN:HA    | 2.06                     | 0.55              |
| 1:A:76:GLU:CD     | 2:B:1159:ARG:HH12 | 2.14                     | 0.55              |
| 1:A:557:ASP:OD2   | 1:A:559:VAL:HB    | 2.06                     | 0.55              |
| 2:B:363:HIS:O     | 2:B:365:THR:N     | 2.39                     | 0.55              |
| 3:C:184:ASN:ND2   | 3:C:189:THR:O     | 2.39                     | 0.55              |
| 9:K:24:ASP:CG     | 9:K:74:ARG:NH1    | 2.65                     | 0.55              |
| 10:L:60:ARG:HG3   | 10:L:61:THR:N     | 2.21                     | 0.55              |
| 11:R:8:G:N2       | 12:T:22:DT:C2     | 2.75                     | 0.55              |
| 1:A:449:SER:OG    | 2:B:1134:GLU:HG3  | 2.07                     | 0.55              |
| 1:A:1257:ASP:OD2  | 1:A:1257:ASP:N    | 2.35                     | 0.55              |
| 2:B:1165:ILE:O    | 2:B:1166:CYS:C    | 2.48                     | 0.55              |
| 3:C:129:ILE:HG23  | 3:C:130:GLY:N     | 2.22                     | 0.55              |
| 1:A:31:SER:HB2    | 1:A:82:GLY:HA2    | 1.87                     | 0.55              |
| 1:A:102:VAL:HB    | 1:A:211:PHE:CZ    | 2.42                     | 0.55              |
| 2:B:942:ARG:HB2   | 2:B:945:GLU:HB2   | 1.89                     | 0.55              |
| 2:B:1060:ARG:C    | 2:B:1062:HIS:H    | 2.14                     | 0.55              |
| 3:C:142:VAL:HG13  | 3:C:143:LEU:N     | 2.21                     | 0.55              |
| 8:J:1:MET:N       | 8:J:56:LEU:H      | 2.04                     | 0.55              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H    | 1.71                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:286:PHE:CZ   | 2:B:378:LEU:HD23  | 2.42                     | 0.55              |
| 12:T:18:DG:C6    | 16:T:29:C7P:H2    | 2.42                     | 0.54              |
| 1:A:256:GLN:HA   | 1:A:257:ARG:CB    | 2.19                     | 0.54              |
| 1:A:753:GLY:HA2  | 1:A:757:ASN:HD22  | 1.72                     | 0.54              |
| 1:A:1062:GLU:O   | 1:A:1064:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:182:VAL:HG12 | 1:A:183:GLY:N     | 2.22                     | 0.54              |
| 1:A:544:ASP:HB2  | 9:K:47:ARG:HH21   | 1.71                     | 0.54              |
| 3:C:35:ARG:NH1   | 9:K:41:THR:OG1    | 2.38                     | 0.54              |
| 1:A:473:SER:C    | 1:A:475:THR:H     | 2.15                     | 0.54              |
| 2:B:756:ILE:HG12 | 2:B:770:GLN:HG2   | 1.89                     | 0.54              |
| 3:C:62:PHE:O     | 3:C:66:ARG:HG3    | 2.07                     | 0.54              |
| 1:A:996:ASN:C    | 1:A:998:LEU:H     | 2.16                     | 0.54              |
| 1:A:996:ASN:HA   | 1:A:998:LEU:HD23  | 1.89                     | 0.54              |
| 3:C:92:CYS:SG    | 3:C:93:ASP:N      | 2.80                     | 0.54              |
| 12:T:20:DC:H2'   | 12:T:21:DC:O4'    | 2.07                     | 0.54              |
| 13:N:2:DT:H72    | 13:N:3:DG:H1      | 1.72                     | 0.54              |
| 1:A:115:LEU:HD21 | 1:A:145:LYS:HE3   | 1.89                     | 0.54              |
| 1:A:203:SER:O    | 1:A:207:ILE:HG13  | 2.08                     | 0.54              |
| 1:A:900:ASP:HA   | 1:A:926:GLN:NE2   | 2.22                     | 0.54              |
| 2:B:313:MET:HG3  | 2:B:390:LEU:HD21  | 1.89                     | 0.54              |
| 2:B:764:SER:O    | 2:B:765:PRO:C     | 2.49                     | 0.54              |
| 1:A:315:LEU:CB   | 1:A:316:GLN:CA    | 2.75                     | 0.54              |
| 2:B:784:ASN:HD21 | 2:B:788:ARG:HD2   | 1.72                     | 0.54              |
| 9:K:46:ILE:O     | 9:K:50:LEU:HB2    | 2.06                     | 0.54              |
| 1:A:830:LYS:HE2  | 1:A:1098:VAL:HB   | 1.90                     | 0.54              |
| 1:A:888:GLY:O    | 1:A:940:ARG:NH2   | 2.40                     | 0.54              |
| 2:B:977:GLY:HA3  | 2:B:1099:VAL:CG1  | 2.37                     | 0.54              |
| 1:A:378:GLU:OE1  | 1:A:434:ARG:NH1   | 2.40                     | 0.54              |
| 1:A:819:GLY:O    | 1:A:820:GLY:C     | 2.51                     | 0.54              |
| 3:C:73:GLN:CA    | 3:C:133:ILE:HD11  | 2.36                     | 0.54              |
| 1:A:122:MET:HE1  | 1:A:138:ILE:HG23  | 1.89                     | 0.54              |
| 1:A:821:ARG:HG3  | 1:A:825:ILE:HD11  | 1.90                     | 0.54              |
| 2:B:805:THR:HG22 | 2:B:809:MET:SD    | 2.48                     | 0.54              |
| 2:B:981:ALA:CB   | 2:B:987:LYS:HA    | 2.37                     | 0.54              |
| 3:C:4:GLU:HG3    | 3:C:5:GLY:N       | 2.23                     | 0.54              |
| 16:T:29:C7P:N3   | 16:T:29:C7P:C5    | 2.69                     | 0.54              |
| 1:A:367:PRO:HD3  | 1:A:467:THR:O     | 2.08                     | 0.53              |
| 1:A:451:HIS:HB3  | 1:A:453:MET:N     | 2.23                     | 0.53              |
| 1:A:674:PRO:O    | 1:A:678:GLU:HB2   | 2.08                     | 0.53              |
| 2:B:263:GLY:O    | 2:B:264:SER:C     | 2.50                     | 0.53              |
| 2:B:486:TYR:CZ   | 2:B:1096:ARG:HB3  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:984:HIS:C    | 2:B:986:GLN:H     | 2.16                     | 0.53              |
| 3:C:183:TRP:O    | 3:C:185:LYS:N     | 2.41                     | 0.53              |
| 3:C:258:ILE:HD11 | 9:K:42:LEU:HD21   | 1.90                     | 0.53              |
| 6:H:113:ALA:HA   | 6:H:125:LEU:O     | 2.09                     | 0.53              |
| 9:K:47:ARG:HD2   | 9:K:60:ALA:HA     | 1.90                     | 0.53              |
| 1:A:902:LEU:O    | 1:A:903:ASN:CB    | 2.56                     | 0.53              |
| 2:B:902:GLY:O    | 10:L:65:VAL:HG11  | 2.08                     | 0.53              |
| 2:B:955:THR:CG2  | 2:B:956:THR:H     | 2.22                     | 0.53              |
| 3:C:43:THR:CG2   | 3:C:44:LEU:H      | 2.21                     | 0.53              |
| 3:C:91:HIS:HB2   | 3:C:96:SER:CB     | 2.38                     | 0.53              |
| 2:B:979:LYS:C    | 2:B:980:PHE:CD1   | 2.86                     | 0.53              |
| 3:C:102:GLN:HG2  | 3:C:154:LYS:HD2   | 1.89                     | 0.53              |
| 3:C:252:GLN:HG3  | 9:K:95:ILE:HG23   | 1.90                     | 0.53              |
| 6:H:24:CYS:O     | 6:H:41:ASP:HA     | 2.09                     | 0.53              |
| 1:A:541:ILE:N    | 1:A:541:ILE:HD12  | 2.23                     | 0.53              |
| 1:A:1434:ALA:CB  | 1:A:1436:ILE:HD13 | 2.39                     | 0.53              |
| 2:B:234:ILE:O    | 2:B:234:ILE:HG12  | 2.09                     | 0.53              |
| 4:E:190:LEU:HD11 | 4:E:196:VAL:HG13  | 1.90                     | 0.53              |
| 1:A:351:THR:HG21 | 1:A:466:SER:O     | 2.09                     | 0.53              |
| 2:B:384:ARG:HH12 | 2:B:579:ARG:NH2   | 2.04                     | 0.53              |
| 2:B:401:PHE:HA   | 2:B:404:LYS:HG3   | 1.89                     | 0.53              |
| 2:B:63:ILE:HD13  | 2:B:95:ILE:HD12   | 1.91                     | 0.53              |
| 2:B:557:PHE:O    | 2:B:561:TRP:HB2   | 2.09                     | 0.53              |
| 2:B:801:LYS:O    | 8:J:52:THR:HG23   | 2.08                     | 0.53              |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H     | 1.74                     | 0.53              |
| 2:B:917:PRO:HA   | 2:B:934:LYS:HA    | 1.91                     | 0.53              |
| 3:C:98:VAL:H     | 3:C:122:SER:HB3   | 1.73                     | 0.53              |
| 1:A:95:PHE:O     | 1:A:99:ILE:HG13   | 2.08                     | 0.53              |
| 1:A:125:ALA:O    | 1:A:128:ILE:HG22  | 2.07                     | 0.53              |
| 1:A:1156:PRO:O   | 1:A:1158:PRO:HD3  | 2.09                     | 0.53              |
| 6:H:109:LYS:HB2  | 6:H:111:LEU:N     | 2.23                     | 0.53              |
| 1:A:446:ARG:NH2  | 11:R:10:A:O2'     | 2.42                     | 0.53              |
| 1:A:697:ALA:HA   | 1:A:702:LEU:HB2   | 1.91                     | 0.53              |
| 2:B:292:ILE:HD11 | 2:B:327:ARG:CG    | 2.39                     | 0.53              |
| 2:B:1084:GLN:NE2 | 3:C:192:TRP:H     | 2.00                     | 0.53              |
| 4:E:7:ARG:C      | 4:E:9:ILE:N       | 2.66                     | 0.53              |
| 8:J:56:LEU:CB    | 8:J:60:PHE:HE2    | 2.20                     | 0.53              |
| 1:A:339:ASN:O    | 2:B:1117:GLN:NE2  | 2.40                     | 0.53              |
| 1:A:364:VAL:O    | 1:A:364:VAL:HG13  | 2.09                     | 0.53              |
| 2:B:857:ARG:NH2  | 12:T:24:DT:OP1    | 2.41                     | 0.53              |
| 1:A:369:SER:HB3  | 9:K:2:ASN:OD1     | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:219:ALA:HB2   | 2:B:405:ARG:HG2   | 1.90                     | 0.52              |
| 2:B:220:GLY:O     | 2:B:222:ILE:HG13  | 2.09                     | 0.52              |
| 2:B:416:LEU:HD22  | 2:B:457:LEU:HD23  | 1.91                     | 0.52              |
| 2:B:485:ARG:CG    | 2:B:485:ARG:NH1   | 2.60                     | 0.52              |
| 2:B:541:LEU:HB2   | 2:B:747:MET:CE    | 2.38                     | 0.52              |
| 4:E:89:GLY:HA2    | 4:E:117:THR:OG1   | 2.08                     | 0.52              |
| 6:H:82:PRO:C      | 6:H:84:ALA:N      | 2.67                     | 0.52              |
| 1:A:33:ALA:HB3    | 1:A:83:HIS:H      | 1.74                     | 0.52              |
| 2:B:841:MET:SD    | 2:B:990:ILE:HD11  | 2.49                     | 0.52              |
| 2:B:882:THR:CG2   | 2:B:884:ARG:H     | 2.22                     | 0.52              |
| 2:B:942:ARG:HB2   | 2:B:945:GLU:CB    | 2.40                     | 0.52              |
| 5:F:92:ARG:O      | 5:F:92:ARG:HG3    | 2.08                     | 0.52              |
| 1:A:76:GLU:OE2    | 2:B:1159:ARG:NH1  | 2.42                     | 0.52              |
| 1:A:135:PHE:C     | 1:A:135:PHE:CD2   | 2.86                     | 0.52              |
| 1:A:299:HIS:HA    | 1:A:302:THR:HG22  | 1.91                     | 0.52              |
| 2:B:269:ILE:HD11  | 2:B:386:LEU:HD21  | 1.92                     | 0.52              |
| 2:B:702:LEU:HD23  | 2:B:737:THR:CG2   | 2.39                     | 0.52              |
| 2:B:791:THR:O     | 2:B:792:MET:CB    | 2.57                     | 0.52              |
| 7:I:8:ARG:O       | 7:I:9:ASP:CB      | 2.57                     | 0.52              |
| 9:K:43:GLY:CA     | 9:K:71:PHE:CE1    | 2.92                     | 0.52              |
| 1:A:705:LYS:HG3   | 1:A:713:SER:HB2   | 1.90                     | 0.52              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HG22  | 2.09                     | 0.52              |
| 1:A:1017:LEU:CB   | 4:E:205:SER:HA    | 2.39                     | 0.52              |
| 1:A:1044:TRP:O    | 1:A:1047:SER:N    | 2.42                     | 0.52              |
| 2:B:64:CYS:O      | 2:B:65:GLU:CB     | 2.57                     | 0.52              |
| 2:B:70:ILE:O      | 2:B:70:ILE:HG22   | 2.09                     | 0.52              |
| 2:B:800:GLN:HB3   | 8:J:52:THR:HG21   | 1.87                     | 0.52              |
| 1:A:567:LYS:O     | 1:A:569:LYS:N     | 2.43                     | 0.52              |
| 2:B:840:ILE:HG12  | 2:B:992:ILE:CG2   | 2.39                     | 0.52              |
| 2:B:1120:GLU:O    | 2:B:1124:ARG:HD3  | 2.09                     | 0.52              |
| 3:C:173:ALA:O     | 3:C:174:ALA:HB3   | 2.09                     | 0.52              |
| 6:H:39:THR:O      | 6:H:123:MET:HA    | 2.10                     | 0.52              |
| 7:I:47:GLU:HB3    | 7:I:50:THR:HG23   | 1.91                     | 0.52              |
| 1:A:134:ARG:CD    | 1:A:221:SER:O     | 2.56                     | 0.52              |
| 1:A:567:LYS:HB2   | 6:H:95:TYR:HA     | 1.92                     | 0.52              |
| 1:A:816:HIS:CE1   | 2:B:764:SER:H     | 2.27                     | 0.52              |
| 1:A:1276:VAL:HG21 | 1:A:1316:VAL:HG22 | 1.92                     | 0.52              |
| 2:B:256:VAL:HG11  | 2:B:382:ILE:HD13  | 1.92                     | 0.52              |
| 2:B:635:ARG:HH22  | 2:B:742:GLU:CD    | 2.17                     | 0.52              |
| 2:B:847:ASP:HB3   | 3:C:167:HIS:NE2   | 2.23                     | 0.52              |
| 4:E:168:TYR:O     | 4:E:169:ARG:HG2   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:553:VAL:HG13  | 1:A:648:ASN:HB3   | 1.91                     | 0.52              |
| 1:A:982:THR:C     | 1:A:984:LYS:N     | 2.65                     | 0.52              |
| 3:C:167:HIS:ND1   | 10:L:70:ARG:HB3   | 2.24                     | 0.52              |
| 1:A:384:ASN:HB2   | 1:A:387:ARG:HH21  | 1.75                     | 0.52              |
| 1:A:902:LEU:O     | 1:A:903:ASN:HB3   | 2.10                     | 0.52              |
| 2:B:214:ALA:HB2   | 2:B:408:LEU:HD13  | 1.92                     | 0.52              |
| 2:B:843:GLN:HA    | 2:B:846:ILE:HD12  | 1.92                     | 0.52              |
| 4:E:156:LEU:HG    | 4:E:195:VAL:O     | 2.09                     | 0.52              |
| 12:T:18:DG:O6     | 16:T:29:C7P:H2    | 2.10                     | 0.52              |
| 1:A:873:MET:HG2   | 1:A:957:PRO:CG    | 2.35                     | 0.52              |
| 1:A:1430:LEU:O    | 2:B:1196:ILE:HG22 | 2.10                     | 0.52              |
| 2:B:384:ARG:HD2   | 2:B:384:ARG:N     | 2.25                     | 0.52              |
| 4:E:7:ARG:C       | 4:E:9:ILE:H       | 2.17                     | 0.52              |
| 1:A:567:LYS:CB    | 6:H:95:TYR:HA     | 2.40                     | 0.51              |
| 1:A:668:ASP:HB3   | 1:A:743:VAL:HG23  | 1.92                     | 0.51              |
| 1:A:896:ARG:HD2   | 1:A:897:TYR:CE1   | 2.46                     | 0.51              |
| 1:A:913:LEU:HD21  | 1:A:981:LEU:O     | 2.10                     | 0.51              |
| 1:A:1152:ILE:HG12 | 1:A:1260:LEU:HD23 | 1.93                     | 0.51              |
| 2:B:102:VAL:HG13  | 2:B:112:LEU:HD22  | 1.92                     | 0.51              |
| 2:B:484:ASN:ND2   | 2:B:490:SER:OG    | 2.24                     | 0.51              |
| 2:B:530:GLY:O     | 2:B:531:GLN:C     | 2.53                     | 0.51              |
| 2:B:874:PHE:CE1   | 2:B:964:VAL:HG23  | 2.45                     | 0.51              |
| 3:C:148:ARG:NH1   | 8:J:64:ASN:HA     | 2.25                     | 0.51              |
| 6:H:139:ASN:O     | 6:H:140:ALA:CB    | 2.59                     | 0.51              |
| 2:B:416:LEU:HD11  | 2:B:460:ALA:HB1   | 1.90                     | 0.51              |
| 2:B:770:GLN:O     | 2:B:770:GLN:NE2   | 2.43                     | 0.51              |
| 2:B:1160:VAL:HG11 | 2:B:1169:MET:HG2  | 1.92                     | 0.51              |
| 4:E:12:LEU:HD22   | 4:E:55:ARG:HH21   | 1.73                     | 0.51              |
| 9:K:90:ALA:O      | 9:K:94:ILE:HG13   | 2.08                     | 0.51              |
| 1:A:304:MET:O     | 1:A:326:ARG:HB2   | 2.10                     | 0.51              |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:HD21 | 1.92                     | 0.51              |
| 2:B:487:THR:CG2   | 2:B:488:TYR:N     | 2.72                     | 0.51              |
| 2:B:807:ARG:HH11  | 2:B:807:ARG:HG3   | 1.76                     | 0.51              |
| 2:B:864:LYS:HD3   | 2:B:871:THR:HG23  | 1.92                     | 0.51              |
| 2:B:1013:ASN:OD1  | 2:B:1014:PRO:HD2  | 2.10                     | 0.51              |
| 3:C:8:VAL:HG11    | 9:K:105:PHE:CD1   | 2.43                     | 0.51              |
| 1:A:668:ASP:OD2   | 1:A:742:ASN:HB2   | 2.09                     | 0.51              |
| 2:B:859:TYR:CD1   | 2:B:859:TYR:N     | 2.78                     | 0.51              |
| 2:B:1166:CYS:SG   | 2:B:1167:GLY:N    | 2.83                     | 0.51              |
| 8:J:8:PHE:HD1     | 8:J:49:MET:HE1    | 1.76                     | 0.51              |
| 1:A:338:GLY:HA2   | 2:B:1129:ARG:HH22 | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:765:VAL:HG13  | 1:A:802:ASN:O     | 2.11                     | 0.51              |
| 1:A:1105:LEU:HD23 | 1:A:1384:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:582:ILE:HD13  | 1:A:629:LEU:HD11  | 1.92                     | 0.51              |
| 1:A:590:ARG:CG    | 1:A:590:ARG:NH1   | 2.74                     | 0.51              |
| 1:A:809:THR:HB    | 1:A:810:PRO:HD2   | 1.93                     | 0.51              |
| 1:A:1383:SER:O    | 1:A:1388:GLY:HA3  | 2.11                     | 0.51              |
| 2:B:287:ARG:NH2   | 2:B:294:ASP:OD2   | 2.43                     | 0.51              |
| 2:B:296:GLU:O     | 2:B:300:HIS:HD2   | 1.94                     | 0.51              |
| 2:B:1147:LEU:O    | 2:B:1151:LEU:HB2  | 2.11                     | 0.51              |
| 8:J:43:ARG:HD2    | 8:J:46:CYS:SG     | 2.51                     | 0.51              |
| 1:A:636:GLU:OE2   | 1:A:962:ARG:NH1   | 2.41                     | 0.51              |
| 1:A:845:LEU:O     | 1:A:848:ILE:HG12  | 2.10                     | 0.51              |
| 1:A:899:VAL:CG2   | 1:A:1029:ARG:HG3  | 2.41                     | 0.51              |
| 2:B:287:ARG:HA    | 2:B:291:ILE:O     | 2.10                     | 0.51              |
| 2:B:770:GLN:OE1   | 2:B:983:ARG:HA    | 2.11                     | 0.51              |
| 4:E:112:TYR:CE1   | 4:E:115:ASN:HA    | 2.46                     | 0.51              |
| 1:A:93:VAL:HG11   | 1:A:305:ASP:HB3   | 1.92                     | 0.51              |
| 1:A:709:THR:HG22  | 1:A:710:LEU:N     | 2.26                     | 0.51              |
| 1:A:834:THR:HG21  | 1:A:1077:THR:HA   | 1.92                     | 0.51              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:N     | 2.25                     | 0.51              |
| 1:A:982:THR:C     | 1:A:984:LYS:H     | 2.18                     | 0.51              |
| 1:A:1101:LEU:HG   | 1:A:1105:LEU:CD1  | 2.41                     | 0.51              |
| 2:B:847:ASP:CB    | 3:C:167:HIS:CD2   | 2.93                     | 0.51              |
| 2:B:986:GLN:HG2   | 2:B:1022:THR:HG21 | 1.92                     | 0.51              |
| 6:H:116:TYR:HB2   | 6:H:123:MET:HB3   | 1.93                     | 0.51              |
| 1:A:709:THR:HG22  | 1:A:710:LEU:H     | 1.76                     | 0.51              |
| 1:A:751:SER:HB2   | 2:B:1015:HIS:CE1  | 2.46                     | 0.51              |
| 1:A:1333:ILE:HG12 | 1:A:1381:LEU:HD12 | 1.93                     | 0.51              |
| 2:B:315:LYS:N     | 2:B:316:PRO:HD2   | 2.26                     | 0.51              |
| 2:B:863:GLU:O     | 2:B:961:LEU:HD22  | 2.11                     | 0.51              |
| 5:F:147:SER:O     | 5:F:151:LEU:HD12  | 2.11                     | 0.51              |
| 1:A:335:ARG:NH1   | 2:B:1202:LEU:CD1  | 2.69                     | 0.51              |
| 1:A:347:PHE:HB2   | 2:B:1150:ARG:NH2  | 2.25                     | 0.51              |
| 1:A:507:VAL:CG1   | 1:A:521:MET:HE1   | 2.41                     | 0.51              |
| 1:A:1161:THR:HG23 | 1:A:1239:ARG:HH21 | 1.74                     | 0.51              |
| 2:B:112:LEU:HD21  | 2:B:117:ALA:HB2   | 1.93                     | 0.51              |
| 2:B:848:ARG:HH22  | 2:B:996:ARG:NH1   | 2.09                     | 0.51              |
| 11:R:8:G:C2       | 12:T:22:DT:C2     | 2.99                     | 0.51              |
| 2:B:915:THR:HG21  | 2:B:934:LYS:HE3   | 1.93                     | 0.50              |
| 6:H:4:THR:HG22    | 6:H:5:LEU:H       | 1.77                     | 0.50              |
| 1:A:361:LEU:HG    | 1:A:361:LEU:O     | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:381:THR:CG2   | 1:A:383:TYR:CD1   | 2.94                     | 0.50              |
| 1:A:456:MET:HG3   | 1:A:478:TYR:CZ    | 2.46                     | 0.50              |
| 2:B:992:ILE:CD1   | 9:K:67:PHE:HE2    | 2.24                     | 0.50              |
| 2:B:1079:LYS:O    | 2:B:1080:LYS:C    | 2.53                     | 0.50              |
| 2:B:1097:HIS:HB3  | 2:B:1102:LYS:CE   | 2.41                     | 0.50              |
| 1:A:1431:GLY:HA3  | 2:B:1197:PRO:HD3  | 1.93                     | 0.50              |
| 2:B:62:ILE:HD12   | 2:B:418:LYS:HG3   | 1.91                     | 0.50              |
| 2:B:942:ARG:HG3   | 2:B:945:GLU:OE1   | 2.11                     | 0.50              |
| 4:E:14:ARG:HH12   | 4:E:142:VAL:HG22  | 1.77                     | 0.50              |
| 1:A:401:GLY:O     | 1:A:435:HIS:CD2   | 2.60                     | 0.50              |
| 1:A:605:MET:HE3   | 1:A:614:PHE:O     | 2.11                     | 0.50              |
| 1:A:648:ASN:O     | 1:A:652:VAL:HG23  | 2.11                     | 0.50              |
| 2:B:483:LEU:HD22  | 2:B:491:THR:HG23  | 1.93                     | 0.50              |
| 5:F:89:GLU:O      | 5:F:93:ILE:HD12   | 2.11                     | 0.50              |
| 5:F:147:SER:C     | 5:F:149:GLU:H     | 2.18                     | 0.50              |
| 8:J:32:GLU:CD     | 8:J:32:GLU:H      | 2.18                     | 0.50              |
| 1:A:318:SER:HA    | 12:T:28:DT:H4'    | 1.92                     | 0.50              |
| 1:A:683:ILE:HG21  | 1:A:801:GLU:CG    | 2.41                     | 0.50              |
| 1:A:910:PRO:HA    | 1:A:916:GLY:HA3   | 1.93                     | 0.50              |
| 1:A:1025:ARG:O    | 1:A:1035:TYR:OH   | 2.23                     | 0.50              |
| 2:B:841:MET:HE1   | 2:B:980:PHE:CE2   | 2.46                     | 0.50              |
| 1:A:525:GLN:HE22  | 1:A:752:LYS:HE2   | 1.77                     | 0.50              |
| 1:A:526:ASP:O     | 1:A:527:THR:C     | 2.54                     | 0.50              |
| 1:A:529:CYS:SG    | 1:A:662:PHE:CE2   | 3.04                     | 0.50              |
| 1:A:858:ASN:C     | 1:A:858:ASN:ND2   | 2.68                     | 0.50              |
| 1:A:1341:ILE:HD13 | 1:A:1379:GLY:O    | 2.11                     | 0.50              |
| 8:J:1:MET:N       | 8:J:57:ILE:H      | 2.09                     | 0.50              |
| 2:B:762:ASN:HD21  | 2:B:1022:THR:HA   | 1.77                     | 0.50              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:HG11 | 1.93                     | 0.50              |
| 2:B:992:ILE:CD1   | 9:K:67:PHE:CE2    | 2.95                     | 0.50              |
| 1:A:129:LYS:O     | 1:A:130:ASP:CB    | 2.58                     | 0.50              |
| 1:A:444:PHE:HE2   | 1:A:470:LEU:CD2   | 2.24                     | 0.50              |
| 1:A:920:LEU:HD23  | 1:A:921:GLY:N     | 2.26                     | 0.50              |
| 1:A:1239:ARG:HH12 | 1:A:1241:ARG:HH12 | 1.58                     | 0.50              |
| 2:B:20:ASP:OD2    | 2:B:20:ASP:C      | 2.55                     | 0.50              |
| 2:B:27:ALA:HB2    | 2:B:708:GLU:CD    | 2.36                     | 0.50              |
| 2:B:731:VAL:O     | 2:B:732:SER:HB2   | 2.10                     | 0.50              |
| 2:B:944:THR:HG21  | 2:B:1122:ARG:NH2  | 2.27                     | 0.50              |
| 2:B:955:THR:HG22  | 2:B:956:THR:O     | 2.12                     | 0.50              |
| 2:B:1073:TYR:OH   | 3:C:179:GLU:HG3   | 2.11                     | 0.50              |
| 1:A:51:GLY:HA2    | 1:A:56:PRO:HG3    | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:609:ASP:O     | 1:A:611:GLN:N     | 2.44                     | 0.50              |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:HD11 | 1.94                     | 0.50              |
| 2:B:825:VAL:HG22  | 2:B:1010:LEU:HB3  | 1.93                     | 0.50              |
| 2:B:827:ILE:HG22  | 2:B:1014:PRO:HG3  | 1.94                     | 0.50              |
| 2:B:852:ARG:HG2   | 2:B:973:ILE:HG23  | 1.94                     | 0.50              |
| 3:C:231:ASN:C     | 3:C:231:ASN:ND2   | 2.55                     | 0.50              |
| 1:A:867:ILE:HD13  | 1:A:1014:ALA:HB2  | 1.94                     | 0.49              |
| 2:B:778:MET:HE2   | 2:B:1094:ARG:HG2  | 1.94                     | 0.49              |
| 2:B:788:ARG:NH1   | 2:B:790:ASP:OD2   | 2.44                     | 0.49              |
| 2:B:916:THR:O     | 2:B:916:THR:CG2   | 2.57                     | 0.49              |
| 8:J:7:CYS:HB2     | 8:J:49:MET:HG2    | 1.93                     | 0.49              |
| 1:A:182:VAL:HG12  | 1:A:183:GLY:H     | 1.77                     | 0.49              |
| 1:A:672:ASP:HB3   | 1:A:675:THR:H     | 1.77                     | 0.49              |
| 1:A:852:TYR:CD2   | 1:A:1060:PRO:HB2  | 2.47                     | 0.49              |
| 1:A:1441:PHE:CZ   | 5:F:89:GLU:HA     | 2.47                     | 0.49              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:H     | 1.77                     | 0.49              |
| 4:E:29:PHE:CD1    | 4:E:65:THR:HG22   | 2.48                     | 0.49              |
| 1:A:568:PRO:HB3   | 3:C:221:TYR:CE1   | 2.48                     | 0.49              |
| 2:B:762:ASN:ND2   | 2:B:1022:THR:HA   | 2.27                     | 0.49              |
| 12:T:9:DA:H2''    | 12:T:10:DA:C8     | 2.46                     | 0.49              |
| 12:T:16:DC:H2''   | 12:T:17:DC:H6     | 1.77                     | 0.49              |
| 1:A:367:PRO:HB3   | 1:A:465:TYR:O     | 2.12                     | 0.49              |
| 3:C:116:LYS:HD3   | 3:C:140:ASN:HB3   | 1.93                     | 0.49              |
| 12:T:27:DA:H2'    | 12:T:27:DA:N3     | 2.26                     | 0.49              |
| 1:A:1313:LEU:C    | 1:A:1315:GLU:H    | 2.20                     | 0.49              |
| 2:B:274:PRO:HB2   | 2:B:359:GLU:HB3   | 1.94                     | 0.49              |
| 2:B:1138:MET:HA   | 2:B:1138:MET:CE   | 2.32                     | 0.49              |
| 3:C:167:HIS:CD2   | 3:C:168:ALA:N     | 2.81                     | 0.49              |
| 4:E:179:GLN:OE1   | 4:E:215:MET:HE2   | 2.13                     | 0.49              |
| 1:A:315:LEU:HD22  | 1:A:315:LEU:H     | 1.77                     | 0.49              |
| 1:A:737:LEU:O     | 1:A:744:LYS:HD2   | 2.12                     | 0.49              |
| 1:A:979:SER:OG    | 1:A:980:ASP:N     | 2.44                     | 0.49              |
| 2:B:431:TYR:CE2   | 2:B:447:ALA:HB2   | 2.48                     | 0.49              |
| 2:B:722:ASP:OD2   | 2:B:723:VAL:HG22  | 2.13                     | 0.49              |
| 2:B:997:GLU:HG3   | 3:C:38:ILE:HG21   | 1.95                     | 0.49              |
| 3:C:27:LEU:HD12   | 3:C:228:PHE:CE2   | 2.45                     | 0.49              |
| 4:E:6:GLU:O       | 4:E:9:ILE:HG22    | 2.13                     | 0.49              |
| 1:A:672:ASP:HB2   | 1:A:736:ASN:ND2   | 2.28                     | 0.49              |
| 2:B:102:VAL:CG2   | 2:B:110:HIS:HB3   | 2.42                     | 0.49              |
| 2:B:474:SER:CB    | 2:B:476:ARG:HG3   | 2.42                     | 0.49              |
| 2:B:1006:ILE:CG2  | 2:B:1007:VAL:N    | 2.76                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:111:LEU:H     | 5:F:111:LEU:CD1  | 2.07                     | 0.49              |
| 12:T:5:DC:H2"     | 12:T:6:DC:OP2    | 2.13                     | 0.49              |
| 1:A:71:GLN:C      | 1:A:73:GLY:H     | 2.21                     | 0.49              |
| 1:A:356:ASP:HB3   | 1:A:359:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:1062:GLU:OE2  | 5:F:88:TYR:OH    | 2.31                     | 0.49              |
| 1:A:1443:VAL:HG22 | 5:F:134:ILE:HD13 | 1.94                     | 0.49              |
| 2:B:20:ASP:OD2    | 2:B:21:GLU:N     | 2.45                     | 0.49              |
| 2:B:168:GLY:H     | 2:B:450:ALA:HB1  | 1.77                     | 0.49              |
| 2:B:313:MET:HE2   | 2:B:390:LEU:HG   | 1.94                     | 0.49              |
| 2:B:496:ARG:HH12  | 2:B:541:LEU:HA   | 1.76                     | 0.49              |
| 2:B:705:MET:HE3   | 2:B:705:MET:HA   | 1.94                     | 0.49              |
| 2:B:882:THR:HG22  | 2:B:884:ARG:H    | 1.78                     | 0.49              |
| 3:C:63:ILE:O      | 3:C:66:ARG:N     | 2.44                     | 0.49              |
| 2:B:119:LEU:HD23  | 2:B:953:LEU:CD1  | 2.43                     | 0.49              |
| 2:B:570:VAL:HB    | 2:B:573:GLN:HB3  | 1.95                     | 0.49              |
| 3:C:46:ILE:HD12   | 3:C:157:CYS:CB   | 2.39                     | 0.49              |
| 7:I:28:GLU:HB3    | 7:I:35:VAL:HG22  | 1.95                     | 0.49              |
| 1:A:113:LEU:HD12  | 1:A:218:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:254:GLU:HA    | 1:A:255:SER:HA   | 1.57                     | 0.49              |
| 1:A:874:ASP:HB2   | 1:A:1058:VAL:HA  | 1.95                     | 0.49              |
| 1:A:1116:LEU:HD13 | 1:A:1329:THR:OG1 | 2.13                     | 0.49              |
| 2:B:293:PRO:HB2   | 7:I:11:ASN:O     | 2.13                     | 0.49              |
| 2:B:848:ARG:NH2   | 2:B:996:ARG:NH1  | 2.60                     | 0.49              |
| 3:C:16:ASP:O      | 3:C:233:GLU:HA   | 2.12                     | 0.49              |
| 3:C:250:THR:HA    | 3:C:253:LYS:HB2  | 1.95                     | 0.49              |
| 1:A:512:VAL:O     | 1:A:512:VAL:HG13 | 2.11                     | 0.48              |
| 2:B:205:ILE:O     | 2:B:206:ASN:C    | 2.55                     | 0.48              |
| 2:B:523:CYS:SG    | 2:B:750:GLY:N    | 2.82                     | 0.48              |
| 2:B:802:PRO:HA    | 2:B:1091:TYR:CD1 | 2.49                     | 0.48              |
| 2:B:1167:GLY:O    | 2:B:1215:ARG:HA  | 2.13                     | 0.48              |
| 7:I:7:CYS:CB      | 7:I:10:CYS:SG    | 3.01                     | 0.48              |
| 7:I:96:SER:HB2    | 7:I:98:VAL:HG23  | 1.94                     | 0.48              |
| 1:A:405:VAL:HG22  | 1:A:432:VAL:HG13 | 1.95                     | 0.48              |
| 2:B:807:ARG:HG3   | 2:B:807:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:1106:ARG:CD   | 2:B:1126:GLY:O   | 2.59                     | 0.48              |
| 7:I:14:LEU:HD13   | 7:I:27:PHE:HB3   | 1.95                     | 0.48              |
| 1:A:846:GLU:CD    | 1:A:1425:SER:HG  | 2.21                     | 0.48              |
| 2:B:258:LEU:HD11  | 2:B:267:ARG:HB3  | 1.94                     | 0.48              |
| 2:B:408:LEU:O     | 2:B:412:LEU:HD12 | 2.13                     | 0.48              |
| 3:C:91:HIS:HB2    | 3:C:96:SER:OG    | 2.13                     | 0.48              |
| 3:C:235:VAL:HG11  | 8:J:6:ARG:NH2    | 2.28                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:K:58:PHE:HB3    | 9:K:76:GLN:HB3   | 1.94                     | 0.48              |
| 1:A:356:ASP:OD2   | 9:K:65:HIS:HE1   | 1.96                     | 0.48              |
| 1:A:482:PHE:C     | 2:B:837:ASP:O    | 2.56                     | 0.48              |
| 1:A:870:GLU:HG2   | 4:E:208:TYR:CD2  | 2.49                     | 0.48              |
| 3:C:46:ILE:HG23   | 3:C:157:CYS:HB3  | 1.93                     | 0.48              |
| 1:A:477:PRO:HG3   | 1:A:521:MET:SD   | 2.53                     | 0.48              |
| 1:A:855:THR:CG2   | 1:A:857:ARG:HE   | 2.26                     | 0.48              |
| 1:A:1098:VAL:N    | 1:A:1099:PRO:HD2 | 2.28                     | 0.48              |
| 2:B:1165:ILE:HG22 | 2:B:1166:CYS:N   | 2.28                     | 0.48              |
| 4:E:161:LYS:O     | 4:E:163:GLU:N    | 2.47                     | 0.48              |
| 12:T:5:DC:H1'     | 12:T:6:DC:O5'    | 2.13                     | 0.48              |
| 1:A:283:GLY:O     | 1:A:285:PRO:HD3  | 2.13                     | 0.48              |
| 2:B:34:ILE:HD13   | 2:B:542:MET:HE3  | 1.96                     | 0.48              |
| 2:B:514:LEU:HD12  | 2:B:518:HIS:CD2  | 2.48                     | 0.48              |
| 2:B:784:ASN:ND2   | 2:B:788:ARG:HD2  | 2.29                     | 0.48              |
| 8:J:26:GLN:O      | 8:J:26:GLN:HG3   | 2.14                     | 0.48              |
| 1:A:15:LYS:HD2    | 2:B:1220:ARG:NH1 | 2.28                     | 0.48              |
| 1:A:15:LYS:HE2    | 2:B:1220:ARG:HG2 | 1.96                     | 0.48              |
| 1:A:1092:LYS:O    | 1:A:1093:LYS:HG3 | 2.13                     | 0.48              |
| 2:B:541:LEU:HD12  | 2:B:747:MET:HE1  | 1.96                     | 0.48              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:CD1  | 2.44                     | 0.48              |
| 3:C:166:GLU:HG3   | 9:K:10:PHE:HZ    | 1.78                     | 0.48              |
| 3:C:178:PHE:C     | 3:C:178:PHE:CD2  | 2.92                     | 0.48              |
| 6:H:24:CYS:HB2    | 6:H:44:VAL:HG23  | 1.95                     | 0.48              |
| 1:A:37:PHE:HB2    | 1:A:52:GLY:CA    | 2.44                     | 0.48              |
| 1:A:55:ASP:O      | 1:A:58:LEU:N     | 2.34                     | 0.48              |
| 1:A:71:GLN:HB2    | 1:A:72:GLU:H     | 1.52                     | 0.48              |
| 1:A:821:ARG:CG    | 1:A:825:ILE:HD11 | 2.44                     | 0.48              |
| 2:B:102:VAL:HG23  | 2:B:110:HIS:HB3  | 1.95                     | 0.48              |
| 2:B:118:ARG:HH22  | 2:B:194:GLU:CD   | 2.21                     | 0.48              |
| 2:B:941:LEU:O     | 2:B:942:ARG:C    | 2.56                     | 0.48              |
| 6:H:115:TYR:HA    | 6:H:123:MET:O    | 2.13                     | 0.48              |
| 6:H:124:ARG:NH1   | 6:H:126:GLU:OE2  | 2.44                     | 0.48              |
| 1:A:322:VAL:HG12  | 1:A:323:LYS:HE2  | 1.95                     | 0.48              |
| 1:A:337:ARG:HD3   | 2:B:1132:GLU:OE1 | 2.13                     | 0.48              |
| 1:A:575:LYS:HD3   | 1:A:612:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:614:PHE:CD1   | 1:A:614:PHE:C    | 2.91                     | 0.48              |
| 2:B:737:THR:O     | 2:B:738:PHE:C    | 2.57                     | 0.48              |
| 2:B:956:THR:HB    | 10:L:46:VAL:CG2  | 2.27                     | 0.48              |
| 5:F:109:VAL:HG11  | 5:F:127:GLU:OE1  | 2.14                     | 0.48              |
| 7:I:78:CYS:SG     | 7:I:105:SER:HB2  | 2.54                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:251:SER:H    | 1:A:253:ASN:ND2   | 2.12                     | 0.48              |
| 2:B:519:TRP:HZ2  | 2:B:705:MET:HE1   | 1.78                     | 0.48              |
| 2:B:708:GLU:CG   | 2:B:709:ASP:H     | 2.27                     | 0.48              |
| 2:B:794:ASN:N    | 2:B:794:ASN:HD22  | 2.12                     | 0.48              |
| 7:I:103:CYS:SG   | 7:I:104:LEU:N     | 2.87                     | 0.48              |
| 8:J:6:ARG:HA     | 8:J:12:LYS:O      | 2.14                     | 0.48              |
| 12:T:11:DC:H2''  | 12:T:12:DC:OP2    | 2.14                     | 0.48              |
| 1:A:919:ILE:O    | 1:A:922:ASP:HB2   | 2.14                     | 0.47              |
| 1:A:1276:VAL:HB  | 1:A:1279:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:1342:GLU:HG3 | 4:E:198:ILE:HD13  | 1.95                     | 0.47              |
| 2:B:474:SER:C    | 2:B:476:ARG:N     | 2.72                     | 0.47              |
| 5:F:125:LEU:HB2  | 5:F:130:ILE:CD1   | 2.43                     | 0.47              |
| 9:K:33:ILE:HD12  | 9:K:73:LEU:HD23   | 1.95                     | 0.47              |
| 12:T:5:DC:OP2    | 12:T:5:DC:H2'     | 2.14                     | 0.47              |
| 1:A:334:GLY:O    | 1:A:335:ARG:C     | 2.56                     | 0.47              |
| 1:A:1153:TYR:CD2 | 1:A:1163:ILE:HD11 | 2.49                     | 0.47              |
| 1:A:1394:THR:HB  | 1:A:1398:MET:HE3  | 1.95                     | 0.47              |
| 6:H:63:LEU:HB2   | 6:H:90:ALA:HB2    | 1.96                     | 0.47              |
| 6:H:108:SER:O    | 6:H:109:LYS:HB2   | 2.12                     | 0.47              |
| 9:K:43:GLY:HA2   | 9:K:71:PHE:CE1    | 2.50                     | 0.47              |
| 1:A:184:SER:HA   | 1:A:199:LEU:HD13  | 1.95                     | 0.47              |
| 1:A:497:THR:HG22 | 2:B:1146:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:587:HIS:HA   | 1:A:607:ILE:O     | 2.14                     | 0.47              |
| 2:B:470:LYS:C    | 2:B:472:ALA:H     | 2.22                     | 0.47              |
| 3:C:183:TRP:O    | 3:C:184:ASN:C     | 2.57                     | 0.47              |
| 3:C:262:LEU:HD11 | 9:K:87:LEU:HD23   | 1.95                     | 0.47              |
| 4:E:108:GLY:O    | 4:E:132:ILE:HG23  | 2.13                     | 0.47              |
| 1:A:372:LYS:HD3  | 1:A:397:ASN:HA    | 1.97                     | 0.47              |
| 3:C:229:TYR:CD1  | 3:C:229:TYR:N     | 2.82                     | 0.47              |
| 6:H:91:ASP:HA    | 6:H:93:TYR:HD1    | 1.79                     | 0.47              |
| 9:K:65:HIS:CD2   | 9:K:66:PRO:HD2    | 2.50                     | 0.47              |
| 10:L:43:THR:HG22 | 10:L:43:THR:O     | 2.14                     | 0.47              |
| 1:A:451:HIS:HB2  | 1:A:454:SER:H     | 1.80                     | 0.47              |
| 2:B:839:MET:O    | 2:B:990:ILE:HA    | 2.14                     | 0.47              |
| 2:B:841:MET:HE3  | 2:B:990:ILE:HD11  | 1.96                     | 0.47              |
| 2:B:1060:ARG:C   | 2:B:1062:HIS:N    | 2.72                     | 0.47              |
| 3:C:144:ILE:HG22 | 3:C:145:CYS:N     | 2.28                     | 0.47              |
| 6:H:44:VAL:HG13  | 6:H:48:PRO:HA     | 1.96                     | 0.47              |
| 9:K:82:ASP:OD1   | 9:K:83:PRO:HD2    | 2.15                     | 0.47              |
| 1:A:335:ARG:O    | 1:A:336:ILE:C     | 2.56                     | 0.47              |
| 1:A:867:ILE:HG22 | 1:A:872:GLY:CA    | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:119:LEU:HD23  | 2:B:953:LEU:HD13  | 1.95                     | 0.47              |
| 3:C:164:ALA:HB2   | 3:C:171:GLY:HA2   | 1.96                     | 0.47              |
| 1:A:756:ILE:HD13  | 1:A:759:ALA:HB3   | 1.95                     | 0.47              |
| 1:A:836:TYR:CE1   | 1:A:840:ARG:HD2   | 2.48                     | 0.47              |
| 1:A:899:VAL:CB    | 1:A:929:LEU:CD1   | 2.85                     | 0.47              |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:HB3  | 1.95                     | 0.47              |
| 2:B:956:THR:CB    | 10:L:46:VAL:HG21  | 2.27                     | 0.47              |
| 3:C:43:THR:CG2    | 3:C:44:LEU:N      | 2.77                     | 0.47              |
| 3:C:51:VAL:HG22   | 3:C:155:LEU:HD22  | 1.97                     | 0.47              |
| 3:C:91:HIS:HB2    | 3:C:96:SER:HB3    | 1.97                     | 0.47              |
| 3:C:235:VAL:HG21  | 8:J:6:ARG:HH21    | 1.79                     | 0.47              |
| 12:T:16:DC:H2''   | 12:T:17:DC:C6     | 2.49                     | 0.47              |
| 1:A:79:GLY:C      | 1:A:243:PRO:HG2   | 2.39                     | 0.47              |
| 1:A:1035:TYR:O    | 1:A:1037:LEU:N    | 2.48                     | 0.47              |
| 9:K:18:LYS:C      | 9:K:19:LEU:HD23   | 2.40                     | 0.47              |
| 1:A:423:ASP:CG    | 1:A:424:ILE:N     | 2.73                     | 0.47              |
| 1:A:1441:PHE:HE1  | 5:F:92:ARG:HD3    | 1.80                     | 0.47              |
| 2:B:296:GLU:O     | 2:B:300:HIS:CD2   | 2.68                     | 0.47              |
| 3:C:40:GLU:HA     | 3:C:163:ILE:HG21  | 1.96                     | 0.47              |
| 1:A:472:LEU:HD11  | 2:B:835:GLN:HE22  | 1.80                     | 0.47              |
| 1:A:784:LEU:C     | 1:A:786:HIS:H     | 2.23                     | 0.47              |
| 1:A:908:LEU:CD1   | 1:A:983:ILE:HD11  | 2.45                     | 0.47              |
| 1:A:1097:GLY:C    | 1:A:1099:PRO:HD2  | 2.40                     | 0.47              |
| 2:B:470:LYS:O     | 2:B:471:LYS:HG3   | 2.15                     | 0.47              |
| 3:C:58:LEU:HD21   | 8:J:57:ILE:HD13   | 1.95                     | 0.47              |
| 5:F:147:SER:C     | 5:F:149:GLU:N     | 2.71                     | 0.47              |
| 1:A:385:ILE:O     | 1:A:388:LEU:N     | 2.48                     | 0.46              |
| 1:A:783:THR:CG2   | 1:A:815:PHE:CE2   | 2.89                     | 0.46              |
| 2:B:981:ALA:O     | 2:B:982:SER:C     | 2.57                     | 0.46              |
| 2:B:1051:THR:O    | 2:B:1055:ILE:HG12 | 2.15                     | 0.46              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:N      | 2.14                     | 0.46              |
| 6:H:84:ALA:HA     | 6:H:87:ARG:HB2    | 1.96                     | 0.46              |
| 12:T:7:DA:OP2     | 12:T:7:DA:H2'     | 2.15                     | 0.46              |
| 1:A:1154:TYR:CE1  | 7:I:18:GLU:HG3    | 2.50                     | 0.46              |
| 2:B:44:VAL:O      | 2:B:45:SER:C      | 2.57                     | 0.46              |
| 2:B:65:GLU:H      | 2:B:67:SER:HB3    | 1.79                     | 0.46              |
| 2:B:175:ARG:CG    | 2:B:175:ARG:NH1   | 2.48                     | 0.46              |
| 2:B:236:HIS:NE2   | 2:B:389:ALA:HA    | 2.30                     | 0.46              |
| 2:B:269:ILE:CD1   | 2:B:386:LEU:HD21  | 2.45                     | 0.46              |
| 2:B:984:HIS:CD2   | 2:B:1024:ALA:HB3  | 2.50                     | 0.46              |
| 3:C:10:ILE:HG12   | 9:K:108:GLU:HB3   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:131:HIS:O    | 3:C:132:PRO:C    | 2.59                     | 0.46              |
| 1:A:7:SER:HB3    | 2:B:1193:GLN:OE1 | 2.15                     | 0.46              |
| 1:A:440:ASP:O    | 1:A:459:ARG:HA   | 2.15                     | 0.46              |
| 1:A:528:LEU:HA   | 1:A:531:ILE:HG22 | 1.96                     | 0.46              |
| 2:B:619:ILE:HG13 | 7:I:65:ASP:HB2   | 1.96                     | 0.46              |
| 2:B:807:ARG:CG   | 2:B:807:ARG:NH1  | 2.72                     | 0.46              |
| 3:C:61:GLU:HA    | 3:C:64:ALA:HB3   | 1.96                     | 0.46              |
| 1:A:343:LYS:NZ   | 2:B:1197:PRO:HB3 | 2.30                     | 0.46              |
| 1:A:384:ASN:O    | 1:A:385:ILE:C    | 2.59                     | 0.46              |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:NH1 | 2.52                     | 0.46              |
| 2:B:956:THR:HA   | 2:B:961:LEU:O    | 2.15                     | 0.46              |
| 4:E:153:HIS:O    | 4:E:154:ILE:HD13 | 2.16                     | 0.46              |
| 9:K:18:LYS:HE3   | 9:K:38:GLU:CG    | 2.45                     | 0.46              |
| 9:K:38:GLU:CD    | 9:K:42:LEU:HD22  | 2.41                     | 0.46              |
| 1:A:92:HIS:HE1   | 2:B:1211:ASN:HB3 | 1.81                     | 0.46              |
| 1:A:397:ASN:OD1  | 1:A:397:ASN:N    | 2.49                     | 0.46              |
| 1:A:943:LEU:O    | 1:A:946:VAL:N    | 2.45                     | 0.46              |
| 1:A:1209:MET:HE3 | 1:A:1228:TRP:HB2 | 1.96                     | 0.46              |
| 1:A:1407:GLU:O   | 1:A:1411:GLU:HG2 | 2.16                     | 0.46              |
| 3:C:29:MET:HE2   | 9:K:94:ILE:HG23  | 1.96                     | 0.46              |
| 3:C:46:ILE:CG2   | 3:C:157:CYS:HB3  | 2.46                     | 0.46              |
| 6:H:109:LYS:NZ   | 6:H:111:LEU:HD12 | 2.30                     | 0.46              |
| 1:A:55:ASP:H     | 1:A:56:PRO:HD2   | 1.81                     | 0.46              |
| 1:A:345:VAL:HG11 | 2:B:1150:ARG:O   | 2.16                     | 0.46              |
| 1:A:419:LYS:HG3  | 1:A:420:ARG:HG3  | 1.98                     | 0.46              |
| 1:A:988:LEU:HD23 | 1:A:988:LEU:O    | 2.15                     | 0.46              |
| 3:C:99:LEU:HD12  | 3:C:118:LEU:HD22 | 1.96                     | 0.46              |
| 1:A:250:ILE:HB   | 1:A:253:ASN:HD21 | 1.80                     | 0.46              |
| 1:A:384:ASN:OD1  | 1:A:385:ILE:N    | 2.49                     | 0.46              |
| 1:A:508:PRO:HA   | 1:A:511:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:856:THR:O    | 1:A:856:THR:HG22 | 2.16                     | 0.46              |
| 1:A:1278:ASN:O   | 1:A:1310:GLY:HA3 | 2.16                     | 0.46              |
| 2:B:755:ILE:HD11 | 2:B:812:LEU:HD12 | 1.98                     | 0.46              |
| 2:B:867:GLY:C    | 2:B:869:SER:H    | 2.24                     | 0.46              |
| 2:B:973:ILE:HG22 | 2:B:974:PRO:HD2  | 1.97                     | 0.46              |
| 3:C:77:ILE:HD12  | 3:C:161:LYS:HE3  | 1.97                     | 0.46              |
| 9:K:43:GLY:HA3   | 9:K:71:PHE:CE1   | 2.50                     | 0.46              |
| 10:L:32:ALA:HB3  | 10:L:55:ILE:HD12 | 1.98                     | 0.46              |
| 12:T:8:DT:H2"    | 12:T:9:DA:OP2    | 2.16                     | 0.46              |
| 12:T:13:DA:H2"   | 12:T:14:DC:OP2   | 2.16                     | 0.46              |
| 1:A:230:ARG:HD2  | 1:A:233:TRP:CH2  | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:679:ILE:HD11  | 1:A:733:ALA:HB2   | 1.98                     | 0.46              |
| 1:A:809:THR:HB    | 1:A:810:PRO:CD    | 2.45                     | 0.46              |
| 1:A:1076:ALA:HA   | 1:A:1079:MET:HG3  | 1.97                     | 0.46              |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:H    | 1.81                     | 0.46              |
| 1:A:1352:VAL:O    | 1:A:1355:VAL:HG12 | 2.16                     | 0.46              |
| 2:B:322:PHE:O     | 2:B:322:PHE:CG    | 2.68                     | 0.46              |
| 2:B:473:MET:C     | 2:B:475:SER:H     | 2.24                     | 0.46              |
| 2:B:478:GLY:O     | 2:B:481:GLN:HG3   | 2.16                     | 0.46              |
| 2:B:636:PRO:HB3   | 2:B:743:ILE:HD12  | 1.98                     | 0.46              |
| 8:J:1:MET:H1      | 8:J:57:ILE:N      | 2.13                     | 0.46              |
| 1:A:332:LYS:C     | 1:A:334:GLY:H     | 2.24                     | 0.46              |
| 1:A:445:ASN:ND2   | 1:A:446:ARG:N     | 2.64                     | 0.46              |
| 1:A:472:LEU:HD21  | 2:B:835:GLN:HB3   | 1.98                     | 0.46              |
| 2:B:179:CYS:O     | 2:B:182:SER:OG    | 2.26                     | 0.46              |
| 2:B:701:ILE:HB    | 2:B:740:HIS:CE1   | 2.50                     | 0.46              |
| 3:C:17:ASN:OD1    | 3:C:233:GLU:HG3   | 2.16                     | 0.46              |
| 3:C:57:VAL:HG11   | 8:J:60:PHE:CB     | 2.45                     | 0.46              |
| 1:A:518:LYS:HE2   | 1:A:624:SER:O     | 2.16                     | 0.46              |
| 2:B:34:ILE:HD13   | 2:B:542:MET:CE    | 2.46                     | 0.46              |
| 2:B:364:ILE:HD13  | 2:B:585:VAL:HG13  | 1.98                     | 0.46              |
| 2:B:411:PRO:HA    | 2:B:414:ALA:HB3   | 1.98                     | 0.46              |
| 2:B:459:TYR:HD2   | 2:B:459:TYR:O     | 1.97                     | 0.46              |
| 2:B:978:ASP:HB2   | 2:B:980:PHE:HE1   | 1.80                     | 0.46              |
| 3:C:102:GLN:HG2   | 3:C:154:LYS:CD    | 2.46                     | 0.46              |
| 8:J:1:MET:O       | 8:J:2:ILE:O       | 2.34                     | 0.46              |
| 1:A:474:VAL:HG22  | 1:A:478:TYR:CE1   | 2.51                     | 0.45              |
| 1:A:770:VAL:C     | 1:A:772:GLY:H     | 2.22                     | 0.45              |
| 1:A:898:ARG:NH1   | 1:A:930:ASP:OD1   | 2.41                     | 0.45              |
| 6:H:14:GLU:HB2    | 6:H:27:GLU:HB3    | 1.98                     | 0.45              |
| 1:A:371:ALA:HA    | 1:A:436:ILE:HG22  | 1.99                     | 0.45              |
| 1:A:423:ASP:O     | 1:A:424:ILE:HB    | 2.16                     | 0.45              |
| 1:A:697:ALA:HB2   | 1:A:702:LEU:HG    | 1.98                     | 0.45              |
| 1:A:1170:ILE:HD13 | 1:A:1170:ILE:HA   | 1.88                     | 0.45              |
| 3:C:12:GLU:HB2    | 3:C:19:ASP:HB3    | 1.97                     | 0.45              |
| 8:J:38:ARG:HE     | 8:J:38:ARG:HB2    | 1.59                     | 0.45              |
| 1:A:407:ARG:HG2   | 1:A:430:TRP:CZ2   | 2.51                     | 0.45              |
| 1:A:672:ASP:HB2   | 1:A:736:ASN:CG    | 2.41                     | 0.45              |
| 1:A:1150:SER:O    | 1:A:1151:GLU:HG3  | 2.16                     | 0.45              |
| 2:B:704:ALA:H     | 2:B:741:CYS:HA    | 1.81                     | 0.45              |
| 2:B:839:MET:HB3   | 2:B:1012:ILE:HG22 | 1.98                     | 0.45              |
| 2:B:973:ILE:CG2   | 2:B:974:PRO:HD2   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:265:MET:C     | 3:C:267:GLN:H     | 2.23                     | 0.45              |
| 4:E:213:ILE:HG12  | 4:E:214:CYS:N     | 2.31                     | 0.45              |
| 1:A:568:PRO:HB2   | 6:H:46:LEU:HD22   | 1.97                     | 0.45              |
| 1:A:816:HIS:ND1   | 2:B:764:SER:HB2   | 2.31                     | 0.45              |
| 1:A:828:ALA:O     | 16:T:29:C7P:H3    | 2.17                     | 0.45              |
| 1:A:845:LEU:O     | 1:A:846:GLU:C     | 2.59                     | 0.45              |
| 1:A:1072:ILE:HD11 | 1:A:1368:MET:HA   | 1.98                     | 0.45              |
| 2:B:616:ILE:HD12  | 2:B:625:LYS:O     | 2.16                     | 0.45              |
| 2:B:801:LYS:O     | 2:B:801:LYS:CG    | 2.65                     | 0.45              |
| 2:B:833:TYR:HH    | 9:K:65:HIS:CD2    | 2.34                     | 0.45              |
| 2:B:848:ARG:NH1   | 8:J:8:PHE:O       | 2.49                     | 0.45              |
| 2:B:852:ARG:NH2   | 10:L:70:ARG:O     | 2.49                     | 0.45              |
| 4:E:205:SER:O     | 4:E:205:SER:OG    | 2.32                     | 0.45              |
| 1:A:554:PRO:HG3   | 1:A:651:LYS:HE3   | 1.98                     | 0.45              |
| 1:A:1193:LEU:C    | 1:A:1193:LEU:HD12 | 2.40                     | 0.45              |
| 1:A:1193:LEU:HB2  | 1:A:1260:LEU:HD21 | 1.98                     | 0.45              |
| 2:B:459:TYR:CD2   | 2:B:459:TYR:O     | 2.69                     | 0.45              |
| 2:B:640:VAL:HB    | 2:B:739:THR:O     | 2.17                     | 0.45              |
| 3:C:100:THR:HG23  | 3:C:155:LEU:O     | 2.17                     | 0.45              |
| 3:C:116:LYS:HB2   | 3:C:140:ASN:HA    | 1.98                     | 0.45              |
| 4:E:23:VAL:HG12   | 4:E:28:TYR:HB2    | 1.98                     | 0.45              |
| 4:E:147:HIS:O     | 4:E:148:GLU:C     | 2.59                     | 0.45              |
| 9:K:58:PHE:O      | 9:K:75:ILE:HA     | 2.17                     | 0.45              |
| 1:A:35:ILE:HG13   | 1:A:241:VAL:HG21  | 1.98                     | 0.45              |
| 1:A:335:ARG:HA    | 1:A:339:ASN:HB2   | 1.99                     | 0.45              |
| 2:B:402:GLY:CA    | 2:B:695:ALA:HB3   | 2.46                     | 0.45              |
| 2:B:514:LEU:HD12  | 2:B:518:HIS:HD2   | 1.80                     | 0.45              |
| 2:B:681:TRP:O     | 2:B:684:LEU:HB2   | 2.16                     | 0.45              |
| 3:C:91:HIS:ND1    | 3:C:158:VAL:HG11  | 2.32                     | 0.45              |
| 6:H:6:PHE:CG      | 6:H:7:ASP:N       | 2.84                     | 0.45              |
| 1:A:954:TRP:HE3   | 1:A:955:PRO:HD2   | 1.82                     | 0.45              |
| 1:A:993:LEU:O     | 1:A:996:ASN:ND2   | 2.50                     | 0.45              |
| 1:A:1021:LEU:O    | 1:A:1024:SER:N    | 2.50                     | 0.45              |
| 2:B:476:ARG:C     | 2:B:478:GLY:H     | 2.24                     | 0.45              |
| 2:B:517:THR:C     | 2:B:519:TRP:H     | 2.25                     | 0.45              |
| 2:B:542:MET:HG3   | 2:B:747:MET:CE    | 2.40                     | 0.45              |
| 8:J:44:TYR:HA     | 8:J:47:ARG:HB2    | 1.99                     | 0.45              |
| 1:A:324:SER:O     | 1:A:326:ARG:N     | 2.50                     | 0.45              |
| 1:A:341:MET:HE1   | 2:B:1135:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:660:ASN:C     | 1:A:660:ASN:HD22  | 2.25                     | 0.45              |
| 2:B:108:VAL:HG12  | 2:B:109:THR:N     | 2.31                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:238:ALA:HB3  | 2:B:256:VAL:HB    | 1.99                     | 0.45              |
| 2:B:766:ARG:HE   | 2:B:1020:ARG:HB2  | 1.82                     | 0.45              |
| 3:C:112:ASN:HB3  | 3:C:114:TYR:CE1   | 2.52                     | 0.45              |
| 1:A:14:VAL:H     | 1:A:1432:GLN:NE2  | 2.06                     | 0.45              |
| 1:A:259:GLU:HG2  | 1:A:260:ASP:N     | 2.31                     | 0.45              |
| 1:A:535:THR:HG23 | 1:A:575:LYS:HG2   | 1.99                     | 0.45              |
| 1:A:890:ASP:H    | 1:A:1296:GLY:HA3  | 1.82                     | 0.45              |
| 1:A:1124:HIS:CD2 | 1:A:1124:HIS:H    | 2.35                     | 0.45              |
| 2:B:882:THR:CG2  | 2:B:935:ARG:HA    | 2.46                     | 0.45              |
| 3:C:167:HIS:CE1  | 10:L:70:ARG:HB3   | 2.52                     | 0.45              |
| 4:E:77:SER:CB    | 4:E:105:PHE:HD2   | 2.28                     | 0.45              |
| 1:A:402:ALA:N    | 1:A:435:HIS:CD2   | 2.80                     | 0.44              |
| 1:A:868:TYR:CD2  | 1:A:1058:VAL:HG21 | 2.51                     | 0.44              |
| 1:A:1029:ARG:HG3 | 1:A:1029:ARG:NH1  | 2.30                     | 0.44              |
| 1:A:1119:TYR:HD1 | 1:A:1326:ARG:CB   | 2.30                     | 0.44              |
| 1:A:1150:SER:HA  | 1:A:1195:LEU:HD23 | 1.99                     | 0.44              |
| 2:B:280:ILE:HG22 | 2:B:281:PRO:O     | 2.18                     | 0.44              |
| 1:A:26:GLU:O     | 1:A:30:ILE:HB     | 2.17                     | 0.44              |
| 1:A:203:SER:HB3  | 1:A:206:GLU:HB2   | 1.98                     | 0.44              |
| 1:A:356:ASP:HA   | 1:A:357:PRO:HD2   | 1.72                     | 0.44              |
| 1:A:899:VAL:HG22 | 1:A:1029:ARG:HG3  | 1.99                     | 0.44              |
| 1:A:1019:CYS:HA  | 1:A:1022:LEU:HB3  | 1.99                     | 0.44              |
| 1:A:1349:TYR:C   | 1:A:1351:GLU:N    | 2.71                     | 0.44              |
| 2:B:273:LEU:HD21 | 2:B:360:PHE:CD1   | 2.36                     | 0.44              |
| 2:B:644:GLU:CD   | 2:B:654:ARG:HH12  | 2.25                     | 0.44              |
| 4:E:181:ALA:HA   | 4:E:186:LEU:HD21  | 1.99                     | 0.44              |
| 6:H:6:PHE:HD2    | 6:H:59:ILE:HG12   | 1.82                     | 0.44              |
| 13:N:6:DT:H2"    | 13:N:7:DA:OP2     | 2.17                     | 0.44              |
| 1:A:534:LEU:O    | 1:A:574:GLY:HA3   | 2.16                     | 0.44              |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:H     | 1.83                     | 0.44              |
| 2:B:875:GLU:O    | 2:B:877:PRO:HD3   | 2.17                     | 0.44              |
| 2:B:1060:ARG:HD2 | 2:B:1060:ARG:HA   | 1.65                     | 0.44              |
| 3:C:44:LEU:HD12  | 3:C:160:LYS:O     | 2.17                     | 0.44              |
| 3:C:70:ILE:HD11  | 3:C:144:ILE:HD11  | 1.98                     | 0.44              |
| 1:A:849:MET:HB3  | 1:A:1063:MET:SD   | 2.58                     | 0.44              |
| 1:A:868:TYR:CE1  | 1:A:1064:VAL:HG21 | 2.52                     | 0.44              |
| 1:A:915:SER:O    | 1:A:919:ILE:HG12  | 2.17                     | 0.44              |
| 1:A:1235:LYS:HG2 | 1:A:1237:ILE:HD11 | 2.00                     | 0.44              |
| 2:B:90:ILE:HA    | 2:B:133:LYS:O     | 2.17                     | 0.44              |
| 2:B:241:ARG:HA   | 2:B:253:THR:HG22  | 1.99                     | 0.44              |
| 2:B:1156:ASP:N   | 2:B:1156:ASP:OD2  | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1160:VAL:CG1  | 2:B:1169:MET:HG2  | 2.47                     | 0.44              |
| 6:H:38:LEU:HD13   | 6:H:125:LEU:HD13  | 1.98                     | 0.44              |
| 1:A:304:MET:CG    | 2:B:1210:MET:HG3  | 2.46                     | 0.44              |
| 1:A:779:PHE:CE1   | 1:A:785:PRO:HD3   | 2.52                     | 0.44              |
| 1:A:875:ALA:HB2   | 1:A:1366:ARG:HD2  | 2.00                     | 0.44              |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N    | 2.33                     | 0.44              |
| 1:A:1336:MET:HE3  | 1:A:1380:GLY:HA2  | 1.98                     | 0.44              |
| 2:B:384:ARG:NH1   | 2:B:579:ARG:HH21  | 2.06                     | 0.44              |
| 2:B:840:ILE:O     | 2:B:1010:LEU:HD12 | 2.18                     | 0.44              |
| 3:C:44:LEU:HA     | 3:C:160:LYS:O     | 2.17                     | 0.44              |
| 6:H:7:ASP:O       | 6:H:8:ASP:HB2     | 2.17                     | 0.44              |
| 8:J:1:MET:N       | 8:J:56:LEU:N      | 2.65                     | 0.44              |
| 1:A:68:GLN:C      | 1:A:70:CYS:H      | 2.26                     | 0.44              |
| 1:A:119:ASN:O     | 1:A:123:ARG:HG3   | 2.18                     | 0.44              |
| 1:A:259:GLU:CG    | 1:A:260:ASP:H     | 2.30                     | 0.44              |
| 1:A:851:HIS:HD2   | 1:A:857:ARG:CG    | 2.24                     | 0.44              |
| 1:A:1372:VAL:O    | 1:A:1373:ASP:C    | 2.59                     | 0.44              |
| 3:C:8:VAL:HG21    | 9:K:105:PHE:HB2   | 2.00                     | 0.44              |
| 7:I:15:TYR:HB3    | 7:I:16:PRO:CD     | 2.48                     | 0.44              |
| 1:A:575:LYS:CB    | 1:A:612:ILE:HD11  | 2.37                     | 0.44              |
| 1:A:690:VAL:HG13  | 1:A:718:VAL:CG2   | 2.48                     | 0.44              |
| 2:B:60:GLN:HE22   | 2:B:95:ILE:H      | 1.65                     | 0.44              |
| 2:B:825:VAL:CG2   | 2:B:1010:LEU:HB3  | 2.47                     | 0.44              |
| 2:B:914:LYS:O     | 2:B:914:LYS:HG2   | 2.18                     | 0.44              |
| 6:H:5:LEU:HD22    | 6:H:133:ASN:O     | 2.18                     | 0.44              |
| 9:K:49:GLU:C      | 9:K:51:LEU:H      | 2.26                     | 0.44              |
| 1:A:265:LYS:HE2   | 1:A:303:TYR:HA    | 2.00                     | 0.44              |
| 1:A:348:SER:OG    | 2:B:1128:LEU:HB2  | 2.18                     | 0.44              |
| 1:A:508:PRO:HA    | 1:A:511:ILE:CD1   | 2.48                     | 0.44              |
| 1:A:949:ASP:OD1   | 1:A:949:ASP:N     | 2.48                     | 0.44              |
| 2:B:723:VAL:O     | 2:B:724:ASP:C     | 2.60                     | 0.44              |
| 2:B:884:ARG:O     | 2:B:936:ASP:CB    | 2.63                     | 0.44              |
| 7:I:63:GLY:HA2    | 7:I:104:LEU:HD21  | 1.98                     | 0.44              |
| 1:A:92:HIS:CD2    | 1:A:92:HIS:O      | 2.71                     | 0.44              |
| 1:A:219:PHE:CE2   | 1:A:231:PRO:HD2   | 2.52                     | 0.44              |
| 1:A:942:PHE:C     | 1:A:942:PHE:HD2   | 2.22                     | 0.44              |
| 1:A:1120:LEU:HD13 | 1:A:1304:TRP:O    | 2.18                     | 0.44              |
| 2:B:189:LEU:O     | 2:B:192:LEU:N     | 2.47                     | 0.44              |
| 2:B:785:TYR:CE2   | 8:J:60:PHE:CE1    | 3.04                     | 0.44              |
| 2:B:1027:ILE:O    | 2:B:1028:GLU:C    | 2.61                     | 0.44              |
| 6:H:92:ASP:OD2    | 6:H:92:ASP:N      | 2.51                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:I:6:PHE:HB3    | 7:I:12:ASN:O      | 2.17                     | 0.44              |
| 1:A:525:GLN:HB2  | 2:B:835:GLN:OE1   | 2.18                     | 0.43              |
| 1:A:567:LYS:HG3  | 1:A:568:PRO:CD    | 2.48                     | 0.43              |
| 1:A:1317:MET:O   | 1:A:1322:ILE:HD11 | 2.17                     | 0.43              |
| 2:B:800:GLN:CG   | 8:J:52:THR:HG22   | 2.48                     | 0.43              |
| 3:C:5:GLY:O      | 3:C:7:GLN:NE2     | 2.48                     | 0.43              |
| 4:E:28:TYR:HE1   | 4:E:78:LEU:HD13   | 1.79                     | 0.43              |
| 6:H:59:ILE:O     | 6:H:60:ALA:HB3    | 2.17                     | 0.43              |
| 7:I:119:THR:O    | 7:I:120:GLN:HB2   | 2.17                     | 0.43              |
| 8:J:3:VAL:HG21   | 8:J:18:TRP:HB2    | 1.99                     | 0.43              |
| 9:K:40:HIS:HE1   | 9:K:63:VAL:CG2    | 2.31                     | 0.43              |
| 1:A:12:ARG:HB3   | 2:B:1218:THR:HG23 | 2.00                     | 0.43              |
| 1:A:225:ASN:C    | 1:A:225:ASN:HD22  | 2.25                     | 0.43              |
| 1:A:714:PHE:C    | 1:A:714:PHE:CD2   | 2.95                     | 0.43              |
| 1:A:770:VAL:C    | 1:A:772:GLY:N     | 2.75                     | 0.43              |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:CG1  | 2.48                     | 0.43              |
| 2:B:640:VAL:CG2  | 2:B:741:CYS:H     | 2.31                     | 0.43              |
| 2:B:857:ARG:HG2  | 2:B:859:TYR:CE1   | 2.53                     | 0.43              |
| 4:E:167:ARG:HD3  | 4:E:167:ARG:HA    | 1.71                     | 0.43              |
| 10:L:60:ARG:HG3  | 10:L:61:THR:H     | 1.83                     | 0.43              |
| 1:A:504:LEU:HD11 | 5:F:91:ALA:CB     | 2.49                     | 0.43              |
| 1:A:596:THR:O    | 1:A:597:LEU:C     | 2.60                     | 0.43              |
| 2:B:65:GLU:CG    | 2:B:66:ASP:N      | 2.69                     | 0.43              |
| 2:B:1038:SER:HA  | 2:B:1062:HIS:HE1  | 1.83                     | 0.43              |
| 3:C:35:ARG:HD3   | 9:K:41:THR:HA     | 1.99                     | 0.43              |
| 3:C:73:GLN:HE21  | 3:C:75:MET:H      | 1.65                     | 0.43              |
| 6:H:42:ILE:HG21  | 6:H:49:VAL:HG23   | 2.01                     | 0.43              |
| 1:A:872:GLY:O    | 1:A:1058:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:986:ILE:HD11 | 1:A:1032:LEU:HD21 | 2.00                     | 0.43              |
| 2:B:90:ILE:HD13  | 2:B:134:LYS:HA    | 2.00                     | 0.43              |
| 2:B:701:ILE:HD11 | 2:B:703:ILE:HD11  | 1.99                     | 0.43              |
| 2:B:862:GLN:HE21 | 2:B:961:LEU:HD13  | 1.82                     | 0.43              |
| 3:C:56:THR:HG21  | 3:C:145:CYS:HG    | 1.82                     | 0.43              |
| 3:C:210:GLU:HG3  | 3:C:229:TYR:OH    | 2.18                     | 0.43              |
| 6:H:44:VAL:HG12  | 6:H:44:VAL:O      | 2.18                     | 0.43              |
| 1:A:140:THR:HA   | 1:A:143:LYS:HE3   | 2.01                     | 0.43              |
| 1:A:452:LYS:O    | 2:B:1141:HIS:CE1  | 2.67                     | 0.43              |
| 1:A:834:THR:O    | 1:A:836:TYR:N     | 2.51                     | 0.43              |
| 1:A:900:ASP:HA   | 1:A:926:GLN:HE22  | 1.83                     | 0.43              |
| 2:B:628:THR:O    | 2:B:628:THR:HG22  | 2.16                     | 0.43              |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:CB    | 2.40                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:878:GLN:HE21  | 2:B:878:GLN:HB2  | 1.56                     | 0.43              |
| 2:B:1017:ILE:H    | 2:B:1018:PRO:HD3 | 1.82                     | 0.43              |
| 3:C:57:VAL:CG1    | 8:J:60:PHE:HB3   | 2.48                     | 0.43              |
| 1:A:332:LYS:O     | 1:A:334:GLY:N    | 2.51                     | 0.43              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:CE   | 2.44                     | 0.43              |
| 1:A:913:LEU:CD1   | 1:A:914:GLU:H    | 2.31                     | 0.43              |
| 1:A:1021:LEU:HD11 | 1:A:1025:ARG:NH1 | 2.34                     | 0.43              |
| 2:B:25:ILE:CD1    | 2:B:651:LEU:HD12 | 2.49                     | 0.43              |
| 2:B:1196:ILE:HG13 | 2:B:1200:ALA:HB3 | 2.01                     | 0.43              |
| 4:E:24:LYS:HD2    | 4:E:30:ILE:HB    | 2.01                     | 0.43              |
| 5:F:81:THR:HG1    | 5:F:144:GLU:CD   | 2.26                     | 0.43              |
| 1:A:442:VAL:HG12  | 1:A:491:VAL:HG22 | 2.01                     | 0.43              |
| 1:A:511:ILE:HA    | 1:A:521:MET:HE2  | 2.01                     | 0.43              |
| 1:A:896:ARG:HB3   | 1:A:897:TYR:CD1  | 2.54                     | 0.43              |
| 1:A:1206:ASP:OD2  | 1:A:1206:ASP:N   | 2.51                     | 0.43              |
| 2:B:120:ARG:NH1   | 10:L:54:ARG:HD2  | 2.34                     | 0.43              |
| 2:B:190:TYR:CE1   | 8:J:62:ARG:HG2   | 2.54                     | 0.43              |
| 2:B:794:ASN:N     | 2:B:794:ASN:ND2  | 2.64                     | 0.43              |
| 3:C:265:MET:C     | 3:C:267:GLN:N    | 2.77                     | 0.43              |
| 9:K:7:PHE:CD1     | 9:K:7:PHE:C      | 2.97                     | 0.43              |
| 9:K:83:PRO:O      | 9:K:86:ALA:HB3   | 2.19                     | 0.43              |
| 1:A:88:LYS:HA     | 1:A:89:PRO:HD2   | 1.72                     | 0.43              |
| 1:A:432:VAL:O     | 1:A:433:GLU:C    | 2.62                     | 0.43              |
| 1:A:741:ASN:HD22  | 1:A:744:LYS:H    | 1.67                     | 0.43              |
| 2:B:357:GLN:HA    | 2:B:374:LYS:NZ   | 2.34                     | 0.43              |
| 2:B:783:THR:HB    | 8:J:63:TYR:OH    | 2.18                     | 0.43              |
| 2:B:845:SER:HB2   | 8:J:8:PHE:HB3    | 2.00                     | 0.43              |
| 2:B:941:LEU:O     | 2:B:942:ARG:O    | 2.37                     | 0.43              |
| 2:B:1149:GLU:C    | 2:B:1151:LEU:H   | 2.26                     | 0.43              |
| 4:E:185:ALA:HA    | 4:E:190:LEU:HD23 | 1.99                     | 0.43              |
| 1:A:565:ILE:CG2   | 1:A:567:LYS:HG2  | 2.46                     | 0.43              |
| 1:A:842:VAL:HG11  | 2:B:1136:ASP:CG  | 2.43                     | 0.43              |
| 1:A:878:ILE:HG21  | 1:A:955:PRO:HB2  | 2.01                     | 0.43              |
| 2:B:46:GLN:OE1    | 2:B:408:LEU:HD21 | 2.17                     | 0.43              |
| 2:B:308:TRP:HA    | 2:B:311:LEU:HD12 | 2.00                     | 0.43              |
| 2:B:516:ASN:H     | 2:B:516:ASN:ND2  | 2.15                     | 0.43              |
| 2:B:563:MET:O     | 2:B:563:MET:HG3  | 2.16                     | 0.43              |
| 3:C:53:THR:O      | 3:C:153:LEU:HA   | 2.19                     | 0.43              |
| 4:E:213:ILE:HG12  | 4:E:214:CYS:H    | 1.84                     | 0.43              |
| 6:H:131:ASN:C     | 6:H:133:ASN:H    | 2.27                     | 0.43              |
| 1:A:168:GLY:O     | 1:A:169:ASN:C    | 2.61                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:218:ASP:O     | 1:A:222:LEU:CD1   | 2.65                     | 0.43              |
| 1:A:784:LEU:HB3   | 1:A:786:HIS:CD2   | 2.54                     | 0.43              |
| 1:A:895:LYS:HE3   | 1:A:895:LYS:HB2   | 1.73                     | 0.43              |
| 1:A:919:ILE:HD12  | 1:A:925:LEU:HD12  | 1.99                     | 0.43              |
| 1:A:1037:LEU:HD22 | 1:A:1042:PHE:HA   | 2.01                     | 0.43              |
| 1:A:1063:MET:HG3  | 1:A:1436:ILE:HG23 | 1.99                     | 0.43              |
| 1:A:1128:GLN:O    | 1:A:1131:ALA:HB3  | 2.19                     | 0.43              |
| 1:A:1202:MET:HE1  | 1:A:1212:VAL:HG21 | 2.00                     | 0.43              |
| 2:B:189:LEU:O     | 2:B:190:TYR:C     | 2.59                     | 0.43              |
| 2:B:190:TYR:CD1   | 8:J:62:ARG:HG2    | 2.54                     | 0.43              |
| 2:B:408:LEU:CG    | 2:B:409:ALA:H     | 2.32                     | 0.43              |
| 2:B:638:PHE:CD2   | 2:B:653:VAL:HG21  | 2.54                     | 0.43              |
| 2:B:640:VAL:CG2   | 2:B:740:HIS:HA    | 2.45                     | 0.43              |
| 2:B:884:ARG:NH1   | 2:B:935:ARG:HE    | 2.17                     | 0.43              |
| 2:B:952:VAL:HG22  | 2:B:966:VAL:HG13  | 2.01                     | 0.43              |
| 3:C:235:VAL:HG21  | 8:J:6:ARG:NH2     | 2.33                     | 0.43              |
| 6:H:24:CYS:HB2    | 6:H:44:VAL:CG2    | 2.49                     | 0.43              |
| 6:H:31:THR:O      | 6:H:32:THR:CB     | 2.67                     | 0.43              |
| 1:A:125:ALA:O     | 1:A:134:ARG:HG3   | 2.19                     | 0.42              |
| 1:A:381:THR:CG2   | 1:A:383:TYR:HD1   | 2.31                     | 0.42              |
| 1:A:1127:ASP:HB3  | 1:A:1130:GLN:HB3  | 2.00                     | 0.42              |
| 1:A:1435:PRO:O    | 1:A:1436:ILE:HD12 | 2.18                     | 0.42              |
| 2:B:753:ALA:C     | 2:B:755:ILE:H     | 2.26                     | 0.42              |
| 4:E:29:PHE:C      | 4:E:30:ILE:HD12   | 2.44                     | 0.42              |
| 4:E:85:GLU:HA     | 4:E:86:PRO:HD3    | 1.87                     | 0.42              |
| 1:A:44:THR:O      | 1:A:45:GLN:CB     | 2.66                     | 0.42              |
| 1:A:49:LYS:HZ1    | 1:A:60:SER:HA     | 1.79                     | 0.42              |
| 1:A:347:PHE:HE2   | 1:A:375:THR:HG22  | 1.83                     | 0.42              |
| 1:A:586:ILE:HD11  | 1:A:637:LYS:HG3   | 2.01                     | 0.42              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:CG2   | 2.67                     | 0.42              |
| 1:A:867:ILE:HG22  | 1:A:872:GLY:HA2   | 2.01                     | 0.42              |
| 2:B:756:ILE:HG12  | 2:B:770:GLN:CG    | 2.48                     | 0.42              |
| 2:B:788:ARG:HH12  | 2:B:790:ASP:CG    | 2.27                     | 0.42              |
| 2:B:1079:LYS:HE3  | 3:C:188:HIS:ND1   | 2.35                     | 0.42              |
| 4:E:13:TRP:CD2    | 4:E:39:LEU:HD13   | 2.54                     | 0.42              |
| 1:A:709:THR:HG23  | 7:I:94:ASP:HA     | 2.01                     | 0.42              |
| 1:A:868:TYR:CE2   | 1:A:1366:ARG:CD   | 2.88                     | 0.42              |
| 2:B:859:TYR:OH    | 2:B:941:LEU:HD22  | 2.19                     | 0.42              |
| 3:C:148:ARG:HB3   | 3:C:151:GLN:HG3   | 2.01                     | 0.42              |
| 4:E:64:PRO:HG2    | 4:E:69:ILE:HD11   | 2.01                     | 0.42              |
| 1:A:350:ARG:HA    | 1:A:487:MET:O     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:443:LEU:HD11  | 2:B:1138:MET:SD   | 2.59                     | 0.42              |
| 1:A:503:GLN:C     | 1:A:504:LEU:HD12  | 2.45                     | 0.42              |
| 1:A:690:VAL:HG13  | 1:A:718:VAL:HG21  | 2.01                     | 0.42              |
| 1:A:1144:LYS:HE3  | 2:B:262:GLU:OE2   | 2.20                     | 0.42              |
| 2:B:862:GLN:HG3   | 2:B:963:PHE:HD1   | 1.83                     | 0.42              |
| 2:B:979:LYS:HG2   | 2:B:1095:LEU:HD12 | 2.02                     | 0.42              |
| 2:B:1106:ARG:HD3  | 2:B:1127:GLY:CA   | 2.50                     | 0.42              |
| 2:B:1115:THR:C    | 2:B:1117:GLN:N    | 2.77                     | 0.42              |
| 4:E:199:ILE:O     | 4:E:199:ILE:CG2   | 2.66                     | 0.42              |
| 8:J:43:ARG:HG3    | 8:J:46:CYS:HB2    | 2.02                     | 0.42              |
| 1:A:388:LEU:O     | 1:A:391:LEU:N     | 2.52                     | 0.42              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:N     | 2.31                     | 0.42              |
| 1:A:779:PHE:CZ    | 2:B:517:THR:HA    | 2.54                     | 0.42              |
| 1:A:1406:VAL:HG12 | 1:A:1407:GLU:OE2  | 2.19                     | 0.42              |
| 2:B:54:PHE:O      | 2:B:56:ASP:N      | 2.53                     | 0.42              |
| 2:B:273:LEU:HD23  | 2:B:274:PRO:HD2   | 2.02                     | 0.42              |
| 2:B:641:GLU:C     | 2:B:643:ASP:H     | 2.27                     | 0.42              |
| 3:C:32:SER:HA     | 3:C:35:ARG:HG3    | 2.01                     | 0.42              |
| 9:K:18:LYS:HE3    | 9:K:38:GLU:HG2    | 2.01                     | 0.42              |
| 1:A:91:PHE:H      | 1:A:297:GLN:NE2   | 2.17                     | 0.42              |
| 1:A:565:ILE:HG23  | 1:A:567:LYS:CE    | 2.50                     | 0.42              |
| 1:A:765:VAL:HG23  | 1:A:800:VAL:HB    | 1.97                     | 0.42              |
| 1:A:1015:VAL:CG1  | 1:A:1019:CYS:SG   | 3.01                     | 0.42              |
| 2:B:65:GLU:N      | 2:B:67:SER:HB3    | 2.33                     | 0.42              |
| 2:B:770:GLN:HG2   | 2:B:983:ARG:O     | 2.20                     | 0.42              |
| 2:B:874:PHE:CE1   | 2:B:964:VAL:CG2   | 3.02                     | 0.42              |
| 3:C:112:ASN:ND2   | 3:C:146:LYS:HG2   | 2.34                     | 0.42              |
| 3:C:129:ILE:CG2   | 3:C:130:GLY:N     | 2.82                     | 0.42              |
| 6:H:32:THR:HG22   | 6:H:33:GLN:HG2    | 2.01                     | 0.42              |
| 6:H:42:ILE:HG21   | 6:H:49:VAL:CG2    | 2.50                     | 0.42              |
| 7:I:7:CYS:SG      | 7:I:8:ARG:O       | 2.77                     | 0.42              |
| 8:J:10:CYS:SG     | 8:J:43:ARG:HD3    | 2.59                     | 0.42              |
| 11:R:3:G:N2       | 12:T:27:DA:H1'    | 2.32                     | 0.42              |
| 1:A:116:ASP:C     | 1:A:118:HIS:H     | 2.27                     | 0.42              |
| 1:A:709:THR:CG2   | 7:I:94:ASP:HA     | 2.48                     | 0.42              |
| 1:A:801:GLU:HG2   | 1:A:801:GLU:O     | 2.19                     | 0.42              |
| 1:A:857:ARG:HB3   | 1:A:863:VAL:HA    | 2.01                     | 0.42              |
| 2:B:277:LYS:H     | 2:B:277:LYS:HD2   | 1.84                     | 0.42              |
| 2:B:472:ALA:O     | 2:B:474:SER:N     | 2.52                     | 0.42              |
| 2:B:477:ALA:HB1   | 2:B:499:ASN:HD21  | 1.85                     | 0.42              |
| 2:B:640:VAL:O     | 2:B:641:GLU:C     | 2.62                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:183:TRP:CD1  | 3:C:183:TRP:H     | 2.38                     | 0.42              |
| 4:E:36:GLU:O     | 4:E:38:PRO:HD3    | 2.20                     | 0.42              |
| 4:E:61:GLN:HB3   | 4:E:79:TRP:CE3    | 2.55                     | 0.42              |
| 4:E:152:LYS:HG3  | 4:E:154:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:503:GLN:NE2  | 5:F:90:ARG:HH21   | 2.18                     | 0.42              |
| 1:A:542:GLU:O    | 1:A:546:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:575:LYS:HB3  | 1:A:612:ILE:CG1   | 2.49                     | 0.42              |
| 1:A:784:LEU:HB3  | 1:A:786:HIS:HD2   | 1.85                     | 0.42              |
| 1:A:1121:GLU:CG  | 1:A:1122:PRO:HD2  | 2.49                     | 0.42              |
| 2:B:37:PHE:O     | 2:B:38:PHE:CB     | 2.66                     | 0.42              |
| 2:B:835:GLN:HA   | 2:B:1013:ASN:HD22 | 1.85                     | 0.42              |
| 2:B:1115:THR:C   | 2:B:1117:GLN:H    | 2.27                     | 0.42              |
| 3:C:91:HIS:CG    | 3:C:158:VAL:HG11  | 2.54                     | 0.42              |
| 5:F:82:THR:C     | 5:F:84:TYR:H      | 2.28                     | 0.42              |
| 8:J:8:PHE:CD1    | 8:J:49:MET:HE1    | 2.54                     | 0.42              |
| 1:A:387:ARG:HE   | 1:A:387:ARG:HB3   | 1.61                     | 0.42              |
| 1:A:399:HIS:CB   | 1:A:400:PRO:HD3   | 2.47                     | 0.42              |
| 1:A:407:ARG:CD   | 1:A:413:ILE:HD11  | 2.35                     | 0.42              |
| 1:A:705:LYS:HG3  | 1:A:713:SER:CB    | 2.50                     | 0.42              |
| 2:B:361:LEU:O    | 2:B:363:HIS:O     | 2.38                     | 0.42              |
| 2:B:851:PHE:HB3  | 2:B:1094:ARG:HD2  | 2.01                     | 0.42              |
| 2:B:1175:LEU:O   | 2:B:1176:ASN:HB3  | 2.20                     | 0.42              |
| 3:C:18:VAL:HG22  | 3:C:240:VAL:HB    | 2.01                     | 0.42              |
| 3:C:39:ALA:CA    | 3:C:164:ALA:HB3   | 2.48                     | 0.42              |
| 3:C:167:HIS:CD2  | 3:C:167:HIS:C     | 2.95                     | 0.42              |
| 6:H:82:PRO:O     | 6:H:83:GLN:CB     | 2.68                     | 0.42              |
| 7:I:65:ASP:HA    | 7:I:66:PRO:HD3    | 1.87                     | 0.42              |
| 9:K:6:ARG:HB3    | 9:K:6:ARG:HH11    | 1.85                     | 0.42              |
| 13:N:9:DG:H2''   | 13:N:10:DG:C8     | 2.55                     | 0.42              |
| 1:A:368:LYS:HB2  | 1:A:368:LYS:HE2   | 1.82                     | 0.42              |
| 1:A:810:PRO:HA   | 2:B:1047:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N     | 2.34                     | 0.42              |
| 1:A:1313:LEU:C   | 1:A:1315:GLU:N    | 2.78                     | 0.42              |
| 2:B:273:LEU:HB2  | 2:B:276:ILE:HD12  | 2.02                     | 0.42              |
| 2:B:890:TYR:O    | 2:B:893:LEU:HD12  | 2.20                     | 0.42              |
| 2:B:1095:LEU:C   | 2:B:1096:ARG:O    | 2.61                     | 0.42              |
| 3:C:261:ALA:HA   | 3:C:264:GLN:NE2   | 2.35                     | 0.42              |
| 8:J:43:ARG:HB3   | 8:J:43:ARG:CZ     | 2.50                     | 0.42              |
| 12:T:14:DC:H2''  | 12:T:15:DC:OP2    | 2.19                     | 0.42              |
| 1:A:112:LYS:NZ   | 1:A:164:ARG:HD2   | 2.35                     | 0.41              |
| 1:A:413:ILE:H    | 1:A:413:ILE:HD13  | 1.80                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:874:ASP:CA    | 1:A:1058:VAL:HG22 | 2.50                     | 0.41              |
| 1:A:898:ARG:O     | 1:A:1029:ARG:NH1  | 2.53                     | 0.41              |
| 2:B:235:SER:HB3   | 2:B:261:ARG:HA    | 2.01                     | 0.41              |
| 2:B:542:MET:HE1   | 2:B:743:ILE:HG21  | 2.00                     | 0.41              |
| 2:B:769:TYR:O     | 2:B:771:SER:N     | 2.53                     | 0.41              |
| 3:C:196:ASP:O     | 3:C:197:SER:C     | 2.63                     | 0.41              |
| 4:E:62:ALA:HB3    | 4:E:78:LEU:HB3    | 2.02                     | 0.41              |
| 1:A:261:ASP:CB    | 1:A:323:LYS:HD2   | 2.35                     | 0.41              |
| 1:A:383:TYR:HB3   | 5:F:115:THR:HG22  | 2.03                     | 0.41              |
| 1:A:535:THR:O     | 1:A:575:LYS:HE2   | 2.19                     | 0.41              |
| 1:A:811:GLN:O     | 1:A:812:GLU:C     | 2.62                     | 0.41              |
| 1:A:874:ASP:N     | 1:A:1058:VAL:HG22 | 2.36                     | 0.41              |
| 1:A:955:PRO:O     | 1:A:956:LEU:HG    | 2.20                     | 0.41              |
| 3:C:3:GLU:CG      | 3:C:4:GLU:H       | 2.28                     | 0.41              |
| 8:J:5:VAL:O       | 8:J:6:ARG:O       | 2.39                     | 0.41              |
| 9:K:58:PHE:HE2    | 9:K:74:ARG:NE     | 2.16                     | 0.41              |
| 9:K:63:VAL:HG23   | 9:K:63:VAL:O      | 2.20                     | 0.41              |
| 1:A:268:ASP:HB3   | 1:A:299:HIS:CE1   | 2.55                     | 0.41              |
| 1:A:443:LEU:HD23  | 1:A:444:PHE:N     | 2.35                     | 0.41              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:HE    | 1.85                     | 0.41              |
| 1:A:947:PHE:CE2   | 1:A:954:TRP:CE2   | 3.07                     | 0.41              |
| 1:A:961:ARG:O     | 1:A:965:GLN:HG3   | 2.20                     | 0.41              |
| 1:A:986:ILE:HG21  | 1:A:1028:THR:HA   | 2.02                     | 0.41              |
| 1:A:1131:ALA:HB1  | 1:A:1284:MET:SD   | 2.60                     | 0.41              |
| 1:A:1438:THR:HG23 | 5:F:92:ARG:HD2    | 2.02                     | 0.41              |
| 2:B:475:SER:O     | 2:B:477:ALA:N     | 2.53                     | 0.41              |
| 2:B:634:TYR:CE1   | 2:B:692:TYR:CG    | 3.08                     | 0.41              |
| 2:B:639:ILE:CD1   | 2:B:691:GLU:HB2   | 2.39                     | 0.41              |
| 2:B:797:TYR:HE1   | 2:B:854:LEU:HG    | 1.86                     | 0.41              |
| 2:B:831:SER:OG    | 2:B:994:TYR:OH    | 2.31                     | 0.41              |
| 2:B:1097:HIS:HB3  | 2:B:1102:LYS:HE2  | 2.03                     | 0.41              |
| 3:C:58:LEU:HD11   | 8:J:2:ILE:HD13    | 2.02                     | 0.41              |
| 4:E:14:ARG:NH2    | 4:E:141:VAL:HG12  | 2.34                     | 0.41              |
| 6:H:4:THR:HA      | 6:H:60:ALA:HA     | 2.01                     | 0.41              |
| 9:K:57:LEU:HB2    | 9:K:76:GLN:HG2    | 2.01                     | 0.41              |
| 9:K:77:THR:HG21   | 9:K:86:ALA:HB2    | 2.02                     | 0.41              |
| 10:L:55:ILE:H     | 10:L:55:ILE:HG12  | 1.65                     | 0.41              |
| 1:A:244:PRO:HB2   | 1:A:245:PRO:CD    | 2.48                     | 0.41              |
| 1:A:834:THR:O     | 1:A:837:ILE:N     | 2.54                     | 0.41              |
| 1:A:1171:GLN:HE21 | 1:A:1171:GLN:HB3  | 1.71                     | 0.41              |
| 2:B:28:GLU:CD     | 2:B:807:ARG:HH22  | 2.28                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:383:ASN:HD22 | 2:B:384:ARG:HD2   | 1.84                     | 0.41              |
| 2:B:1033:LYS:HE2 | 2:B:1087:PHE:O    | 2.20                     | 0.41              |
| 3:C:97:VAL:HG21  | 3:C:129:ILE:CG2   | 2.50                     | 0.41              |
| 6:H:94:ASP:N     | 6:H:94:ASP:OD1    | 2.52                     | 0.41              |
| 1:A:18:GLN:HB3   | 2:B:1215:ARG:HB2  | 2.03                     | 0.41              |
| 1:A:56:PRO:O     | 1:A:57:ARG:CB     | 2.68                     | 0.41              |
| 1:A:215:SER:HB3  | 1:A:218:ASP:HB2   | 2.02                     | 0.41              |
| 1:A:382:PRO:CA   | 1:A:428:TYR:HE2   | 2.33                     | 0.41              |
| 1:A:414:ASP:OD1  | 1:A:416:ARG:HG3   | 2.21                     | 0.41              |
| 1:A:709:THR:HB   | 1:A:712:GLU:H     | 1.86                     | 0.41              |
| 2:B:216:GLU:HB2  | 2:B:406:LEU:HD22  | 2.02                     | 0.41              |
| 2:B:493:SER:OG   | 2:B:775:LYS:HE2   | 2.20                     | 0.41              |
| 2:B:562:GLY:HA3  | 2:B:590:HIS:CE1   | 2.55                     | 0.41              |
| 2:B:1100:ASP:OD1 | 9:K:1:MET:HB3     | 2.20                     | 0.41              |
| 4:E:46:TYR:CD2   | 4:E:58:MET:HG2    | 2.55                     | 0.41              |
| 11:R:8:G:C2'     | 11:R:9:G:H5'      | 2.51                     | 0.41              |
| 1:A:244:PRO:C    | 1:A:246:VAL:H     | 2.28                     | 0.41              |
| 1:A:456:MET:HB2  | 1:A:478:TYR:OH    | 2.20                     | 0.41              |
| 1:A:947:PHE:HE2  | 1:A:954:TRP:CD2   | 2.38                     | 0.41              |
| 1:A:1121:GLU:O   | 1:A:1122:PRO:C    | 2.64                     | 0.41              |
| 2:B:360:PHE:HD2  | 2:B:374:LYS:HD3   | 1.86                     | 0.41              |
| 2:B:569:TYR:CD1  | 2:B:589:VAL:HG21  | 2.56                     | 0.41              |
| 4:E:68:SER:C     | 4:E:70:SER:N      | 2.79                     | 0.41              |
| 5:F:85:MET:SD    | 5:F:153:VAL:HG22  | 2.60                     | 0.41              |
| 10:L:40:LEU:HD11 | 10:L:49:LYS:HE2   | 2.03                     | 0.41              |
| 1:A:18:GLN:HB3   | 2:B:1215:ARG:HD2  | 2.02                     | 0.41              |
| 1:A:550:LEU:HD21 | 1:A:561:PRO:CD    | 2.50                     | 0.41              |
| 1:A:963:ILE:HD12 | 1:A:1049:ILE:HG13 | 2.02                     | 0.41              |
| 2:B:217:ARG:NH1  | 2:B:407:ASP:OD1   | 2.54                     | 0.41              |
| 2:B:728:ARG:NH1  | 2:B:760:ASP:OD2   | 2.52                     | 0.41              |
| 3:C:41:ILE:HA    | 3:C:42:PRO:HD3    | 1.92                     | 0.41              |
| 3:C:119:VAL:O    | 3:C:121:VAL:HG23  | 2.19                     | 0.41              |
| 11:R:5:A:C2      | 11:R:6:G:C5       | 3.08                     | 0.41              |
| 1:A:265:LYS:HD2  | 1:A:302:THR:HG23  | 2.02                     | 0.41              |
| 1:A:711:ARG:HG3  | 7:I:97:MET:CE     | 2.50                     | 0.41              |
| 1:A:960:ILE:O    | 1:A:961:ARG:C     | 2.63                     | 0.41              |
| 2:B:181:LEU:H    | 2:B:181:LEU:HG    | 1.53                     | 0.41              |
| 7:I:7:CYS:O      | 7:I:11:ASN:HA     | 2.20                     | 0.41              |
| 1:A:90:VAL:HA    | 1:A:204:THR:HG21  | 2.03                     | 0.41              |
| 1:A:313:GLN:HB3  | 1:A:314:ALA:H     | 1.54                     | 0.41              |
| 1:A:406:ILE:HD11 | 1:A:412:ARG:HH12  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:655:PHE:O     | 1:A:656:TRP:C     | 2.63                     | 0.41              |
| 1:A:1004:ASN:CG   | 4:E:167:ARG:HD2   | 2.45                     | 0.41              |
| 1:A:1158:PRO:HB3  | 1:A:1188:GLN:OE1  | 2.21                     | 0.41              |
| 2:B:228:LYS:NZ    | 2:B:234:ILE:HD11  | 2.36                     | 0.41              |
| 2:B:240:ILE:O     | 2:B:240:ILE:HG23  | 2.21                     | 0.41              |
| 2:B:557:PHE:CD2   | 2:B:557:PHE:C     | 2.99                     | 0.41              |
| 2:B:1023:VAL:O    | 2:B:1023:VAL:HG12 | 2.21                     | 0.41              |
| 2:B:1028:GLU:HG2  | 2:B:1090:THR:HG23 | 2.02                     | 0.41              |
| 2:B:1200:ALA:O    | 2:B:1201:LYS:C    | 2.64                     | 0.41              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:HD13  | 2.02                     | 0.41              |
| 3:C:120:ILE:H     | 3:C:120:ILE:HG12  | 1.57                     | 0.41              |
| 6:H:109:LYS:CB    | 6:H:110:ASP:C     | 2.94                     | 0.41              |
| 7:I:75:CYS:HB3    | 7:I:110:PHE:CE2   | 2.55                     | 0.41              |
| 1:A:25:GLU:O      | 1:A:29:ALA:HB3    | 2.20                     | 0.41              |
| 1:A:80:HIS:H      | 1:A:80:HIS:CD2    | 2.39                     | 0.41              |
| 1:A:116:ASP:C     | 1:A:118:HIS:N     | 2.79                     | 0.41              |
| 1:A:335:ARG:HB3   | 1:A:336:ILE:H     | 1.64                     | 0.41              |
| 1:A:523:ILE:HG22  | 1:A:528:LEU:HB2   | 2.03                     | 0.41              |
| 1:A:1092:LYS:HD3  | 1:A:1092:LYS:HA   | 1.90                     | 0.41              |
| 1:A:1337:GLU:O    | 4:E:183:PRO:HG3   | 2.21                     | 0.41              |
| 2:B:1064:TYR:N    | 2:B:1064:TYR:CD1  | 2.89                     | 0.41              |
| 3:C:41:ILE:HG13   | 3:C:172:PRO:CG    | 2.51                     | 0.41              |
| 3:C:109:SER:O     | 3:C:110:THR:C     | 2.64                     | 0.41              |
| 4:E:24:LYS:HB3    | 4:E:30:ILE:HD13   | 2.02                     | 0.41              |
| 4:E:35:VAL:C      | 4:E:37:LEU:H      | 2.29                     | 0.41              |
| 1:A:15:LYS:HG2    | 2:B:1218:THR:O    | 2.21                     | 0.40              |
| 1:A:99:ILE:O      | 1:A:102:VAL:HG23  | 2.21                     | 0.40              |
| 1:A:362:ASP:OD1   | 1:A:459:ARG:HD3   | 2.21                     | 0.40              |
| 1:A:770:VAL:O     | 1:A:772:GLY:N     | 2.54                     | 0.40              |
| 1:A:1152:ILE:HG23 | 1:A:1260:LEU:HD23 | 2.03                     | 0.40              |
| 1:A:1394:THR:O    | 1:A:1395:GLY:C    | 2.64                     | 0.40              |
| 2:B:101:MET:SD    | 2:B:109:THR:HG23  | 2.60                     | 0.40              |
| 2:B:410:GLY:O     | 2:B:413:LEU:N     | 2.52                     | 0.40              |
| 2:B:915:THR:HB    | 2:B:934:LYS:CB    | 2.52                     | 0.40              |
| 4:E:164:LEU:HD22  | 4:E:211:TYR:CD2   | 2.55                     | 0.40              |
| 6:H:99:GLY:HA3    | 6:H:118:PHE:CD2   | 2.56                     | 0.40              |
| 7:I:26:LEU:HB3    | 7:I:35:VAL:CG1    | 2.51                     | 0.40              |
| 1:A:67:CYS:C      | 1:A:68:GLN:HG3    | 2.47                     | 0.40              |
| 1:A:69:THR:C      | 1:A:71:GLN:H      | 2.28                     | 0.40              |
| 1:A:107:CYS:HB2   | 1:A:114:LEU:CD2   | 2.49                     | 0.40              |
| 1:A:445:ASN:HD22  | 1:A:446:ARG:N     | 2.19                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:451:HIS:CB    | 1:A:454:SER:H     | 2.34                     | 0.40              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:HB3  | 2.02                     | 0.40              |
| 2:B:408:LEU:HD22  | 2:B:545:ILE:CD1   | 2.43                     | 0.40              |
| 2:B:940:PRO:O     | 2:B:941:LEU:C     | 2.62                     | 0.40              |
| 2:B:1001:PHE:HE1  | 3:C:178:PHE:HB3   | 1.86                     | 0.40              |
| 2:B:1010:LEU:HD12 | 2:B:1010:LEU:HA   | 1.70                     | 0.40              |
| 3:C:241:ASP:O     | 3:C:245:VAL:HG23  | 2.22                     | 0.40              |
| 1:A:356:ASP:CB    | 1:A:359:LEU:HD12  | 2.52                     | 0.40              |
| 1:A:475:THR:HG22  | 1:A:476:SER:N     | 2.36                     | 0.40              |
| 2:B:94:LYS:HD2    | 2:B:96:TYR:CE2    | 2.57                     | 0.40              |
| 2:B:849:GLY:CA    | 2:B:852:ARG:HD2   | 2.48                     | 0.40              |
| 6:H:77:ARG:O      | 6:H:78:SER:C      | 2.64                     | 0.40              |
| 10:L:38:LEU:CD2   | 10:L:48:CYS:HA    | 2.52                     | 0.40              |
| 1:A:91:PHE:HB2    | 1:A:297:GLN:HE22  | 1.86                     | 0.40              |
| 1:A:171:GLN:HA    | 1:A:172:PRO:HD3   | 1.84                     | 0.40              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HB    | 2.21                     | 0.40              |
| 1:A:1434:ALA:HB1  | 1:A:1436:ILE:HD13 | 2.01                     | 0.40              |
| 1:A:1438:THR:HG23 | 5:F:92:ARG:HB2    | 2.03                     | 0.40              |
| 2:B:66:ASP:O      | 2:B:67:SER:C      | 2.64                     | 0.40              |
| 3:C:166:GLU:O     | 3:C:167:HIS:HB2   | 2.21                     | 0.40              |
| 6:H:41:ASP:OD2    | 6:H:122:LEU:N     | 2.52                     | 0.40              |
| 6:H:98:TYR:C      | 6:H:118:PHE:HD2   | 2.30                     | 0.40              |
| 7:I:37:GLU:H      | 7:I:37:GLU:HG2    | 1.64                     | 0.40              |
| 1:A:508:PRO:C     | 1:A:511:ILE:HG13  | 2.46                     | 0.40              |
| 1:A:853:ASP:C     | 1:A:855:THR:H     | 2.29                     | 0.40              |
| 1:A:1063:MET:HE3  | 1:A:1063:MET:HB3  | 1.80                     | 0.40              |
| 2:B:242:SER:OG    | 2:B:252:SER:O     | 2.27                     | 0.40              |
| 2:B:284:ILE:HD11  | 2:B:321:GLY:HA2   | 2.02                     | 0.40              |
| 2:B:815:ARG:H     | 2:B:815:ARG:HG2   | 1.42                     | 0.40              |
| 2:B:848:ARG:NE    | 8:J:11:GLY:HA2    | 2.36                     | 0.40              |
| 2:B:1131:GLY:HA3  | 2:B:1134:GLU:OE1  | 2.22                     | 0.40              |
| 4:E:54:GLN:HA     | 4:E:54:GLN:HE21   | 1.87                     | 0.40              |
| 6:H:98:TYR:HD1    | 6:H:141:TYR:CE1   | 2.39                     | 0.40              |
| 9:K:40:HIS:CE1    | 9:K:63:VAL:HG21   | 2.57                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 1383/1733 (80%) | 1080 (78%) | 219 (16%) | 84 (6%)  | 1           | 13 |
| 2   | B     | 1088/1224 (89%) | 855 (79%)  | 169 (16%) | 64 (6%)  | 1           | 13 |
| 3   | C     | 264/318 (83%)   | 213 (81%)  | 38 (14%)  | 13 (5%)  | 1           | 16 |
| 4   | E     | 212/215 (99%)   | 178 (84%)  | 25 (12%)  | 9 (4%)   | 2           | 19 |
| 5   | F     | 82/155 (53%)    | 65 (79%)   | 13 (16%)  | 4 (5%)   | 1           | 16 |
| 6   | H     | 129/146 (88%)   | 97 (75%)   | 19 (15%)  | 13 (10%) | 0           | 6  |
| 7   | I     | 117/122 (96%)   | 87 (74%)   | 21 (18%)  | 9 (8%)   | 1           | 9  |
| 8   | J     | 63/70 (90%)     | 54 (86%)   | 5 (8%)    | 4 (6%)   | 1           | 12 |
| 9   | K     | 112/120 (93%)   | 94 (84%)   | 15 (13%)  | 3 (3%)   | 4           | 26 |
| 10  | L     | 44/70 (63%)     | 26 (59%)   | 14 (32%)  | 4 (9%)   | 0           | 7  |
| All | All   | 3494/4173 (84%) | 2749 (79%) | 538 (15%) | 207 (6%) | 1           | 13 |

All (207) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | ASN  |
| 1   | A     | 56  | PRO  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 214 | ILE  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 257 | ARG  |
| 1   | A     | 312 | PRO  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 321 | PRO  |
| 1   | A     | 335 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 385  | ILE  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 404  | TYR  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 672  | ASP  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 986  | ILE  |
| 1   | A     | 1036 | ARG  |
| 1   | A     | 1062 | GLU  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1335 | ILE  |
| 1   | A     | 1393 | ASN  |
| 2   | B     | 55   | VAL  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 473  | MET  |
| 2   | B     | 476  | ARG  |
| 2   | B     | 480  | SER  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 563  | MET  |
| 2   | B     | 636  | PRO  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 879  | ARG  |
| 2   | B     | 942  | ARG  |
| 2   | B     | 958  | GLN  |
| 2   | B     | 982  | SER  |
| 2   | B     | 1165 | ILE  |
| 3   | C     | 110  | THR  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 184  | ASN  |
| 3   | C     | 215  | GLU  |
| 4   | E     | 3    | GLN  |
| 4   | E     | 59   | SER  |
| 4   | E     | 206  | GLY  |
| 5   | F     | 73   | ALA  |
| 5   | F     | 74   | ILE  |
| 5   | F     | 128  | LYS  |
| 6   | H     | 32   | THR  |
| 6   | H     | 61   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | H     | 77   | ARG  |
| 6   | H     | 82   | PRO  |
| 6   | H     | 90   | ALA  |
| 6   | H     | 135  | LEU  |
| 6   | H     | 140  | ALA  |
| 7   | I     | 9    | ASP  |
| 7   | I     | 15   | TYR  |
| 8   | J     | 2    | ILE  |
| 8   | J     | 6    | ARG  |
| 8   | J     | 8    | PHE  |
| 1   | A     | 45   | GLN  |
| 1   | A     | 50   | ILE  |
| 1   | A     | 55   | ASP  |
| 1   | A     | 248  | PRO  |
| 1   | A     | 254  | GLU  |
| 1   | A     | 258  | GLY  |
| 1   | A     | 336  | ILE  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 609  | ASP  |
| 1   | A     | 610  | GLY  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 824  | LEU  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 983  | ILE  |
| 1   | A     | 1002 | GLY  |
| 1   | A     | 1049 | ILE  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1395 | GLY  |
| 1   | A     | 1437 | GLY  |
| 2   | B     | 100  | PRO  |
| 2   | B     | 264  | SER  |
| 2   | B     | 489  | SER  |
| 2   | B     | 575  | PRO  |
| 2   | B     | 708  | GLU  |
| 2   | B     | 737  | THR  |
| 2   | B     | 738  | PHE  |
| 2   | B     | 774  | GLY  |
| 2   | B     | 1021 | MET  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1181 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | C     | 212  | PRO  |
| 3   | C     | 227  | THR  |
| 4   | E     | 162  | ARG  |
| 5   | F     | 111  | LEU  |
| 6   | H     | 3    | ASN  |
| 6   | H     | 18   | GLY  |
| 6   | H     | 108  | SER  |
| 7   | I     | 3    | THR  |
| 7   | I     | 11   | ASN  |
| 7   | I     | 16   | PRO  |
| 9   | K     | 50   | LEU  |
| 10  | L     | 45   | ALA  |
| 1   | A     | 63   | ARG  |
| 1   | A     | 66   | LYS  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 89   | PRO  |
| 1   | A     | 168  | GLY  |
| 1   | A     | 178  | GLY  |
| 1   | A     | 245  | PRO  |
| 1   | A     | 419  | LYS  |
| 1   | A     | 568  | PRO  |
| 1   | A     | 835  | GLY  |
| 1   | A     | 854  | ASN  |
| 1   | A     | 972  | HIS  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1221 | LYS  |
| 1   | A     | 1270 | ASN  |
| 2   | B     | 38   | PHE  |
| 2   | B     | 67   | SER  |
| 2   | B     | 318  | VAL  |
| 2   | B     | 577  | ALA  |
| 2   | B     | 712  | PRO  |
| 2   | B     | 732  | SER  |
| 2   | B     | 792  | MET  |
| 2   | B     | 869  | SER  |
| 2   | B     | 959  | ASP  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1176 | ASN  |
| 3   | C     | 197  | SER  |
| 3   | C     | 240  | VAL  |
| 4   | E     | 50   | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | H     | 43   | ASN  |
| 6   | H     | 132  | LEU  |
| 7   | I     | 20   | LYS  |
| 9   | K     | 53   | ASP  |
| 10  | L     | 47   | ARG  |
| 1   | A     | 333  | GLU  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 441  | PRO  |
| 1   | A     | 823  | GLY  |
| 1   | A     | 834  | THR  |
| 1   | A     | 1388 | GLY  |
| 2   | B     | 364  | ILE  |
| 2   | B     | 394  | ASP  |
| 2   | B     | 467  | GLY  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 635  | ARG  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 735  | ALA  |
| 2   | B     | 770  | GLN  |
| 2   | B     | 799  | PRO  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 865  | LYS  |
| 2   | B     | 901  | PRO  |
| 2   | B     | 1080 | LYS  |
| 2   | B     | 1178 | ASN  |
| 3   | C     | 267  | GLN  |
| 4   | E     | 148  | GLU  |
| 4   | E     | 183  | PRO  |
| 6   | H     | 131  | ASN  |
| 7   | I     | 34   | TYR  |
| 7   | I     | 42   | LEU  |
| 9   | K     | 10   | PHE  |
| 10  | L     | 56   | LEU  |
| 1   | A     | 324  | SER  |
| 1   | A     | 591  | PHE  |
| 1   | A     | 639  | PRO  |
| 1   | A     | 820  | GLY  |
| 1   | A     | 1174 | PHE  |
| 2   | B     | 54   | PHE  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 363  | HIS  |
| 2   | B     | 410  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 648  | HIS  |
| 2   | B     | 1061 | GLU  |
| 2   | B     | 1143 | ALA  |
| 3   | C     | 174  | ALA  |
| 4   | E     | 86   | PRO  |
| 1   | A     | 578  | LEU  |
| 1   | A     | 987  | VAL  |
| 3   | C     | 88   | CYS  |
| 10  | L     | 59   | ALA  |
| 2   | B     | 1017 | ILE  |
| 7   | I     | 84   | VAL  |
| 1   | A     | 331  | GLY  |
| 1   | A     | 775  | ILE  |
| 1   | A     | 1435 | PRO  |
| 2   | B     | 436  | VAL  |
| 8   | J     | 57   | ILE  |
| 1   | A     | 51   | GLY  |
| 1   | A     | 325  | ILE  |
| 1   | A     | 338  | GLY  |
| 2   | B     | 647  | GLY  |
| 4   | E     | 76   | GLY  |
| 1   | A     | 1384 | VAL  |
| 2   | B     | 724  | ASP  |
| 3   | C     | 130  | GLY  |
| 1   | A     | 948  | VAL  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 1218/1520 (80%) | 973 (80%) | 245 (20%) | 1           | 8  |
| 2   | B     | 960/1061 (90%)  | 756 (79%) | 204 (21%) | 1           | 7  |
| 3   | C     | 234/274 (85%)   | 190 (81%) | 44 (19%)  | 1           | 9  |
| 4   | E     | 196/197 (100%)  | 170 (87%) | 26 (13%)  | 4           | 21 |
| 5   | F     | 74/137 (54%)    | 56 (76%)  | 18 (24%)  | 1           | 5  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 6   | H     | 117/128 (91%)   | 98 (84%)   | 19 (16%)  | 2           | 15 |
| 7   | I     | 113/116 (97%)   | 96 (85%)   | 17 (15%)  | 3           | 17 |
| 8   | J     | 60/65 (92%)     | 47 (78%)   | 13 (22%)  | 1           | 7  |
| 9   | K     | 99/102 (97%)    | 82 (83%)   | 17 (17%)  | 2           | 12 |
| 10  | L     | 40/57 (70%)     | 29 (72%)   | 11 (28%)  | 0           | 3  |
| All | All   | 3111/3657 (85%) | 2497 (80%) | 614 (20%) | 1           | 8  |

All (614) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | THR  |
| 1   | A     | 18  | GLN  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 28  | ARG  |
| 1   | A     | 32  | VAL  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 40  | THR  |
| 1   | A     | 43  | GLU  |
| 1   | A     | 44  | THR  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 63  | ARG  |
| 1   | A     | 67  | CYS  |
| 1   | A     | 68  | GLN  |
| 1   | A     | 69  | THR  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 71  | GLN  |
| 1   | A     | 74  | MET  |
| 1   | A     | 80  | HIS  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 98  | LYS  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 110 | CYS  |
| 1   | A     | 133 | LYS  |
| 1   | A     | 169 | ASN  |
| 1   | A     | 180 | LYS  |
| 1   | A     | 204 | THR  |
| 1   | A     | 206 | GLU  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 214 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 222 | LEU  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 235 | ILE  |
| 1   | A     | 237 | THR  |
| 1   | A     | 239 | LEU  |
| 1   | A     | 247 | ARG  |
| 1   | A     | 249 | SER  |
| 1   | A     | 250 | ILE  |
| 1   | A     | 254 | GLU  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 257 | ARG  |
| 1   | A     | 263 | THR  |
| 1   | A     | 266 | LEU  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 271 | LYS  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 290 | GLU  |
| 1   | A     | 297 | GLN  |
| 1   | A     | 303 | TYR  |
| 1   | A     | 304 | MET  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 307 | ASP  |
| 1   | A     | 308 | ILE  |
| 1   | A     | 313 | GLN  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 318 | SER  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 323 | LYS  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 340 | LEU  |
| 1   | A     | 354 | SER  |
| 1   | A     | 372 | LYS  |
| 1   | A     | 375 | THR  |
| 1   | A     | 381 | THR  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 387 | ARG  |
| 1   | A     | 389 | THR  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 397 | ASN  |
| 1   | A     | 403 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 413 | ILE  |
| 1   | A     | 416 | ARG  |
| 1   | A     | 419 | LYS  |
| 1   | A     | 433 | GLU  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 436 | ILE  |
| 1   | A     | 438 | ASP  |
| 1   | A     | 450 | LEU  |
| 1   | A     | 454 | SER  |
| 1   | A     | 460 | VAL  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 469 | ARG  |
| 1   | A     | 470 | LEU  |
| 1   | A     | 475 | THR  |
| 1   | A     | 476 | SER  |
| 1   | A     | 486 | GLU  |
| 1   | A     | 494 | SER  |
| 1   | A     | 501 | LEU  |
| 1   | A     | 521 | MET  |
| 1   | A     | 523 | ILE  |
| 1   | A     | 525 | GLN  |
| 1   | A     | 533 | LYS  |
| 1   | A     | 538 | ASP  |
| 1   | A     | 550 | LEU  |
| 1   | A     | 559 | VAL  |
| 1   | A     | 560 | ILE  |
| 1   | A     | 573 | SER  |
| 1   | A     | 576 | GLN  |
| 1   | A     | 577 | ILE  |
| 1   | A     | 578 | LEU  |
| 1   | A     | 582 | ILE  |
| 1   | A     | 590 | ARG  |
| 1   | A     | 593 | GLU  |
| 1   | A     | 596 | THR  |
| 1   | A     | 597 | LEU  |
| 1   | A     | 599 | SER  |
| 1   | A     | 601 | LYS  |
| 1   | A     | 612 | ILE  |
| 1   | A     | 618 | GLU  |
| 1   | A     | 629 | LEU  |
| 1   | A     | 660 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 666 | ILE  |
| 1   | A     | 670 | ILE  |
| 1   | A     | 676 | MET  |
| 1   | A     | 678 | GLU  |
| 1   | A     | 679 | ILE  |
| 1   | A     | 680 | THR  |
| 1   | A     | 695 | LYS  |
| 1   | A     | 702 | LEU  |
| 1   | A     | 709 | THR  |
| 1   | A     | 711 | ARG  |
| 1   | A     | 728 | LYS  |
| 1   | A     | 732 | LEU  |
| 1   | A     | 734 | GLU  |
| 1   | A     | 735 | VAL  |
| 1   | A     | 738 | LYS  |
| 1   | A     | 740 | LEU  |
| 1   | A     | 743 | VAL  |
| 1   | A     | 747 | VAL  |
| 1   | A     | 754 | SER  |
| 1   | A     | 756 | ILE  |
| 1   | A     | 758 | ILE  |
| 1   | A     | 764 | CYS  |
| 1   | A     | 768 | GLN  |
| 1   | A     | 788 | SER  |
| 1   | A     | 795 | GLU  |
| 1   | A     | 800 | VAL  |
| 1   | A     | 806 | ARG  |
| 1   | A     | 809 | THR  |
| 1   | A     | 821 | ARG  |
| 1   | A     | 827 | THR  |
| 1   | A     | 829 | VAL  |
| 1   | A     | 830 | LYS  |
| 1   | A     | 854 | ASN  |
| 1   | A     | 855 | THR  |
| 1   | A     | 856 | THR  |
| 1   | A     | 857 | ARG  |
| 1   | A     | 858 | ASN  |
| 1   | A     | 864 | ILE  |
| 1   | A     | 867 | ILE  |
| 1   | A     | 878 | ILE  |
| 1   | A     | 880 | LYS  |
| 1   | A     | 882 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 884  | ASP  |
| 1   | A     | 886  | ILE  |
| 1   | A     | 895  | LYS  |
| 1   | A     | 896  | ARG  |
| 1   | A     | 902  | LEU  |
| 1   | A     | 908  | LEU  |
| 1   | A     | 911  | SER  |
| 1   | A     | 913  | LEU  |
| 1   | A     | 914  | GLU  |
| 1   | A     | 918  | GLU  |
| 1   | A     | 929  | LEU  |
| 1   | A     | 934  | LYS  |
| 1   | A     | 936  | LEU  |
| 1   | A     | 948  | VAL  |
| 1   | A     | 949  | ASP  |
| 1   | A     | 976  | THR  |
| 1   | A     | 982  | THR  |
| 1   | A     | 990  | VAL  |
| 1   | A     | 996  | ASN  |
| 1   | A     | 1001 | ARG  |
| 1   | A     | 1007 | ILE  |
| 1   | A     | 1017 | LEU  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1037 | LEU  |
| 1   | A     | 1045 | VAL  |
| 1   | A     | 1049 | ILE  |
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1080 | THR  |
| 1   | A     | 1081 | LEU  |
| 1   | A     | 1094 | VAL  |
| 1   | A     | 1095 | THR  |
| 1   | A     | 1104 | ILE  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1112 | LYS  |
| 1   | A     | 1118 | VAL  |
| 1   | A     | 1128 | GLN  |
| 1   | A     | 1142 | THR  |
| 1   | A     | 1146 | VAL  |
| 1   | A     | 1148 | ILE  |
| 1   | A     | 1170 | ILE  |
| 1   | A     | 1172 | LEU  |
| 1   | A     | 1173 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1193 | LEU  |
| 1   | A     | 1203 | ASN  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1208 | THR  |
| 1   | A     | 1219 | THR  |
| 1   | A     | 1227 | ILE  |
| 1   | A     | 1256 | GLU  |
| 1   | A     | 1257 | ASP  |
| 1   | A     | 1262 | LYS  |
| 1   | A     | 1264 | GLU  |
| 1   | A     | 1267 | MET  |
| 1   | A     | 1269 | GLU  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1281 | ARG  |
| 1   | A     | 1282 | VAL  |
| 1   | A     | 1283 | VAL  |
| 1   | A     | 1285 | MET  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1297 | GLU  |
| 1   | A     | 1299 | VAL  |
| 1   | A     | 1301 | GLU  |
| 1   | A     | 1307 | GLU  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1322 | ILE  |
| 1   | A     | 1333 | ILE  |
| 1   | A     | 1334 | ASP  |
| 1   | A     | 1354 | ASN  |
| 1   | A     | 1359 | ASP  |
| 1   | A     | 1361 | SER  |
| 1   | A     | 1368 | MET  |
| 1   | A     | 1376 | THR  |
| 1   | A     | 1378 | GLN  |
| 1   | A     | 1382 | THR  |
| 1   | A     | 1384 | VAL  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1392 | SER  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1400 | CYS  |
| 1   | A     | 1406 | VAL  |
| 1   | A     | 1407 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1411 | GLU  |
| 1   | A     | 1420 | ASP  |
| 1   | A     | 1425 | SER  |
| 1   | A     | 1426 | GLU  |
| 1   | A     | 1445 | ILE  |
| 2   | B     | 22   | SER  |
| 2   | B     | 25   | ILE  |
| 2   | B     | 26   | THR  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 34   | ILE  |
| 2   | B     | 67   | SER  |
| 2   | B     | 94   | LYS  |
| 2   | B     | 97   | VAL  |
| 2   | B     | 98   | THR  |
| 2   | B     | 104  | GLU  |
| 2   | B     | 106  | ASP  |
| 2   | B     | 109  | THR  |
| 2   | B     | 120  | ARG  |
| 2   | B     | 128  | LEU  |
| 2   | B     | 134  | LYS  |
| 2   | B     | 165  | VAL  |
| 2   | B     | 167  | ILE  |
| 2   | B     | 172  | ILE  |
| 2   | B     | 174  | LEU  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 181  | LEU  |
| 2   | B     | 188  | ASP  |
| 2   | B     | 194  | GLU  |
| 2   | B     | 199  | MET  |
| 2   | B     | 208  | SER  |
| 2   | B     | 217  | ARG  |
| 2   | B     | 218  | SER  |
| 2   | B     | 223  | VAL  |
| 2   | B     | 225  | VAL  |
| 2   | B     | 228  | LYS  |
| 2   | B     | 234  | ILE  |
| 2   | B     | 237  | VAL  |
| 2   | B     | 246  | LYS  |
| 2   | B     | 248  | SER  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 261  | ARG  |
| 2   | B     | 262  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 264 | SER  |
| 2   | B     | 268 | THR  |
| 2   | B     | 272 | THR  |
| 2   | B     | 273 | LEU  |
| 2   | B     | 282 | ILE  |
| 2   | B     | 283 | VAL  |
| 2   | B     | 294 | ASP  |
| 2   | B     | 297 | ILE  |
| 2   | B     | 305 | VAL  |
| 2   | B     | 306 | ASN  |
| 2   | B     | 313 | MET  |
| 2   | B     | 314 | LEU  |
| 2   | B     | 315 | LYS  |
| 2   | B     | 322 | PHE  |
| 2   | B     | 347 | LYS  |
| 2   | B     | 349 | ILE  |
| 2   | B     | 365 | THR  |
| 2   | B     | 367 | LEU  |
| 2   | B     | 368 | GLU  |
| 2   | B     | 373 | ARG  |
| 2   | B     | 382 | ILE  |
| 2   | B     | 384 | ARG  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 391 | ASP  |
| 2   | B     | 399 | ASP  |
| 2   | B     | 404 | LYS  |
| 2   | B     | 415 | GLN  |
| 2   | B     | 422 | LYS  |
| 2   | B     | 424 | LEU  |
| 2   | B     | 451 | LYS  |
| 2   | B     | 453 | ILE  |
| 2   | B     | 454 | THR  |
| 2   | B     | 459 | TYR  |
| 2   | B     | 461 | LEU  |
| 2   | B     | 463 | THR  |
| 2   | B     | 469 | GLN  |
| 2   | B     | 471 | LYS  |
| 2   | B     | 479 | VAL  |
| 2   | B     | 482 | VAL  |
| 2   | B     | 485 | ARG  |
| 2   | B     | 490 | SER  |
| 2   | B     | 498 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 513 | GLN  |
| 2   | B     | 527 | THR  |
| 2   | B     | 529 | GLU  |
| 2   | B     | 537 | LYS  |
| 2   | B     | 544 | CYS  |
| 2   | B     | 547 | VAL  |
| 2   | B     | 549 | THR  |
| 2   | B     | 552 | MET  |
| 2   | B     | 554 | ILE  |
| 2   | B     | 556 | THR  |
| 2   | B     | 563 | MET  |
| 2   | B     | 570 | VAL  |
| 2   | B     | 591 | ARG  |
| 2   | B     | 603 | LEU  |
| 2   | B     | 604 | ARG  |
| 2   | B     | 612 | GLU  |
| 2   | B     | 616 | ILE  |
| 2   | B     | 619 | ILE  |
| 2   | B     | 626 | ILE  |
| 2   | B     | 628 | THR  |
| 2   | B     | 629 | ASP  |
| 2   | B     | 635 | ARG  |
| 2   | B     | 641 | GLU  |
| 2   | B     | 643 | ASP  |
| 2   | B     | 653 | VAL  |
| 2   | B     | 658 | ILE  |
| 2   | B     | 665 | GLU  |
| 2   | B     | 668 | ASP  |
| 2   | B     | 682 | SER  |
| 2   | B     | 686 | ASN  |
| 2   | B     | 701 | ILE  |
| 2   | B     | 710 | LEU  |
| 2   | B     | 737 | THR  |
| 2   | B     | 740 | HIS  |
| 2   | B     | 743 | ILE  |
| 2   | B     | 751 | VAL  |
| 2   | B     | 754 | SER  |
| 2   | B     | 762 | ASN  |
| 2   | B     | 764 | SER  |
| 2   | B     | 778 | MET  |
| 2   | B     | 780 | VAL  |
| 2   | B     | 783 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 791 | THR  |
| 2   | B     | 792 | MET  |
| 2   | B     | 794 | ASN  |
| 2   | B     | 801 | LYS  |
| 2   | B     | 807 | ARG  |
| 2   | B     | 812 | LEU  |
| 2   | B     | 821 | GLN  |
| 2   | B     | 822 | ASN  |
| 2   | B     | 825 | VAL  |
| 2   | B     | 831 | SER  |
| 2   | B     | 844 | SER  |
| 2   | B     | 854 | LEU  |
| 2   | B     | 859 | TYR  |
| 2   | B     | 866 | TYR  |
| 2   | B     | 868 | MET  |
| 2   | B     | 873 | THR  |
| 2   | B     | 878 | GLN  |
| 2   | B     | 879 | ARG  |
| 2   | B     | 880 | THR  |
| 2   | B     | 882 | THR  |
| 2   | B     | 883 | LEU  |
| 2   | B     | 886 | LYS  |
| 2   | B     | 894 | ASP  |
| 2   | B     | 901 | PRO  |
| 2   | B     | 911 | ILE  |
| 2   | B     | 914 | LYS  |
| 2   | B     | 934 | LYS  |
| 2   | B     | 939 | THR  |
| 2   | B     | 944 | THR  |
| 2   | B     | 945 | GLU  |
| 2   | B     | 953 | LEU  |
| 2   | B     | 959 | ASP  |
| 2   | B     | 970 | THR  |
| 2   | B     | 973 | ILE  |
| 2   | B     | 976 | ILE  |
| 2   | B     | 983 | ARG  |
| 2   | B     | 984 | HIS  |
| 2   | B     | 986 | GLN  |
| 2   | B     | 989 | THR  |
| 2   | B     | 993 | THR  |
| 2   | B     | 997 | GLU  |
| 2   | B     | 999 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1004 | GLU  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1012 | ILE  |
| 2   | B     | 1019 | SER  |
| 2   | B     | 1020 | ARG  |
| 2   | B     | 1022 | THR  |
| 2   | B     | 1028 | GLU  |
| 2   | B     | 1040 | ASN  |
| 2   | B     | 1048 | THR  |
| 2   | B     | 1050 | ILE  |
| 2   | B     | 1051 | THR  |
| 2   | B     | 1058 | LEU  |
| 2   | B     | 1061 | GLU  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1071 | VAL  |
| 2   | B     | 1082 | MET  |
| 2   | B     | 1092 | TYR  |
| 2   | B     | 1093 | GLN  |
| 2   | B     | 1096 | ARG  |
| 2   | B     | 1099 | VAL  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1113 | VAL  |
| 2   | B     | 1115 | THR  |
| 2   | B     | 1119 | VAL  |
| 2   | B     | 1124 | ARG  |
| 2   | B     | 1132 | GLU  |
| 2   | B     | 1135 | ARG  |
| 2   | B     | 1138 | MET  |
| 2   | B     | 1147 | LEU  |
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1159 | ARG  |
| 2   | B     | 1160 | VAL  |
| 2   | B     | 1170 | THR  |
| 2   | B     | 1181 | GLU  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1189 | ILE  |
| 2   | B     | 1191 | ILE  |
| 2   | B     | 1194 | ILE  |
| 2   | B     | 1196 | ILE  |
| 2   | B     | 1202 | LEU  |
| 2   | B     | 1221 | SER  |
| 3   | C     | 4    | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 18  | VAL  |
| 3   | C     | 21  | ILE  |
| 3   | C     | 23  | SER  |
| 3   | C     | 25  | VAL  |
| 3   | C     | 27  | LEU  |
| 3   | C     | 38  | ILE  |
| 3   | C     | 40  | GLU  |
| 3   | C     | 41  | ILE  |
| 3   | C     | 53  | THR  |
| 3   | C     | 56  | THR  |
| 3   | C     | 77  | ILE  |
| 3   | C     | 89  | GLU  |
| 3   | C     | 92  | CYS  |
| 3   | C     | 97  | VAL  |
| 3   | C     | 99  | LEU  |
| 3   | C     | 101 | LEU  |
| 3   | C     | 119 | VAL  |
| 3   | C     | 120 | ILE  |
| 3   | C     | 123 | ASN  |
| 3   | C     | 129 | ILE  |
| 3   | C     | 133 | ILE  |
| 3   | C     | 140 | ASN  |
| 3   | C     | 142 | VAL  |
| 3   | C     | 143 | LEU  |
| 3   | C     | 144 | ILE  |
| 3   | C     | 149 | LYS  |
| 3   | C     | 154 | LYS  |
| 3   | C     | 156 | THR  |
| 3   | C     | 157 | CYS  |
| 3   | C     | 163 | ILE  |
| 3   | C     | 166 | GLU  |
| 3   | C     | 183 | TRP  |
| 3   | C     | 215 | GLU  |
| 3   | C     | 224 | GLN  |
| 3   | C     | 227 | THR  |
| 3   | C     | 229 | TYR  |
| 3   | C     | 231 | ASN  |
| 3   | C     | 233 | GLU  |
| 3   | C     | 240 | VAL  |
| 3   | C     | 244 | VAL  |
| 3   | C     | 265 | MET  |
| 3   | C     | 267 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 268 | ASP  |
| 4   | E     | 2   | ASP  |
| 4   | E     | 4   | GLU  |
| 4   | E     | 6   | GLU  |
| 4   | E     | 7   | ARG  |
| 4   | E     | 9   | ILE  |
| 4   | E     | 37  | LEU  |
| 4   | E     | 41  | ASP  |
| 4   | E     | 50  | MET  |
| 4   | E     | 54  | GLN  |
| 4   | E     | 57  | MET  |
| 4   | E     | 61  | GLN  |
| 4   | E     | 78  | LEU  |
| 4   | E     | 94  | LYS  |
| 4   | E     | 98  | ILE  |
| 4   | E     | 101 | GLN  |
| 4   | E     | 102 | GLU  |
| 4   | E     | 107 | THR  |
| 4   | E     | 127 | ILE  |
| 4   | E     | 131 | THR  |
| 4   | E     | 150 | VAL  |
| 4   | E     | 165 | LEU  |
| 4   | E     | 169 | ARG  |
| 4   | E     | 175 | LEU  |
| 4   | E     | 184 | VAL  |
| 4   | E     | 191 | LYS  |
| 4   | E     | 198 | ILE  |
| 5   | F     | 72  | LYS  |
| 5   | F     | 79  | ARG  |
| 5   | F     | 81  | THR  |
| 5   | F     | 82  | THR  |
| 5   | F     | 90  | ARG  |
| 5   | F     | 92  | ARG  |
| 5   | F     | 93  | ILE  |
| 5   | F     | 97  | ARG  |
| 5   | F     | 109 | VAL  |
| 5   | F     | 111 | LEU  |
| 5   | F     | 112 | GLU  |
| 5   | F     | 119 | ARG  |
| 5   | F     | 120 | ILE  |
| 5   | F     | 123 | LYS  |
| 5   | F     | 125 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 128 | LYS  |
| 5   | F     | 148 | VAL  |
| 5   | F     | 155 | LEU  |
| 6   | H     | 2   | SER  |
| 6   | H     | 11  | GLN  |
| 6   | H     | 15  | VAL  |
| 6   | H     | 26  | ILE  |
| 6   | H     | 31  | THR  |
| 6   | H     | 33  | GLN  |
| 6   | H     | 54  | SER  |
| 6   | H     | 55  | LEU  |
| 6   | H     | 89  | LEU  |
| 6   | H     | 92  | ASP  |
| 6   | H     | 94  | ASP  |
| 6   | H     | 95  | TYR  |
| 6   | H     | 107 | VAL  |
| 6   | H     | 110 | ASP  |
| 6   | H     | 112 | ILE  |
| 6   | H     | 130 | ARG  |
| 6   | H     | 132 | LEU  |
| 6   | H     | 136 | LYS  |
| 6   | H     | 142 | LEU  |
| 7   | I     | 8   | ARG  |
| 7   | I     | 13  | MET  |
| 7   | I     | 14  | LEU  |
| 7   | I     | 29  | CYS  |
| 7   | I     | 30  | ARG  |
| 7   | I     | 40  | SER  |
| 7   | I     | 50  | THR  |
| 7   | I     | 52  | ILE  |
| 7   | I     | 55  | THR  |
| 7   | I     | 70  | ARG  |
| 7   | I     | 83  | ASN  |
| 7   | I     | 84  | VAL  |
| 7   | I     | 91  | ARG  |
| 7   | I     | 95  | THR  |
| 7   | I     | 106 | CYS  |
| 7   | I     | 107 | SER  |
| 7   | I     | 111 | THR  |
| 8   | J     | 2   | ILE  |
| 8   | J     | 3   | VAL  |
| 8   | J     | 7   | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | J     | 10  | CYS  |
| 8   | J     | 13  | VAL  |
| 8   | J     | 14  | VAL  |
| 8   | J     | 23  | ASN  |
| 8   | J     | 31  | ASP  |
| 8   | J     | 34  | THR  |
| 8   | J     | 48  | ARG  |
| 8   | J     | 55  | ASP  |
| 8   | J     | 59  | LYS  |
| 8   | J     | 64  | ASN  |
| 9   | K     | 6   | ARG  |
| 9   | K     | 18  | LYS  |
| 9   | K     | 19  | LEU  |
| 9   | K     | 21  | ILE  |
| 9   | K     | 26  | LYS  |
| 9   | K     | 31  | VAL  |
| 9   | K     | 33  | ILE  |
| 9   | K     | 46  | ILE  |
| 9   | K     | 50  | LEU  |
| 9   | K     | 51  | LEU  |
| 9   | K     | 75  | ILE  |
| 9   | K     | 77  | THR  |
| 9   | K     | 78  | THR  |
| 9   | K     | 101 | LEU  |
| 9   | K     | 106 | GLU  |
| 9   | K     | 111 | LEU  |
| 9   | K     | 113 | THR  |
| 10  | L     | 27  | LEU  |
| 10  | L     | 30  | ILE  |
| 10  | L     | 38  | LEU  |
| 10  | L     | 46  | VAL  |
| 10  | L     | 50  | ASP  |
| 10  | L     | 51  | CYS  |
| 10  | L     | 55  | ILE  |
| 10  | L     | 61  | THR  |
| 10  | L     | 65  | VAL  |
| 10  | L     | 66  | GLN  |
| 10  | L     | 70  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 64   | ASN  |
| 1   | A     | 68   | GLN  |
| 1   | A     | 75   | ASN  |
| 1   | A     | 83   | HIS  |
| 1   | A     | 92   | HIS  |
| 1   | A     | 109  | HIS  |
| 1   | A     | 118  | HIS  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 225  | ASN  |
| 1   | A     | 297  | GLN  |
| 1   | A     | 390  | GLN  |
| 1   | A     | 394  | ASN  |
| 1   | A     | 435  | HIS  |
| 1   | A     | 445  | ASN  |
| 1   | A     | 503  | GLN  |
| 1   | A     | 525  | GLN  |
| 1   | A     | 631  | HIS  |
| 1   | A     | 650  | GLN  |
| 1   | A     | 660  | ASN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 745  | GLN  |
| 1   | A     | 757  | ASN  |
| 1   | A     | 851  | HIS  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 996  | ASN  |
| 1   | A     | 1078 | GLN  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1173 | HIS  |
| 1   | A     | 1232 | ASN  |
| 1   | A     | 1258 | HIS  |
| 1   | A     | 1270 | ASN  |
| 1   | A     | 1312 | ASN  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1387 | HIS  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1432 | GLN  |
| 2   | B     | 60   | GLN  |
| 2   | B     | 115  | GLN  |
| 2   | B     | 206  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 215  | GLN  |
| 2   | B     | 236  | HIS  |
| 2   | B     | 300  | HIS  |
| 2   | B     | 366  | GLN  |
| 2   | B     | 383  | ASN  |
| 2   | B     | 433  | GLN  |
| 2   | B     | 469  | GLN  |
| 2   | B     | 484  | ASN  |
| 2   | B     | 515  | HIS  |
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 573  | GLN  |
| 2   | B     | 590  | HIS  |
| 2   | B     | 592  | ASN  |
| 2   | B     | 657  | HIS  |
| 2   | B     | 740  | HIS  |
| 2   | B     | 744  | HIS  |
| 2   | B     | 794  | ASN  |
| 2   | B     | 822  | ASN  |
| 2   | B     | 862  | GLN  |
| 2   | B     | 878  | GLN  |
| 2   | B     | 986  | GLN  |
| 2   | B     | 1015 | HIS  |
| 2   | B     | 1062 | HIS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1076 | HIS  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1141 | HIS  |
| 2   | B     | 1187 | ASN  |
| 3   | C     | 73   | GLN  |
| 3   | C     | 91   | HIS  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 123  | ASN  |
| 3   | C     | 131  | HIS  |
| 3   | C     | 135  | GLN  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 188  | HIS  |
| 3   | C     | 203  | GLN  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 224  | GLN  |
| 3   | C     | 231  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 242 | GLN  |
| 3   | C     | 264 | GLN  |
| 4   | E     | 54  | GLN  |
| 4   | E     | 101 | GLN  |
| 4   | E     | 114 | ASN  |
| 4   | E     | 147 | HIS  |
| 6   | H     | 33  | GLN  |
| 6   | H     | 35  | GLN  |
| 6   | H     | 83  | GLN  |
| 6   | H     | 131 | ASN  |
| 6   | H     | 137 | GLN  |
| 6   | H     | 139 | ASN  |
| 7   | I     | 83  | ASN  |
| 7   | I     | 114 | GLN  |
| 9   | K     | 29  | ASN  |
| 9   | K     | 40  | HIS  |
| 9   | K     | 65  | HIS  |
| 9   | K     | 89  | ASN  |
| 10  | L     | 53  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 11  | R     | 9/10 (90%) | 2 (22%)           | 0               |

All (2) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | R     | 2   | U    |
| 11  | R     | 9   | G    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 16  | C7P  | T     | 29  | 12   | 5,9,10       | 0.97 | 0           | 2,11,14     | 1.14 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 16  | C7P  | T     | 29  | 12   | -       | -        | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | T     | 29  | C7P  | 5       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 1395/1733 (80%) | 0.21   | 21 (1%) 72 44 | 50, 115, 229, 314     | 0     |
| 2   | B     | 1106/1224 (90%) | 0.06   | 6 (0%) 87 66  | 50, 103, 169, 240     | 0     |
| 3   | C     | 266/318 (83%)   | -0.09  | 0 100 100     | 69, 105, 142, 159     | 0     |
| 4   | E     | 214/215 (99%)   | 0.39   | 3 (1%) 73 45  | 91, 175, 245, 258     | 0     |
| 5   | F     | 84/155 (54%)    | -0.07  | 0 100 100     | 88, 118, 148, 152     | 0     |
| 6   | H     | 133/146 (91%)   | 0.68   | 7 (5%) 32 18  | 117, 162, 209, 217    | 0     |
| 7   | I     | 119/122 (97%)   | 0.49   | 4 (3%) 48 27  | 104, 143, 186, 208    | 0     |
| 8   | J     | 65/70 (92%)     | -0.23  | 0 100 100     | 67, 86, 118, 130      | 0     |
| 9   | K     | 114/120 (95%)   | -0.15  | 0 100 100     | 67, 109, 139, 151     | 0     |
| 10  | L     | 46/70 (65%)     | 0.54   | 2 (4%) 40 21  | 78, 155, 178, 185     | 0     |
| 11  | R     | 10/10 (100%)    | 4.07   | 10 (100%) 0 0 | 183, 210, 307, 319    | 0     |
| 12  | T     | 28/28 (100%)    | 2.02   | 14 (50%) 0 1  | 199, 326, 403, 414    | 0     |
| 13  | N     | 14/14 (100%)    | 1.16   | 0 100 100     | 313, 367, 380, 399    | 0     |
| All | All   | 3594/4225 (85%) | 0.19   | 67 (1%) 66 38 | 50, 116, 220, 414     | 0     |

All (67) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | R     | 2   | U    | 7.0  |
| 11  | R     | 1   | A    | 5.0  |
| 1   | A     | 173 | THR  | 4.5  |
| 1   | A     | 79  | GLY  | 4.4  |
| 11  | R     | 7   | A    | 4.3  |
| 11  | R     | 8   | G    | 4.1  |
| 2   | B     | 643 | ASP  | 4.1  |
| 11  | R     | 9   | G    | 4.1  |
| 11  | R     | 3   | G    | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | R     | 10   | A    | 3.9  |
| 2   | B     | 882  | THR  | 3.8  |
| 12  | T     | 20   | DC   | 3.7  |
| 12  | T     | 26   | DC   | 3.7  |
| 12  | T     | 23   | DC   | 3.6  |
| 11  | R     | 6    | G    | 3.5  |
| 1   | A     | 104  | GLU  | 3.5  |
| 2   | B     | 335  | GLY  | 3.4  |
| 12  | T     | 27   | DA   | 3.2  |
| 4   | E     | 124  | VAL  | 3.2  |
| 12  | T     | 25   | DC   | 3.1  |
| 1   | A     | 59   | GLY  | 3.1  |
| 12  | T     | 21   | DC   | 3.1  |
| 10  | L     | 27   | LEU  | 3.0  |
| 12  | T     | 19   | DT   | 2.9  |
| 7   | I     | 49   | ILE  | 2.8  |
| 12  | T     | 28   | DT   | 2.7  |
| 12  | T     | 24   | DT   | 2.7  |
| 12  | T     | 22   | DT   | 2.7  |
| 1   | A     | 1321 | GLY  | 2.6  |
| 6   | H     | 114  | VAL  | 2.6  |
| 6   | H     | 90   | ALA  | 2.6  |
| 1   | A     | 97   | ALA  | 2.6  |
| 1   | A     | 174  | ILE  | 2.5  |
| 11  | R     | 5    | A    | 2.5  |
| 6   | H     | 140  | ALA  | 2.5  |
| 6   | H     | 63   | LEU  | 2.4  |
| 1   | A     | 54   | ASN  | 2.4  |
| 1   | A     | 145  | LYS  | 2.4  |
| 11  | R     | 4    | G    | 2.4  |
| 1   | A     | 175  | ARG  | 2.4  |
| 12  | T     | 18   | DG   | 2.3  |
| 1   | A     | 114  | LEU  | 2.2  |
| 1   | A     | 1330 | ASN  | 2.2  |
| 4   | E     | 20   | LYS  | 2.2  |
| 1   | A     | 1162 | VAL  | 2.2  |
| 6   | H     | 86   | ASP  | 2.1  |
| 1   | A     | 93   | VAL  | 2.1  |
| 1   | A     | 91   | PHE  | 2.1  |
| 2   | B     | 478  | GLY  | 2.1  |
| 7   | I     | 41   | PRO  | 2.1  |
| 1   | A     | 121  | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1110 | ASN  | 2.1  |
| 7   | I     | 43   | VAL  | 2.1  |
| 12  | T     | 1    | DC   | 2.1  |
| 12  | T     | 2    | DT   | 2.1  |
| 4   | E     | 98   | ILE  | 2.1  |
| 6   | H     | 84   | ALA  | 2.1  |
| 7   | I     | 107  | SER  | 2.1  |
| 1   | A     | 308  | ILE  | 2.1  |
| 1   | A     | 171  | GLN  | 2.1  |
| 1   | A     | 311  | GLN  | 2.1  |
| 6   | H     | 85   | GLY  | 2.0  |
| 1   | A     | 44   | THR  | 2.0  |
| 10  | L     | 45   | ALA  | 2.0  |
| 2   | B     | 883  | LEU  | 2.0  |
| 12  | T     | 17   | DC   | 2.0  |
| 2   | B     | 709  | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 16  | C7P  | T     | 29   | 9/10  | 0.86 | 0.20 | 314,324,360,369             | 1     |
| 14  | ZN   | A     | 1734 | 1/1   | 0.94 | 0.06 | 90,90,90,90                 | 1     |
| 14  | ZN   | L     | 105  | 1/1   | 0.95 | 0.07 | 106,106,106,106             | 1     |
| 14  | ZN   | A     | 1735 | 1/1   | 0.98 | 0.04 | 103,103,103,103             | 1     |
| 14  | ZN   | I     | 203  | 1/1   | 0.99 | 0.02 | 81,81,81,81                 | 0     |
| 14  | ZN   | J     | 101  | 1/1   | 0.99 | 0.03 | 87,87,87,87                 | 1     |
| 14  | ZN   | B     | 1307 | 1/1   | 0.99 | 0.06 | 95,95,95,95                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 14  | ZN   | C     | 319  | 1/1   | 0.99 | 0.04 | 83,83,83,83                 | 0     |
| 15  | MG   | A     | 2001 | 1/1   | 1.00 | 0.02 | 9,9,9,9                     | 0     |
| 14  | ZN   | I     | 204  | 1/1   | 1.00 | 0.04 | 81,81,81,81                 | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.