



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 12:13 PM EDT

PDB ID : 5TMC  
Title : Re-refinement of Thermus thermopiles DNA-directed RNA polymerase structure  
Authors : Wang, J.  
Deposited on : 2016-10-12  
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

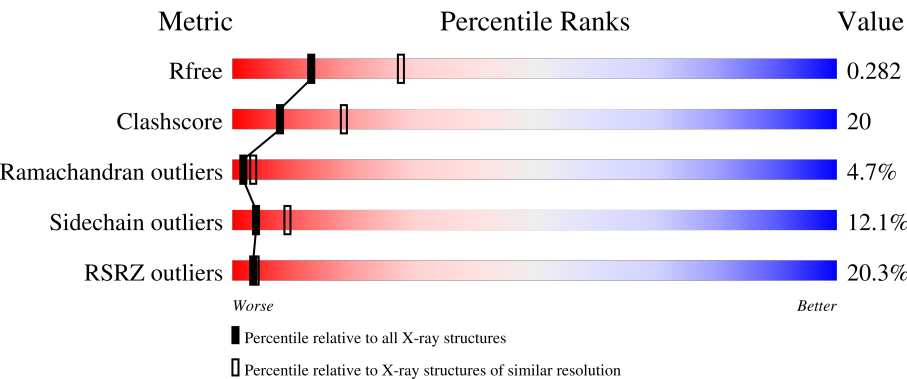
|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                       |
| Xtriage (Phenix)               | : | 1.20.1   |
| EDS                            | : | 3.0  |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4                           | : | 9.0.003 (Gargrove)   |
| Density-Fitness                | : | 1.0.11   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.39   |

# 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 2.71 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 164625                      | 4050 (2.74-2.70)                                      |
| Clashscore            | 180529                      | 4439 (2.74-2.70)                                      |
| Ramachandran outliers | 177936                      | 4374 (2.74-2.70)                                      |
| Sidechain outliers    | 177891                      | 4375 (2.74-2.70)                                      |
| RSRZ outliers         | 164620                      | 4050 (2.74-2.70)                                      |

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     | 315    | <div><div>6%</div><div>34%</div><div>31%</div><div>8%</div><div>27%</div></div> |
| 1   | B     | 315    | <div><div>21%</div><div>46%</div><div>27%</div><div>•</div><div>24%</div></div> |
| 2   | C     | 1119   | <div><div>17%</div><div>52%</div><div>41%</div><div>7%</div></div>              |
| 3   | D     | 1524   | <div><div>20%</div><div>52%</div><div>40%</div><div>7%</div><div>•</div></div>  |
| 4   | E     | 99     | <div><div>14%</div><div>69%</div><div>23%</div><div>•••</div></div>             |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | F     | 423    | <div><div></div><div>27%</div><div>56%</div><div>23%</div><div>17%</div></div> |
| 6   | Z     | 48     | <div><div></div><div>96%</div></div>   |

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28419 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 subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1816  | 1159 | 315 | 339 | 3 |         |         |       |
| 1   | B     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1863  | 1188 | 322 | 350 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1504     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11864 | 7518 | 2091 | 2219 | 36 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 61      | GLU      | VAL    | conflict | UNP Q72ID6 |
| E     | 92      | ILE      | LEU    | conflict | UNP Q72ID6 |
| E     | 95      | GLY      | VAL    | conflict | UNP Q72ID6 |

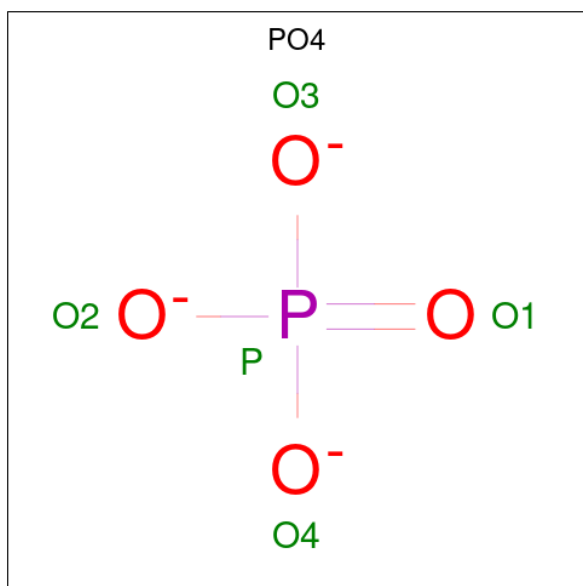
- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 351      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2844  | 1794 | 515 | 531 | 4 |         |         |       |

- Molecule 6 is a protein called unknown protein.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 6   | Z     | 48       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 240   | 144 | 48 | 48 |         |         |       |

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

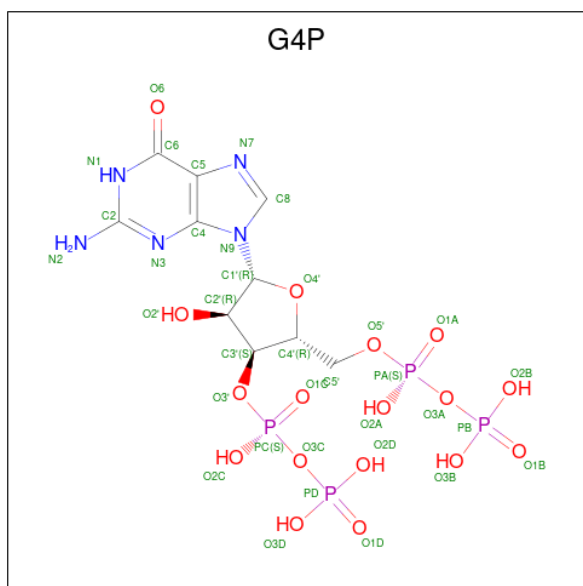
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 8   | D     | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 10 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula:  $C_{10}H_{17}N_5O_{17}P_4$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 10  | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 36    | 10 | 5 | 17 | 4 |         |         |

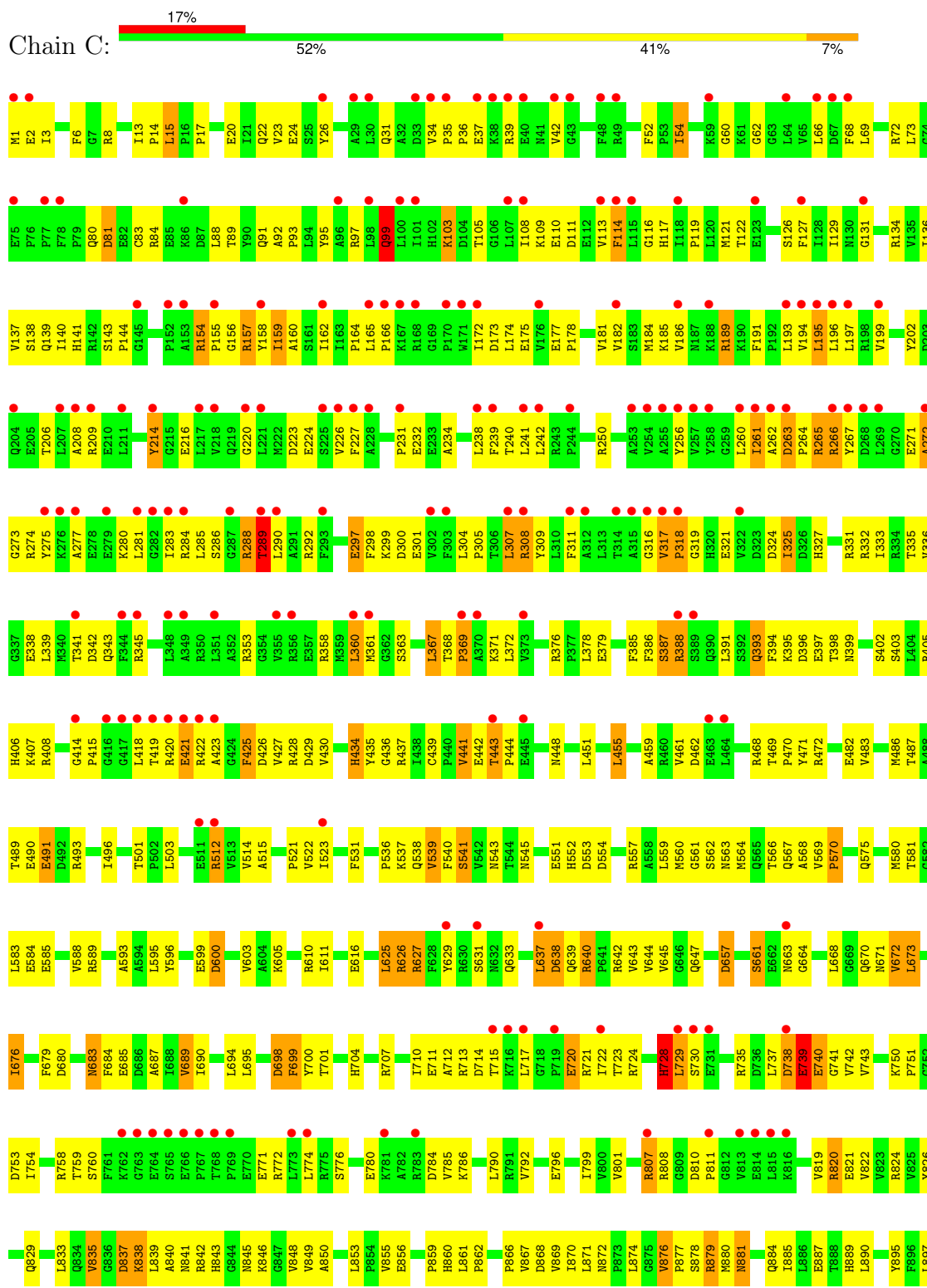
- Molecule 11 is water.

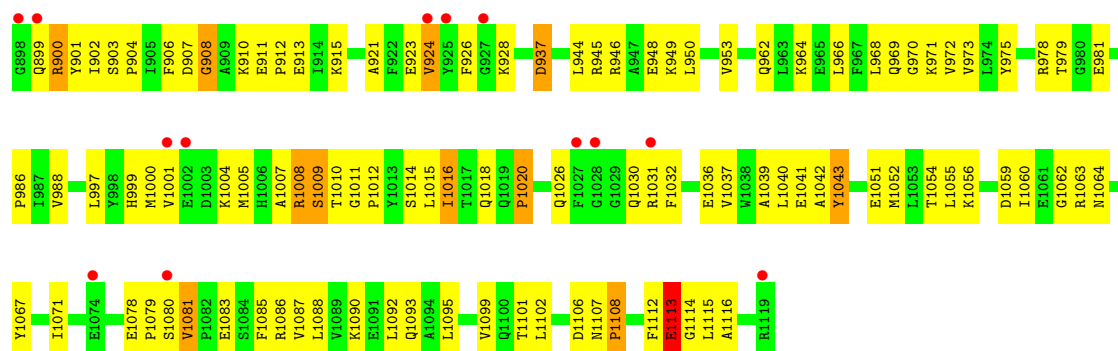
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | A     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 11  | B     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 11  | C     | 54       | Total | O  | 0       | 0       |
|     |       |          | 54    | 54 |         |         |
| 11  | D     | 62       | Total | O  | 0       | 0       |
|     |       |          | 62    | 62 |         |         |
| 11  | E     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 11  | F     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |



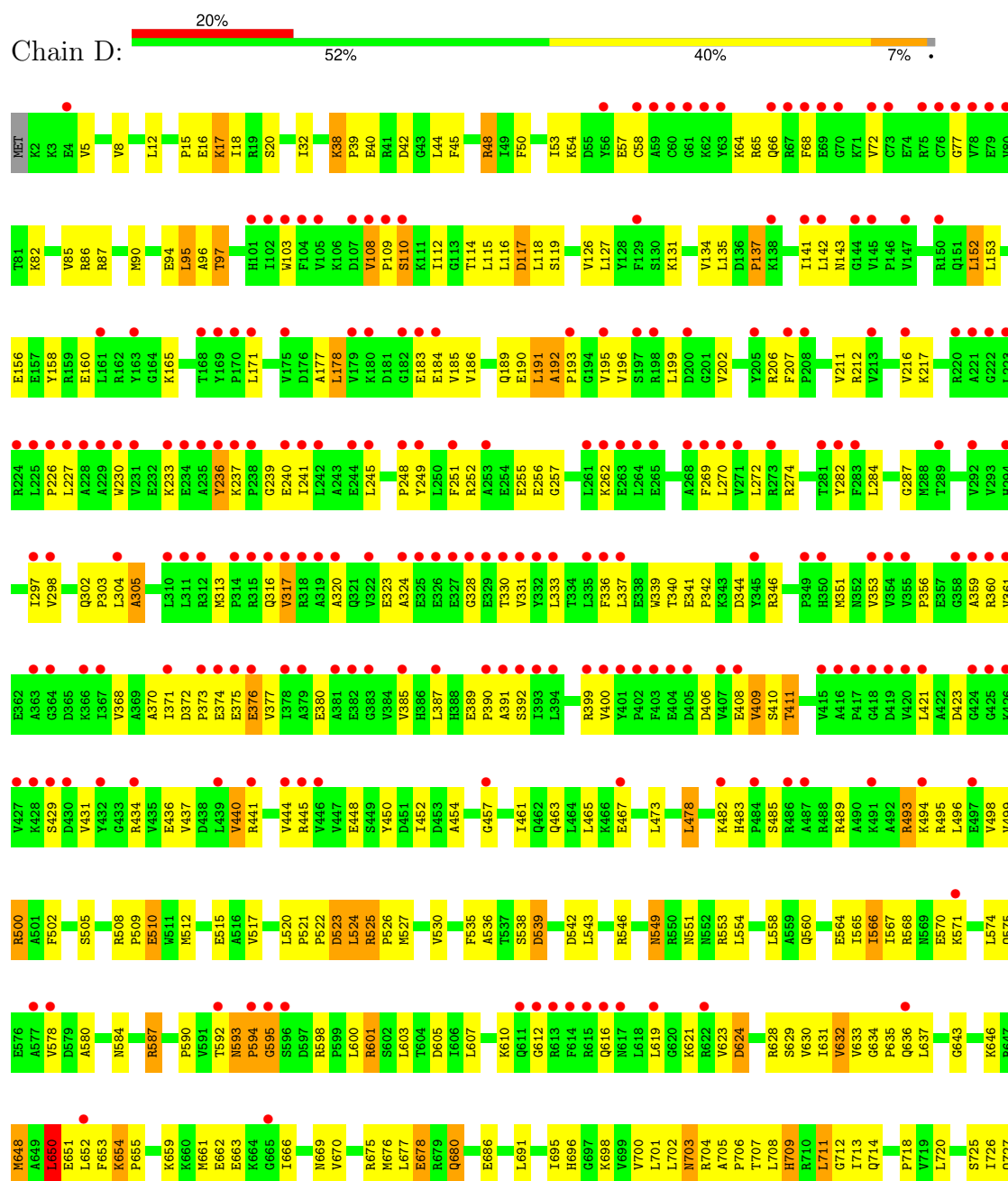
GLY  
GLU  
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GLU  
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LYS  
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PHE  
THR  
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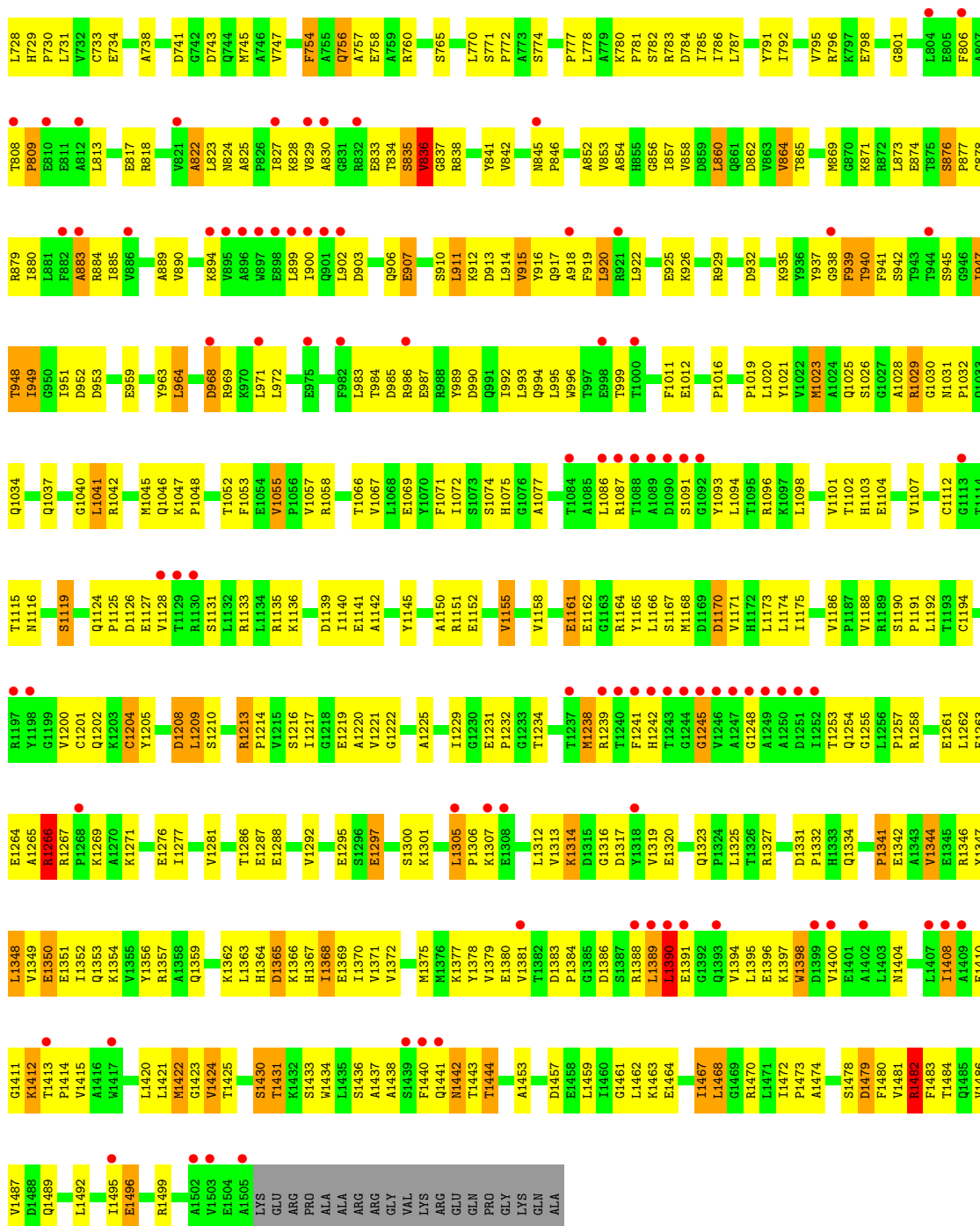
● Molecule 2: DNA-directed RNA polymerase subunit beta





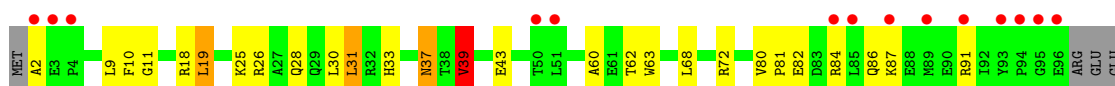
• Molecule 3: DNA-directed RNA polymerase subunit beta'







- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  14% 69% 23% ...



- Molecule 5: RNA polymerase sigma factor SigA

Chain Z:  96% •



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 65  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 236.35Å 236.35Å 249.04Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 48.51 – 2.71<br>48.51 – 2.71                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.9 (48.51-2.71)<br>97.1 (48.51-2.71)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.06 (at 2.73Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0109   | Depositor        |
| R, $R_{free}$   | 0.265 , 0.286<br>0.262 , 0.282                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7447 reflections (3.61%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.2  | Xtriage          |
| Anisotropy  | 0.049   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 102.2  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction   | 0.086 for h,-h-k,-l   | Xtriage          |
| Reported twinning fraction  | 0.875 for H, K, L<br>0.125 for -H-K, K, -L                  | Depositor        |
| Outliers  | 1 of 206105 reflections (0.000%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 28419   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 121.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: ZN, G4P, MG, PO4

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     | 0.47         | 0/1848  | 0.64        | 0/2512         |
| 1   | B     | 0.39         | 0/1896  | 0.57        | 0/2579         |
| 2   | C     | 0.46         | 0/8997  | 0.65        | 0/12164        |
| 3   | D     | 0.45         | 0/12073 | 0.65        | 2/16324 (0.0%) |
| 4   | E     | 0.44         | 0/783   | 0.63        | 0/1054         |
| 5   | F     | 0.35         | 0/2890  | 0.55        | 0/3888         |
| All | All   | 0.44         | 0/28487 | 0.63        | 2/38521 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | D     | 0                   | 1                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | D     | 95  | LEU  | CA-CB-CG | 5.47 | 127.89      | 115.30   |
| 3   | D     | 650 | LEU  | CA-CB-CG | 5.43 | 127.79      | 115.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 3   | D     | 1126 | ASP  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1816  | 0        | 1871     | 90      | 0            |
| 1   | B     | 1863  | 0        | 1914     | 59      | 0            |
| 2   | C     | 8829  | 0        | 8933     | 408     | 0            |
| 3   | D     | 11864 | 0        | 12094    | 544     | 0            |
| 4   | E     | 769   | 0        | 775      | 20      | 0            |
| 5   | F     | 2844  | 0        | 2926     | 68      | 0            |
| 6   | Z     | 240   | 0        | 50       | 1       | 0            |
| 7   | A     | 5     | 0        | 0        | 0       | 0            |
| 8   | C     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 3     | 0        | 0        | 0       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 36    | 0        | 11       | 1       | 0            |
| 11  | A     | 15    | 0        | 0        | 0       | 0            |
| 11  | B     | 2     | 0        | 0        | 2       | 0            |
| 11  | C     | 54    | 0        | 0        | 4       | 0            |
| 11  | D     | 62    | 0        | 0        | 7       | 0            |
| 11  | E     | 9     | 0        | 0        | 1       | 0            |
| 11  | F     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 28419 | 0        | 28574    | 1111    | 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 20.

All (1111) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1265:ALA:HA  | 3:D:1266:ARG:CB   | 1.60                     | 1.29              |
| 3:D:1265:ALA:HA  | 3:D:1266:ARG:HB2  | 1.23                     | 1.13              |
| 3:D:96:ALA:HB3   | 3:D:554:LEU:HD23  | 1.32                     | 1.07              |
| 2:C:93:PRO:HA    | 2:C:117:HIS:HB2   | 1.36                     | 1.06              |
| 2:C:567:GLN:HB2  | 2:C:997:LEU:HD22  | 1.41                     | 1.01              |
| 3:D:703:ASN:HA   | 3:D:712:GLY:O     | 1.59                     | 1.01              |
| 3:D:836:VAL:H    | 3:D:837:GLY:HA3   | 1.26                     | 0.97              |
| 3:D:1213:ARG:HG2 | 3:D:1213:ARG:HH11 | 1.26                     | 0.96              |
| 3:D:728:LEU:HD13 | 3:D:745:MET:HE1   | 1.47                     | 0.95              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:964:LEU:HD21 | 3:D:1058:ARG:HG2  | 1.45                     | 0.95              |
| 3:D:1265:ALA:HA  | 3:D:1266:ARG:HB3  | 1.49                     | 0.95              |
| 3:D:8:VAL:HG12   | 3:D:1434:TRP:HZ2  | 1.32                     | 0.94              |
| 2:C:838:LYS:HG3  | 2:C:997:LEU:HB2   | 1.48                     | 0.93              |
| 2:C:881:ASN:H    | 2:C:881:ASN:ND2   | 1.67                     | 0.93              |
| 2:C:676:ILE:O    | 3:D:948:THR:HG22  | 1.69                     | 0.91              |
| 2:C:881:ASN:HD22 | 2:C:881:ASN:N     | 1.62                     | 0.91              |
| 3:D:1496:GLU:HA  | 3:D:1499:ARG:HB2  | 1.50                     | 0.91              |
| 3:D:1265:ALA:CA  | 3:D:1266:ARG:HB2  | 2.01                     | 0.90              |
| 3:D:845:ASN:HB2  | 3:D:846:PRO:HD2   | 1.53                     | 0.90              |
| 2:C:724:ARG:HE   | 2:C:738:ASP:HA    | 1.35                     | 0.89              |
| 2:C:263:ASP:H    | 2:C:264:PRO:CD    | 1.86                     | 0.88              |
| 2:C:575:GLN:NE2  | 2:C:671:ASN:H     | 1.71                     | 0.88              |
| 3:D:192:ALA:HB1  | 3:D:193:PRO:HD2   | 1.55                     | 0.88              |
| 2:C:199:VAL:HG21 | 2:C:238:LEU:HD11  | 1.56                     | 0.88              |
| 3:D:1265:ALA:CA  | 3:D:1266:ARG:CB   | 2.51                     | 0.88              |
| 2:C:22:GLN:HG3   | 2:C:407:LYS:HB3   | 1.55                     | 0.87              |
| 2:C:889:HIS:HE1  | 3:D:951:ILE:H     | 1.21                     | 0.87              |
| 2:C:396:ASP:HA   | 2:C:633:GLN:HE22  | 1.40                     | 0.87              |
| 3:D:493:ARG:HH12 | 3:D:1390:LEU:H    | 1.23                     | 0.86              |
| 3:D:675:ARG:HA   | 3:D:678:GLU:OE1   | 1.76                     | 0.86              |
| 2:C:469:THR:HG22 | 2:C:538:GLN:HE21  | 1.37                     | 0.85              |
| 2:C:1059:ASP:OD1 | 2:C:1062:GLY:N    | 2.10                     | 0.85              |
| 1:B:2:LEU:N      | 1:B:3:ASP:HA      | 1.91                     | 0.85              |
| 3:D:654:LYS:HB3  | 3:D:655:PRO:HD3   | 1.58                     | 0.85              |
| 3:D:1258:ARG:CZ  | 3:D:1262:LEU:HD21 | 2.07                     | 0.85              |
| 3:D:1377:LYS:HD2 | 3:D:1378:TYR:CE2  | 2.12                     | 0.84              |
| 3:D:584:ASN:OD1  | 3:D:590:PRO:HD2   | 1.78                     | 0.84              |
| 3:D:1047:LYS:HB3 | 3:D:1048:PRO:HD2  | 1.60                     | 0.83              |
| 1:A:128:HIS:HE1  | 1:A:131:THR:HG23  | 1.43                     | 0.82              |
| 1:B:167:VAL:HG12 | 1:B:168:ASP:H     | 1.44                     | 0.82              |
| 2:C:881:ASN:H    | 2:C:881:ASN:HD22  | 0.84                     | 0.82              |
| 2:C:34:VAL:N     | 2:C:35:PRO:HD2    | 1.93                     | 0.82              |
| 5:F:370:LYS:HA   | 5:F:374:GLY:HA3   | 1.62                     | 0.81              |
| 3:D:984:THR:HG22 | 3:D:987:GLU:HG3   | 1.61                     | 0.81              |
| 3:D:730:PRO:O    | 11:D:1701:HOH:O   | 1.97                     | 0.81              |
| 3:D:1094:LEU:O   | 3:D:1098:LEU:HD13 | 1.80                     | 0.81              |
| 2:C:263:ASP:H    | 2:C:264:PRO:HD3   | 1.44                     | 0.81              |
| 2:C:157:ARG:HG3  | 2:C:158:TYR:H     | 1.44                     | 0.81              |
| 3:D:580:ALA:O    | 3:D:584:ASN:HB2   | 1.80                     | 0.80              |
| 3:D:907:GLU:OE2  | 3:D:910:SER:HB3   | 1.81                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:93:PRO:HA     | 2:C:117:HIS:CB    | 2.10                     | 0.80              |
| 2:C:581:THR:HA    | 2:C:903:SER:O     | 1.81                     | 0.80              |
| 3:D:1042:ARG:HH11 | 3:D:1042:ARG:HB3  | 1.45                     | 0.80              |
| 3:D:96:ALA:CB     | 3:D:554:LEU:HD23  | 2.09                     | 0.80              |
| 2:C:13:ILE:HD12   | 2:C:14:PRO:HD2    | 1.63                     | 0.80              |
| 3:D:1011:PHE:HB3  | 3:D:1021:TYR:CD2  | 2.16                     | 0.80              |
| 2:C:1081:VAL:HG13 | 2:C:1086:ARG:HE   | 1.46                     | 0.79              |
| 3:D:117:ASP:HB2   | 3:D:495:ARG:HH12  | 1.47                     | 0.79              |
| 3:D:964:LEU:O     | 3:D:968:ASP:HB2   | 1.82                     | 0.79              |
| 2:C:971:LYS:HA    | 2:C:988:VAL:HA    | 1.65                     | 0.79              |
| 3:D:1434:TRP:NE1  | 3:D:1457:ASP:HB2  | 1.98                     | 0.78              |
| 2:C:1092:LEU:HD13 | 2:C:1099:VAL:HG21 | 1.63                     | 0.78              |
| 3:D:836:VAL:N     | 3:D:837:GLY:HA3   | 1.96                     | 0.78              |
| 2:C:737:LEU:O     | 2:C:739:GLU:N     | 2.16                     | 0.78              |
| 3:D:1091:SER:C    | 3:D:1093:TYR:H    | 1.87                     | 0.78              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:H     | 1.49                     | 0.78              |
| 2:C:695:LEU:HD21  | 2:C:833:LEU:HB3   | 1.65                     | 0.78              |
| 2:C:1083:GLU:OE1  | 3:D:87:ARG:NH1    | 2.18                     | 0.77              |
| 1:B:86:VAL:HG13   | 1:B:123:MET:HB2   | 1.66                     | 0.77              |
| 3:D:1312:LEU:HD13 | 3:D:1327:ARG:HG2  | 1.67                     | 0.76              |
| 3:D:1201:CYS:SG   | 3:D:1204:CYS:HB2  | 2.25                     | 0.76              |
| 1:A:128:HIS:CE1   | 1:A:131:THR:HG23  | 2.18                     | 0.76              |
| 2:C:878:SER:N     | 11:C:1301:HOH:O   | 2.07                     | 0.76              |
| 2:C:436:GLY:HA2   | 2:C:538:GLN:O     | 1.86                     | 0.76              |
| 1:A:23:PHE:HE2    | 1:A:208:LEU:HD13  | 1.51                     | 0.75              |
| 3:D:1041:LEU:HD12 | 3:D:1058:ARG:HA   | 1.66                     | 0.75              |
| 3:D:1031:ASN:H    | 3:D:1034:GLN:HE21 | 1.34                     | 0.75              |
| 4:E:26:ARG:HH21   | 4:E:30:LEU:HD13   | 1.52                     | 0.75              |
| 3:D:8:VAL:HG12    | 3:D:1434:TRP:CZ2  | 2.18                     | 0.75              |
| 3:D:632:VAL:O     | 3:D:727:GLN:HA    | 1.87                     | 0.75              |
| 2:C:859:PRO:O     | 2:C:867:VAL:HG22  | 1.87                     | 0.74              |
| 3:D:1496:GLU:HA   | 3:D:1499:ARG:CB   | 2.16                     | 0.74              |
| 2:C:490:GLU:HG2   | 2:C:493:ARG:HH21  | 1.51                     | 0.74              |
| 3:D:97:THR:HG21   | 3:D:571:LYS:HD3   | 1.69                     | 0.74              |
| 1:B:58:ILE:HD12   | 1:B:61:VAL:HB     | 1.70                     | 0.74              |
| 3:D:351:MET:HG2   | 3:D:370:ALA:HA    | 1.69                     | 0.74              |
| 3:D:885:ILE:HG21  | 3:D:937:TYR:HD1   | 1.53                     | 0.74              |
| 2:C:261:ILE:O     | 2:C:264:PRO:HD3   | 1.88                     | 0.73              |
| 3:D:907:GLU:O     | 3:D:911:LEU:HD12  | 1.89                     | 0.73              |
| 2:C:325:ILE:HD12  | 2:C:325:ILE:H     | 1.54                     | 0.73              |
| 1:A:96:THR:HB     | 1:A:145:ASP:OD2   | 1.88                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:776:SER:HA    | 2:C:780:GLU:HB2   | 1.69                     | 0.72              |
| 3:D:698:LYS:HA    | 3:D:756:GLN:HE22  | 1.53                     | 0.72              |
| 3:D:947:ILE:HG13  | 3:D:948:THR:N     | 2.04                     | 0.72              |
| 3:D:1378:TYR:HD1  | 3:D:1422:MET:SD   | 2.11                     | 0.72              |
| 5:F:152:ASP:N     | 5:F:153:PRO:HD3   | 2.05                     | 0.72              |
| 5:F:208:SER:O     | 5:F:212:LEU:HG    | 1.88                     | 0.72              |
| 3:D:1368:ILE:HD12 | 3:D:1368:ILE:H    | 1.55                     | 0.71              |
| 2:C:738:ASP:O     | 2:C:740:GLU:N     | 2.22                     | 0.71              |
| 3:D:646:LYS:HA    | 3:D:720:LEU:HD22  | 1.72                     | 0.71              |
| 3:D:1459:LEU:HA   | 3:D:1464:GLU:HG3  | 1.72                     | 0.71              |
| 3:D:661:MET:HA    | 3:D:666:ILE:HD12  | 1.71                     | 0.70              |
| 3:D:1380:GLU:HB2  | 3:D:1420:LEU:HD11 | 1.73                     | 0.70              |
| 1:B:38:ASN:ND2    | 2:C:979:THR:HA    | 2.06                     | 0.70              |
| 2:C:181:VAL:HA    | 2:C:220:GLY:HA2   | 1.74                     | 0.70              |
| 2:C:214:TYR:CE1   | 2:C:311:PHE:HB3   | 2.26                     | 0.70              |
| 5:F:135:ILE:HD11  | 5:F:178:ARG:HA    | 1.72                     | 0.70              |
| 3:D:1208:ASP:O    | 3:D:1209:LEU:HB2  | 1.90                     | 0.70              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:H      | 1.57                     | 0.70              |
| 2:C:425:PHE:O     | 2:C:429:ASP:HB2   | 1.92                     | 0.69              |
| 2:C:724:ARG:NE    | 2:C:738:ASP:HA    | 2.07                     | 0.69              |
| 3:D:158:TYR:HE1   | 3:D:454:ALA:HB3   | 1.57                     | 0.69              |
| 2:C:277:ALA:HA    | 2:C:280:LYS:HB2   | 1.74                     | 0.69              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CG    | 2.22                     | 0.69              |
| 2:C:672:VAL:HG22  | 2:C:868:ASP:CB    | 2.23                     | 0.69              |
| 2:C:536:PRO:O     | 2:C:539:VAL:HG23  | 1.92                     | 0.69              |
| 2:C:848:VAL:CG1   | 3:D:632:VAL:HG23  | 2.23                     | 0.69              |
| 3:D:791:TYR:CE2   | 3:D:945:SER:HB2   | 2.28                     | 0.69              |
| 3:D:1213:ARG:HH11 | 3:D:1213:ARG:CG   | 2.05                     | 0.69              |
| 2:C:430:VAL:HG13  | 3:D:1075:HIS:HD2  | 1.58                     | 0.68              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:CG2   | 2.23                     | 0.68              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:HG22  | 1.75                     | 0.68              |
| 2:C:1093:GLN:HB3  | 3:D:90:MET:HE2    | 1.76                     | 0.68              |
| 3:D:631:ILE:HG21  | 3:D:745:MET:HG3   | 1.75                     | 0.68              |
| 3:D:1139:ASP:O    | 3:D:1142:ALA:HB3  | 1.94                     | 0.68              |
| 2:C:838:LYS:CG    | 2:C:997:LEU:HB2   | 2.21                     | 0.67              |
| 2:C:263:ASP:N     | 2:C:264:PRO:HD3   | 2.10                     | 0.67              |
| 2:C:193:LEU:HD21  | 2:C:307:LEU:HD21  | 1.76                     | 0.67              |
| 2:C:840:ALA:HA    | 2:C:845:ASN:O     | 1.95                     | 0.67              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:HG2   | 1.76                     | 0.67              |
| 3:D:317:VAL:HG23  | 3:D:337:LEU:HA    | 1.76                     | 0.67              |
| 3:D:482:LYS:H     | 3:D:489:ARG:HG3   | 1.60                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:592:THR:HG23  | 3:D:600:LEU:HD21  | 1.76                     | 0.67              |
| 2:C:1008:ARG:NH2  | 2:C:1020:PRO:HB3  | 2.09                     | 0.67              |
| 5:F:222:ARG:HG2   | 5:F:242:TRP:CZ3   | 2.30                     | 0.67              |
| 2:C:704:HIS:HB3   | 11:C:1308:HOH:O   | 1.95                     | 0.66              |
| 2:C:843:HIS:HE1   | 2:C:887:GLU:OE1   | 1.78                     | 0.66              |
| 3:D:1351:GLU:HA   | 3:D:1354:LYS:HD3  | 1.76                     | 0.66              |
| 3:D:836:VAL:H     | 3:D:837:GLY:CA    | 2.05                     | 0.66              |
| 1:B:45:LEU:HD11   | 11:B:401:HOH:O    | 1.95                     | 0.66              |
| 3:D:1261:GLU:O    | 3:D:1265:ALA:HB2  | 1.96                     | 0.66              |
| 3:D:630:VAL:HG13  | 3:D:725:SER:HB3   | 1.76                     | 0.66              |
| 3:D:964:LEU:CD2   | 3:D:1058:ARG:HG2  | 2.23                     | 0.66              |
| 5:F:370:LYS:HA    | 5:F:374:GLY:CA    | 2.25                     | 0.66              |
| 3:D:1225:ALA:O    | 3:D:1229:ILE:HG13 | 1.96                     | 0.65              |
| 3:D:1397:LYS:HB2  | 3:D:1398:TRP:CZ3  | 2.32                     | 0.65              |
| 3:D:1442:ASN:HD21 | 3:D:1444:THR:HB   | 1.60                     | 0.65              |
| 2:C:1102:LEU:HB3  | 2:C:1106:ASP:HA   | 1.78                     | 0.65              |
| 3:D:108:VAL:HG12  | 3:D:109:PRO:HA    | 1.79                     | 0.65              |
| 2:C:140:ILE:HD12  | 2:C:331:ARG:NH2   | 2.12                     | 0.65              |
| 2:C:846:LYS:HE2   | 3:D:741:ASP:O     | 1.97                     | 0.65              |
| 3:D:885:ILE:CG2   | 3:D:937:TYR:HD1   | 2.10                     | 0.65              |
| 3:D:1258:ARG:NH2  | 3:D:1262:LEU:HD21 | 2.10                     | 0.65              |
| 3:D:702:LEU:O     | 3:D:713:ILE:HA    | 1.96                     | 0.65              |
| 2:C:949:LYS:HD2   | 3:D:796:ARG:NH2   | 2.11                     | 0.65              |
| 2:C:91:GLN:HB3    | 2:C:119:PRO:HA    | 1.79                     | 0.64              |
| 2:C:399:ASN:ND2   | 2:C:568:ALA:HB3   | 2.12                     | 0.64              |
| 2:C:673:LEU:HD11  | 2:C:895:TYR:CZ    | 2.31                     | 0.64              |
| 1:A:38:ASN:O      | 1:A:41:ARG:N      | 2.30                     | 0.64              |
| 2:C:317:VAL:N     | 2:C:318:PRO:HD3   | 2.13                     | 0.64              |
| 2:C:1086:ARG:HD3  | 2:C:1112:PHE:CD2  | 2.33                     | 0.64              |
| 2:C:588:VAL:HG13  | 2:C:593:ALA:HB3   | 1.79                     | 0.64              |
| 3:D:633:VAL:HG13  | 3:D:635:PRO:HD3   | 1.78                     | 0.64              |
| 2:C:707:ARG:HG3   | 2:C:826:TYR:CE2   | 2.33                     | 0.64              |
| 5:F:379:ARG:HD3   | 5:F:382:THR:HB    | 1.78                     | 0.64              |
| 1:A:200:TRP:HE3   | 1:A:200:TRP:H     | 1.45                     | 0.64              |
| 2:C:1081:VAL:CG1  | 2:C:1086:ARG:HE   | 2.09                     | 0.64              |
| 2:C:116:GLY:HA3   | 2:C:378:LEU:HD23  | 1.78                     | 0.64              |
| 2:C:911:GLU:N     | 2:C:912:PRO:HD2   | 2.11                     | 0.64              |
| 2:C:1090:LYS:HA   | 2:C:1093:GLN:HB2  | 1.80                     | 0.64              |
| 3:D:659:LYS:HE3   | 3:D:663:GLU:HG3   | 1.77                     | 0.64              |
| 3:D:1102:THR:HG21 | 3:D:1371:VAL:HG22 | 1.79                     | 0.64              |
| 3:D:1232:PRO:HG2  | 3:D:1356:TYR:HE2  | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:574:LEU:O     | 3:D:578:VAL:HG23  | 1.98                     | 0.63              |
| 2:C:640:ARG:HH11  | 2:C:642:ARG:HH22  | 1.46                     | 0.63              |
| 3:D:183:GLU:O     | 3:D:202:VAL:HG13  | 1.98                     | 0.63              |
| 2:C:1052:MET:HG3  | 3:D:623:VAL:HG21  | 1.79                     | 0.63              |
| 3:D:791:TYR:CD2   | 3:D:945:SER:HB2   | 2.34                     | 0.63              |
| 2:C:1009:SER:HB3  | 3:D:651:GLU:OE2   | 1.98                     | 0.63              |
| 3:D:941:PHE:O     | 3:D:945:SER:HB3   | 1.98                     | 0.63              |
| 1:A:111:ALA:HB2   | 1:A:127:LEU:HD23  | 1.79                     | 0.63              |
| 3:D:885:ILE:CG2   | 3:D:937:TYR:CD1   | 2.82                     | 0.63              |
| 5:F:367:MET:HA    | 5:F:370:LYS:HB2   | 1.80                     | 0.63              |
| 1:A:24:VAL:HG13   | 1:A:196:THR:HG23  | 1.80                     | 0.63              |
| 2:C:575:GLN:NE2   | 2:C:670:GLN:HG2   | 2.14                     | 0.63              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:HD3   | 1.81                     | 0.62              |
| 1:A:73:GLU:HB3    | 1:A:78:ILE:HG12   | 1.81                     | 0.62              |
| 3:D:535:PHE:O     | 5:F:314:PRO:HB2   | 1.99                     | 0.62              |
| 3:D:969:ARG:O     | 3:D:972:LEU:HB2   | 1.99                     | 0.62              |
| 2:C:202:TYR:HE2   | 2:C:300:ASP:HB3   | 1.63                     | 0.62              |
| 2:C:396:ASP:HA    | 2:C:633:GLN:NE2   | 2.11                     | 0.62              |
| 2:C:1012:PRO:HD3  | 2:C:1026:GLN:HG2  | 1.81                     | 0.62              |
| 2:C:710:ILE:HB    | 2:C:790:LEU:HD22  | 1.80                     | 0.62              |
| 3:D:45:PHE:O      | 3:D:86:ARG:NH2    | 2.32                     | 0.62              |
| 2:C:363:SER:H     | 2:C:367:LEU:HD21  | 1.64                     | 0.62              |
| 3:D:1127:GLU:HB3  | 3:D:1131:SER:HB3  | 1.82                     | 0.62              |
| 1:A:110:LYS:HB2   | 1:A:112:ARG:HG2   | 1.81                     | 0.62              |
| 2:C:430:VAL:HG13  | 3:D:1075:HIS:CD2  | 2.34                     | 0.62              |
| 2:C:1018:GLN:HG3  | 2:C:1060:ILE:HD11 | 1.80                     | 0.62              |
| 3:D:845:ASN:HB2   | 3:D:846:PRO:CD    | 2.29                     | 0.62              |
| 1:A:206:THR:HG22  | 1:A:208:LEU:H     | 1.65                     | 0.61              |
| 3:D:728:LEU:HD13  | 3:D:745:MET:CE    | 2.27                     | 0.61              |
| 2:C:575:GLN:HE21  | 2:C:671:ASN:H     | 1.48                     | 0.61              |
| 3:D:1074:SER:HA   | 3:D:1077:ALA:HB3  | 1.81                     | 0.61              |
| 3:D:1341:PRO:HD2  | 3:D:1342:GLU:OE2  | 2.00                     | 0.61              |
| 2:C:441:VAL:O     | 2:C:441:VAL:CG2   | 2.48                     | 0.61              |
| 2:C:1087:VAL:HG22 | 3:D:524:LEU:HD22  | 1.81                     | 0.61              |
| 3:D:1397:LYS:C    | 3:D:1398:TRP:HE3  | 2.03                     | 0.61              |
| 2:C:194:VAL:HA    | 2:C:197:LEU:HD12  | 1.81                     | 0.61              |
| 3:D:1152:GLU:HG3  | 3:D:1161:GLU:HA   | 1.83                     | 0.61              |
| 2:C:843:HIS:CE1   | 2:C:887:GLU:OE1   | 2.53                     | 0.61              |
| 2:C:1030:GLN:OE1  | 3:D:628:ARG:HB2   | 2.00                     | 0.61              |
| 3:D:703:ASN:HB2   | 3:D:713:ILE:HG12  | 1.81                     | 0.61              |
| 2:C:720:GLU:HB3   | 2:C:760:SER:HA    | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:838:ARG:HH11  | 3:D:874:GLU:HB3   | 1.66                     | 0.61              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HB    | 1.82                     | 0.61              |
| 3:D:703:ASN:ND2   | 3:D:707:THR:OG1   | 2.33                     | 0.61              |
| 3:D:520:LEU:O     | 3:D:525:ARG:NH1   | 2.34                     | 0.60              |
| 3:D:616:GLN:HA    | 3:D:619:LEU:HD12  | 1.81                     | 0.60              |
| 3:D:711:LEU:HD13  | 3:D:778:LEU:HD23  | 1.82                     | 0.60              |
| 2:C:469:THR:HG22  | 2:C:538:GLN:NE2   | 2.12                     | 0.60              |
| 2:C:971:LYS:HB2   | 2:C:986:PRO:HB2   | 1.83                     | 0.60              |
| 2:C:711:GLU:O     | 2:C:758:ARG:NH1   | 2.32                     | 0.60              |
| 2:C:553:ASP:OD1   | 2:C:843:HIS:CD2   | 2.54                     | 0.60              |
| 3:D:781:PRO:HG2   | 3:D:911:LEU:HD22  | 1.84                     | 0.60              |
| 2:C:1039:ALA:HB2  | 3:D:707:THR:HG21  | 1.84                     | 0.60              |
| 1:B:124:ASN:HD22  | 1:B:127:LEU:HD13  | 1.67                     | 0.60              |
| 2:C:469:THR:CG2   | 2:C:538:GLN:HE21  | 2.10                     | 0.60              |
| 2:C:807:ARG:HA    | 2:C:821:GLU:HB2   | 1.84                     | 0.60              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:OE1    | 2.01                     | 0.60              |
| 3:D:1433:SER:HA   | 3:D:1457:ASP:OD2  | 2.01                     | 0.60              |
| 2:C:807:ARG:CZ    | 2:C:807:ARG:HB3   | 2.31                     | 0.60              |
| 3:D:729:HIS:HE1   | 3:D:932:ASP:OD1   | 1.85                     | 0.60              |
| 3:D:795:VAL:HG12  | 3:D:876:SER:HB3   | 1.84                     | 0.60              |
| 3:D:885:ILE:HG23  | 3:D:937:TYR:CE1   | 2.36                     | 0.60              |
| 2:C:772:ARG:HG2   | 5:F:373:LYS:HD3   | 1.84                     | 0.59              |
| 2:C:885:ILE:HG22  | 2:C:889:HIS:CE1   | 2.36                     | 0.59              |
| 3:D:64:LYS:HB3    | 5:F:376:ILE:HB    | 1.84                     | 0.59              |
| 3:D:1145:TYR:CE2  | 3:D:1168:MET:HB2  | 2.36                     | 0.59              |
| 2:C:91:GLN:CB     | 2:C:119:PRO:HA    | 2.33                     | 0.59              |
| 2:C:177:GLU:HG2   | 2:C:178:PRO:HD2   | 1.84                     | 0.59              |
| 2:C:551:GLU:HG2   | 2:C:552:HIS:CD2   | 2.37                     | 0.59              |
| 5:F:101:GLU:HG3   | 5:F:104:ARG:HH12  | 1.66                     | 0.59              |
| 2:C:877:PRO:HG3   | 3:D:1023:MET:CE   | 2.32                     | 0.59              |
| 3:D:808:THR:N     | 3:D:809:PRO:HD2   | 2.17                     | 0.59              |
| 3:D:1140:ILE:HD13 | 3:D:1175:ILE:HG12 | 1.83                     | 0.59              |
| 10:D:1605:G4P:O3C | 10:D:1605:G4P:H4' | 2.02                     | 0.59              |
| 1:B:209:GLU:O     | 1:B:213:GLN:HG2   | 2.01                     | 0.59              |
| 3:D:1127:GLU:HB3  | 3:D:1131:SER:CB   | 2.32                     | 0.59              |
| 1:B:226:SER:O     | 1:B:228:PRO:HD3   | 2.02                     | 0.59              |
| 2:C:3:ILE:HG22    | 2:C:900:ARG:HB2   | 1.84                     | 0.59              |
| 3:D:17:LYS:O      | 3:D:20:SER:HB3    | 2.03                     | 0.59              |
| 3:D:709:HIS:ND1   | 3:D:1231:GLU:HG3  | 2.18                     | 0.59              |
| 1:A:42:ARG:HH21   | 2:C:978:ARG:HG3   | 1.67                     | 0.59              |
| 2:C:1009:SER:HB2  | 3:D:651:GLU:O     | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1352:ILE:HG21 | 3:D:1368:ILE:HG21 | 1.85                     | 0.59              |
| 1:B:66:SER:O      | 1:B:75:VAL:HG23   | 2.03                     | 0.59              |
| 3:D:770:LEU:HA    | 3:D:777:PRO:HA    | 1.85                     | 0.59              |
| 3:D:890:VAL:O     | 3:D:926:LYS:HD3   | 2.02                     | 0.59              |
| 3:D:628:ARG:HG2   | 3:D:629:SER:N     | 2.18                     | 0.58              |
| 1:A:58:ILE:HB     | 1:A:61:VAL:HG22   | 1.85                     | 0.58              |
| 3:D:558:LEU:HD23  | 3:D:567:ILE:HD12  | 1.85                     | 0.58              |
| 3:D:838:ARG:HD3   | 3:D:874:GLU:CD    | 2.22                     | 0.58              |
| 5:F:79:ASP:N      | 5:F:80:PRO:HD2    | 2.18                     | 0.58              |
| 3:D:527:MET:O     | 3:D:527:MET:HG3   | 2.03                     | 0.58              |
| 5:F:319:THR:O     | 5:F:329:TYR:N     | 2.32                     | 0.58              |
| 2:C:640:ARG:NH1   | 2:C:642:ARG:HH22  | 2.01                     | 0.58              |
| 2:C:1032:PHE:HZ   | 2:C:1040:LEU:HD11 | 1.67                     | 0.58              |
| 3:D:1091:SER:C    | 3:D:1093:TYR:N    | 2.55                     | 0.58              |
| 2:C:405:ARG:HD2   | 2:C:442:GLU:OE2   | 2.03                     | 0.58              |
| 2:C:971:LYS:CB    | 2:C:986:PRO:HB2   | 2.34                     | 0.58              |
| 3:D:65:ARG:HG3    | 3:D:66:GLN:H      | 1.67                     | 0.58              |
| 3:D:1440:PHE:HE2  | 3:D:1463:LYS:HZ3  | 1.52                     | 0.58              |
| 3:D:1378:TYR:CE1  | 3:D:1430:SER:HB2  | 2.39                     | 0.58              |
| 2:C:435:TYR:HA    | 3:D:1071:PHE:HE2  | 1.69                     | 0.58              |
| 3:D:1400:VAL:HG12 | 3:D:1404:ASN:HD21 | 1.69                     | 0.58              |
| 2:C:395:LYS:HE2   | 2:C:403:SER:OG    | 2.04                     | 0.58              |
| 2:C:877:PRO:HG3   | 3:D:1023:MET:HE3  | 1.85                     | 0.58              |
| 2:C:281:LEU:HB3   | 2:C:305:PRO:HB2   | 1.86                     | 0.57              |
| 3:D:374:GLU:HB3   | 3:D:376:GLU:HG3   | 1.86                     | 0.57              |
| 5:F:367:MET:O     | 5:F:371:LEU:HG    | 2.04                     | 0.57              |
| 1:B:151:VAL:HB    | 1:B:169:ALA:HB3   | 1.84                     | 0.57              |
| 3:D:1362:LYS:HD3  | 11:D:1752:HOH:O   | 2.04                     | 0.57              |
| 3:D:1481:VAL:CG1  | 4:E:18:ARG:HA     | 2.34                     | 0.57              |
| 5:F:350:LEU:O     | 5:F:354:LEU:HG    | 2.03                     | 0.57              |
| 2:C:140:ILE:HD12  | 2:C:331:ARG:HH22  | 1.67                     | 0.57              |
| 2:C:441:VAL:O     | 2:C:441:VAL:HG23  | 2.03                     | 0.57              |
| 3:D:112:ILE:HG22  | 3:D:512:MET:HE3   | 1.86                     | 0.57              |
| 3:D:860:LEU:HA    | 3:D:877:PRO:HD2   | 1.85                     | 0.57              |
| 3:D:634:GLY:O     | 3:D:637:LEU:HB2   | 2.03                     | 0.57              |
| 3:D:852:ALA:HB1   | 3:D:857:ILE:HG12  | 1.85                     | 0.57              |
| 3:D:1205:TYR:CZ   | 3:D:1221:VAL:HG22 | 2.39                     | 0.57              |
| 1:A:38:ASN:O      | 1:A:39:PRO:C      | 2.41                     | 0.57              |
| 3:D:568:ARG:O     | 3:D:571:LYS:N     | 2.37                     | 0.57              |
| 3:D:992:ILE:O     | 3:D:995:LEU:HB3   | 2.03                     | 0.57              |
| 3:D:1115:THR:O    | 3:D:1151:ARG:NH2  | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1295:GLU:HG2  | 3:D:1300:SER:HA   | 1.86                     | 0.57              |
| 1:A:41:ARG:HG3    | 1:A:45:LEU:HD12   | 1.86                     | 0.57              |
| 3:D:770:LEU:HD11  | 3:D:919:PHE:CE1   | 2.39                     | 0.57              |
| 3:D:262:LYS:HD3   | 3:D:269:PHE:HD2   | 1.70                     | 0.57              |
| 3:D:549:ASN:O     | 3:D:553:ARG:HB2   | 2.04                     | 0.57              |
| 1:A:181:VAL:HG12  | 1:A:181:VAL:O     | 2.05                     | 0.56              |
| 3:D:320:ALA:HB3   | 3:D:336:PHE:HD1   | 1.70                     | 0.56              |
| 2:C:271:GLU:H     | 2:C:274:ARG:HD3   | 1.70                     | 0.56              |
| 2:C:274:ARG:HD2   | 2:C:285:LEU:HB3   | 1.87                     | 0.56              |
| 2:C:728:HIS:NE2   | 2:C:730:SER:O     | 2.38                     | 0.56              |
| 2:C:889:HIS:CD2   | 2:C:970:GLY:HA3   | 2.41                     | 0.56              |
| 3:D:421:LEU:HD22  | 3:D:429:SER:HB2   | 1.85                     | 0.56              |
| 1:B:167:VAL:HG12  | 1:B:168:ASP:N     | 2.17                     | 0.56              |
| 2:C:712:ALA:HB3   | 2:C:821:GLU:H     | 1.70                     | 0.56              |
| 2:C:713:ARG:HG2   | 2:C:819:VAL:HG22  | 1.86                     | 0.56              |
| 2:C:890:LEU:HG    | 2:C:901:TYR:CD1   | 2.40                     | 0.56              |
| 3:D:1155:VAL:HG11 | 3:D:1174:LEU:HD23 | 1.88                     | 0.56              |
| 2:C:501:THR:O     | 2:C:503:LEU:HD13  | 2.06                     | 0.56              |
| 5:F:417:LYS:HB2   | 5:F:418:LEU:HD12  | 1.87                     | 0.56              |
| 2:C:6:PHE:HB2     | 2:C:902:ILE:O     | 2.06                     | 0.56              |
| 2:C:712:ALA:O     | 2:C:820:ARG:N     | 2.38                     | 0.56              |
| 2:C:1008:ARG:HH21 | 2:C:1020:PRO:HB3  | 1.68                     | 0.56              |
| 3:D:935:LYS:HG2   | 3:D:939:PHE:CE1   | 2.41                     | 0.56              |
| 2:C:17:PRO:O      | 2:C:20:GLU:HB2    | 2.05                     | 0.56              |
| 2:C:234:ALA:O     | 2:C:238:LEU:HG    | 2.05                     | 0.56              |
| 2:C:469:THR:HG22  | 2:C:470:PRO:HD2   | 1.88                     | 0.56              |
| 2:C:695:LEU:HD21  | 2:C:833:LEU:CB    | 2.36                     | 0.56              |
| 3:D:408:GLU:O     | 3:D:409:VAL:HG22  | 2.06                     | 0.56              |
| 3:D:1190:SER:OG   | 3:D:1191:PRO:HD2  | 2.06                     | 0.56              |
| 1:B:86:VAL:HG22   | 1:B:123:MET:HG3   | 1.88                     | 0.56              |
| 2:C:99:GLN:HB2    | 2:C:109:LYS:HA    | 1.88                     | 0.56              |
| 3:D:400:VAL:HG12  | 3:D:445:ARG:HG2   | 1.86                     | 0.56              |
| 3:D:729:HIS:CD2   | 3:D:730:PRO:HD2   | 2.41                     | 0.56              |
| 3:D:824:ASN:ND2   | 3:D:862:ASP:OD2   | 2.39                     | 0.56              |
| 3:D:127:LEU:HD11  | 3:D:461:ILE:HG13  | 1.87                     | 0.56              |
| 3:D:1030:GLY:HA2  | 3:D:1034:GLN:NE2  | 2.21                     | 0.56              |
| 3:D:1379:VAL:HG13 | 3:D:1395:LEU:HB2  | 1.87                     | 0.56              |
| 2:C:426:ASP:O     | 2:C:428:ARG:N     | 2.38                     | 0.55              |
| 3:D:879:ARG:HB3   | 3:D:902:LEU:CD1   | 2.36                     | 0.55              |
| 3:D:916:TYR:CE2   | 3:D:920:LEU:HD21  | 2.40                     | 0.55              |
| 2:C:368:THR:HB    | 2:C:369:PRO:HD3   | 1.86                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:835:VAL:HA    | 2:C:849:VAL:O     | 2.05                     | 0.55              |
| 2:C:1015:LEU:HA   | 5:F:335:ASP:HB2   | 1.89                     | 0.55              |
| 3:D:711:LEU:HD13  | 3:D:778:LEU:CD2   | 2.35                     | 0.55              |
| 2:C:881:ASN:O     | 2:C:884:GLN:HG2   | 2.06                     | 0.55              |
| 3:D:272:LEU:HG    | 3:D:282:TYR:HE1   | 1.71                     | 0.55              |
| 2:C:496:ILE:HG12  | 2:C:531:PHE:HB2   | 1.88                     | 0.55              |
| 5:F:207:LEU:HB3   | 5:F:212:LEU:HD21  | 1.88                     | 0.55              |
| 2:C:672:VAL:HG22  | 2:C:868:ASP:HB2   | 1.89                     | 0.55              |
| 2:C:99:GLN:H      | 2:C:110:GLU:HB2   | 1.71                     | 0.55              |
| 1:A:32:PHE:HA     | 1:A:35:THR:HB     | 1.88                     | 0.55              |
| 2:C:557:ARG:HD3   | 2:C:879:ARG:HG3   | 1.89                     | 0.55              |
| 2:C:1032:PHE:CE1  | 2:C:1052:MET:HG2  | 2.42                     | 0.55              |
| 3:D:522:PRO:HA    | 3:D:525:ARG:NH1   | 2.21                     | 0.55              |
| 3:D:798:GLU:HG3   | 3:D:824:ASN:HB2   | 1.89                     | 0.55              |
| 4:E:39:VAL:O      | 4:E:72:ARG:HD2    | 2.07                     | 0.55              |
| 2:C:553:ASP:OD1   | 2:C:843:HIS:HD2   | 1.89                     | 0.55              |
| 2:C:1081:VAL:HG13 | 2:C:1086:ARG:NE   | 2.20                     | 0.55              |
| 3:D:634:GLY:HA3   | 3:D:637:LEU:HD12  | 1.88                     | 0.55              |
| 3:D:770:LEU:HB2   | 3:D:1210:SER:HA   | 1.87                     | 0.55              |
| 3:D:1229:ILE:O    | 3:D:1229:ILE:HG22 | 2.06                     | 0.55              |
| 3:D:1353:GLN:O    | 3:D:1357:ARG:HG2  | 2.06                     | 0.55              |
| 3:D:1127:GLU:HB3  | 3:D:1131:SER:OG   | 2.07                     | 0.54              |
| 2:C:595:LEU:HD12  | 2:C:639:GLN:NE2   | 2.22                     | 0.54              |
| 3:D:1047:LYS:HB3  | 3:D:1048:PRO:CD   | 2.30                     | 0.54              |
| 1:A:181:VAL:N     | 2:C:937:ASP:OD2   | 2.32                     | 0.54              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:HD3   | 2.42                     | 0.54              |
| 2:C:34:VAL:N      | 2:C:35:PRO:CD     | 2.68                     | 0.54              |
| 3:D:216:VAL:HG22  | 3:D:340:THR:HG22  | 1.87                     | 0.54              |
| 3:D:1314:LYS:HB3  | 3:D:1317:ASP:OD2  | 2.07                     | 0.54              |
| 2:C:83:CYS:HB3    | 2:C:88:LEU:O      | 2.07                     | 0.54              |
| 2:C:164:PRO:HB2   | 2:C:166:PRO:HD3   | 1.89                     | 0.54              |
| 2:C:512:ARG:HD3   | 2:C:523:ILE:HD12  | 1.90                     | 0.54              |
| 3:D:570:GLU:OE2   | 5:F:214:GLN:NE2   | 2.36                     | 0.54              |
| 3:D:835:SER:N     | 3:D:838:ARG:HE    | 2.06                     | 0.54              |
| 3:D:1369:GLU:O    | 3:D:1372:VAL:HG12 | 2.08                     | 0.54              |
| 3:D:822:ALA:HB3   | 3:D:825:ALA:HB2   | 1.88                     | 0.54              |
| 2:C:108:ILE:HD12  | 2:C:368:THR:HG21  | 1.90                     | 0.54              |
| 3:D:1145:TYR:HE2  | 3:D:1168:MET:HB2  | 1.71                     | 0.54              |
| 2:C:181:VAL:HG12  | 2:C:182:VAL:H     | 1.73                     | 0.54              |
| 3:D:436:GLU:HB2   | 3:D:445:ARG:HB2   | 1.88                     | 0.54              |
| 3:D:835:SER:H     | 3:D:838:ARG:HE    | 1.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1459:LEU:HD12 | 3:D:1470:ARG:HH11 | 1.73                     | 0.54              |
| 2:C:637:LEU:O     | 2:C:638:ASP:HB3   | 2.08                     | 0.54              |
| 3:D:353:VAL:HG12  | 3:D:368:VAL:HG22  | 1.90                     | 0.54              |
| 1:A:38:ASN:O      | 1:A:40:LEU:N      | 2.41                     | 0.53              |
| 1:A:24:VAL:HG11   | 1:A:194:LYS:HE2   | 1.90                     | 0.53              |
| 4:E:33:HIS:HB2    | 4:E:37:ASN:HD21   | 1.72                     | 0.53              |
| 5:F:200:LYS:HA    | 5:F:209:PHE:CE1   | 2.44                     | 0.53              |
| 3:D:1332:PRO:HB2  | 3:D:1421:LEU:CD2  | 2.38                     | 0.53              |
| 5:F:300:ASP:HB3   | 5:F:303:ARG:HB2   | 1.89                     | 0.53              |
| 1:A:23:PHE:CE2    | 1:A:208:LEU:HD13  | 2.39                     | 0.53              |
| 2:C:861:LEU:CD2   | 2:C:972:VAL:HG21  | 2.38                     | 0.53              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:OE1   | 2.08                     | 0.53              |
| 1:B:85:LEU:HA     | 1:B:124:ASN:HD21  | 1.72                     | 0.53              |
| 2:C:89:THR:HG23   | 2:C:129:ILE:HA    | 1.90                     | 0.53              |
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HB2   | 1.89                     | 0.53              |
| 2:C:393:GLN:OE1   | 2:C:406:HIS:HE1   | 1.92                     | 0.53              |
| 2:C:1114:GLY:O    | 2:C:1116:ALA:N    | 2.41                     | 0.53              |
| 3:D:1066:THR:HB   | 3:D:1069:GLU:H    | 1.74                     | 0.53              |
| 2:C:1020:PRO:HG3  | 3:D:624:ASP:OD1   | 2.09                     | 0.53              |
| 3:D:38:LYS:HG3    | 3:D:39:PRO:HD2    | 1.90                     | 0.53              |
| 3:D:698:LYS:HA    | 3:D:756:GLN:NE2   | 2.22                     | 0.53              |
| 3:D:1012:GLU:HA   | 3:D:1012:GLU:OE1  | 2.08                     | 0.53              |
| 3:D:1264:GLU:HA   | 3:D:1423:GLY:HA3  | 1.91                     | 0.53              |
| 5:F:117:SER:HB2   | 5:F:122:LEU:O     | 2.09                     | 0.53              |
| 2:C:84:ARG:HA     | 2:C:131:GLY:HA2   | 1.90                     | 0.53              |
| 2:C:455:LEU:HG    | 2:C:459:ALA:HB3   | 1.89                     | 0.53              |
| 2:C:862:PRO:HA    | 2:C:975:TYR:HE1   | 1.74                     | 0.53              |
| 3:D:15:PRO:HA     | 3:D:18:ILE:HD12   | 1.90                     | 0.53              |
| 3:D:1046:GLN:N    | 11:D:1702:HOH:O   | 2.29                     | 0.53              |
| 2:C:468:ARG:HE    | 2:C:487:THR:HG23  | 1.73                     | 0.53              |
| 3:D:792:ILE:O     | 3:D:878:GLY:HA3   | 2.08                     | 0.53              |
| 3:D:165:LYS:HD3   | 3:D:199:LEU:HD11  | 1.90                     | 0.53              |
| 3:D:925:GLU:HG3   | 4:E:2:ALA:HB3     | 1.91                     | 0.53              |
| 3:D:1397:LYS:HB2  | 3:D:1398:TRP:HZ3  | 1.73                     | 0.53              |
| 3:D:1481:VAL:O    | 3:D:1482:ARG:C    | 2.47                     | 0.53              |
| 5:F:152:ASP:N     | 5:F:153:PRO:CD    | 2.72                     | 0.53              |
| 5:F:416:ARG:HG2   | 5:F:419:ARG:HD2   | 1.91                     | 0.53              |
| 1:A:70:GLY:HA2    | 1:A:133:GLU:HG2   | 1.90                     | 0.52              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:HA2   | 1.91                     | 0.52              |
| 3:D:1370:ILE:HG22 | 3:D:1371:VAL:N    | 2.22                     | 0.52              |
| 5:F:172:ARG:O     | 5:F:176:ILE:HG12  | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:885:ILE:HG23  | 3:D:937:TYR:CD1   | 2.43                     | 0.52              |
| 3:D:1042:ARG:HB3  | 3:D:1042:ARG:NH1  | 2.19                     | 0.52              |
| 3:D:1462:LEU:HD23 | 3:D:1473:PRO:HG2  | 1.91                     | 0.52              |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA     | 1.92                     | 0.52              |
| 2:C:292:ARG:HB2   | 2:C:299:LYS:H     | 1.75                     | 0.52              |
| 2:C:444:PRO:HG2   | 2:C:448:ASN:O     | 2.09                     | 0.52              |
| 3:D:108:VAL:HA    | 3:D:109:PRO:C     | 2.30                     | 0.52              |
| 3:D:270:LEU:O     | 3:D:282:TYR:HB2   | 2.09                     | 0.52              |
| 2:C:1092:LEU:CD1  | 2:C:1099:VAL:HG21 | 2.34                     | 0.52              |
| 3:D:72:VAL:HG13   | 3:D:77:GLY:HA2    | 1.90                     | 0.52              |
| 5:F:137:GLY:HA2   | 5:F:140:ARG:HB3   | 1.91                     | 0.52              |
| 2:C:333:ILE:HD11  | 2:C:461:VAL:HG11  | 1.90                     | 0.52              |
| 3:D:94:GLU:O      | 3:D:551:ASN:ND2   | 2.43                     | 0.52              |
| 3:D:871:LYS:HD3   | 3:D:873:LEU:HD21  | 1.91                     | 0.52              |
| 2:C:1063:ARG:HG3  | 5:F:341:PRO:HG3   | 1.92                     | 0.52              |
| 3:D:1372:VAL:O    | 3:D:1375:MET:HB3  | 2.10                     | 0.52              |
| 3:D:1379:VAL:HG11 | 3:D:1395:LEU:HD13 | 1.90                     | 0.52              |
| 5:F:263:HIS:O     | 5:F:267:THR:HG23  | 2.10                     | 0.52              |
| 3:D:730:PRO:HA    | 3:D:733:CYS:SG    | 2.50                     | 0.52              |
| 3:D:704:ARG:CD    | 3:D:738:ALA:HB2   | 2.40                     | 0.52              |
| 3:D:1213:ARG:HG2  | 3:D:1213:ARG:NH1  | 2.05                     | 0.52              |
| 5:F:157:GLU:O     | 5:F:161:GLN:N     | 2.43                     | 0.52              |
| 2:C:551:GLU:HB3   | 2:C:906:PHE:CD2   | 2.45                     | 0.52              |
| 2:C:603:VAL:HG21  | 2:C:643:VAL:HG11  | 1.91                     | 0.51              |
| 1:A:225:PHE:HD2   | 1:B:11:PHE:CE1    | 2.28                     | 0.51              |
| 2:C:521:PRO:HG2   | 3:D:1055:VAL:HG21 | 1.93                     | 0.51              |
| 3:D:948:THR:O     | 3:D:949:ILE:CG1   | 2.58                     | 0.51              |
| 3:D:1381:VAL:HG13 | 3:D:1389:LEU:O    | 2.10                     | 0.51              |
| 1:B:177:VAL:HB    | 11:B:401:HOH:O    | 2.11                     | 0.51              |
| 2:C:72:ARG:HG3    | 2:C:95:TYR:HB2    | 1.92                     | 0.51              |
| 2:C:157:ARG:HG3   | 2:C:158:TYR:N     | 2.21                     | 0.51              |
| 2:C:1008:ARG:HD3  | 2:C:1010:THR:HA   | 1.92                     | 0.51              |
| 3:D:1489:GLN:HA   | 3:D:1492:LEU:HD12 | 1.92                     | 0.51              |
| 2:C:545:ASN:HB3   | 2:C:583:LEU:HD12  | 1.91                     | 0.51              |
| 3:D:57:GLU:HG2    | 3:D:58:CYS:H      | 1.76                     | 0.51              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:CD2   | 2.22                     | 0.51              |
| 1:A:106:PRO:HG3   | 1:A:134:GLU:HG2   | 1.93                     | 0.51              |
| 2:C:496:ILE:O     | 2:C:515:ALA:HB1   | 2.11                     | 0.51              |
| 3:D:361:VAL:HG21  | 3:D:385:VAL:HG23  | 1.93                     | 0.51              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:HB3   | 1.93                     | 0.51              |
| 2:C:81:ASP:HB3    | 2:C:626:ARG:HH22  | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:387:SER:HB3   | 2:C:388:ARG:HD3   | 1.92                     | 0.51              |
| 2:C:1052:MET:HG3  | 3:D:623:VAL:CG2   | 2.41                     | 0.51              |
| 3:D:440:VAL:HG23  | 3:D:441:ARG:H     | 1.75                     | 0.51              |
| 5:F:95:THR:HB     | 5:F:98:GLU:H      | 1.75                     | 0.51              |
| 2:C:603:VAL:HG23  | 2:C:647:GLN:O     | 2.10                     | 0.51              |
| 2:C:1067:TYR:CE2  | 2:C:1071:ILE:HG13 | 2.45                     | 0.51              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:HB    | 1.91                     | 0.51              |
| 2:C:443:THR:HG22  | 2:C:559:LEU:HD11  | 1.93                     | 0.51              |
| 2:C:810:ASP:N     | 2:C:811:PRO:CD    | 2.74                     | 0.51              |
| 2:C:1031:ARG:HA   | 3:D:621:LYS:O     | 2.10                     | 0.51              |
| 3:D:593:ASN:CB    | 3:D:594:PRO:HD3   | 2.40                     | 0.51              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:CD    | 2.35                     | 0.51              |
| 3:D:1281:VAL:HB   | 3:D:1316:GLY:H    | 1.75                     | 0.51              |
| 1:A:56:VAL:HG22   | 1:A:142:VAL:HG22  | 1.93                     | 0.51              |
| 1:A:156:HIS:HD2   | 1:A:158:ILE:HB    | 1.76                     | 0.51              |
| 3:D:95:LEU:HD21   | 3:D:517:VAL:HG23  | 1.91                     | 0.51              |
| 3:D:651:GLU:O     | 3:D:654:LYS:HB2   | 2.11                     | 0.51              |
| 3:D:778:LEU:HG    | 3:D:778:LEU:O     | 2.11                     | 0.51              |
| 3:D:1264:GLU:CD   | 3:D:1425:THR:HG1  | 2.13                     | 0.51              |
| 2:C:585:GLU:HA    | 2:C:664:GLY:O     | 2.11                     | 0.50              |
| 2:C:672:VAL:HG22  | 2:C:868:ASP:HB3   | 1.93                     | 0.50              |
| 3:D:731:LEU:HA    | 11:D:1701:HOH:O   | 2.11                     | 0.50              |
| 3:D:1292:VAL:HG11 | 3:D:1325:LEU:HD22 | 1.93                     | 0.50              |
| 2:C:657:ASP:OD1   | 2:C:661:SER:OG    | 2.29                     | 0.50              |
| 2:C:742:VAL:HG12  | 2:C:743:VAL:N     | 2.25                     | 0.50              |
| 3:D:1342:GLU:CD   | 3:D:1342:GLU:H    | 2.15                     | 0.50              |
| 1:A:139:ASN:C     | 1:A:139:ASN:OD1   | 2.50                     | 0.50              |
| 1:A:228:PRO:O     | 1:A:229:GLN:HB2   | 2.10                     | 0.50              |
| 1:B:63:HIS:CE1    | 3:D:809:PRO:HB3   | 2.47                     | 0.50              |
| 2:C:141:HIS:CE1   | 2:C:332:ARG:NH1   | 2.80                     | 0.50              |
| 2:C:625:LEU:O     | 2:C:626:ARG:C     | 2.50                     | 0.50              |
| 3:D:127:LEU:CD1   | 3:D:461:ILE:HG13  | 2.41                     | 0.50              |
| 3:D:917:GLN:C     | 3:D:919:PHE:H     | 2.14                     | 0.50              |
| 3:D:1397:LYS:HB2  | 3:D:1398:TRP:CE3  | 2.45                     | 0.50              |
| 5:F:120:THR:HB    | 5:F:122:LEU:HG    | 1.92                     | 0.50              |
| 2:C:842:ARG:NH1   | 11:C:1302:HOH:O   | 2.29                     | 0.50              |
| 3:D:137:PRO:HA    | 3:D:452:ILE:HG23  | 1.92                     | 0.50              |
| 3:D:860:LEU:HB3   | 3:D:878:GLY:N     | 2.25                     | 0.50              |
| 2:C:728:HIS:CG    | 2:C:729:LEU:H     | 2.29                     | 0.50              |
| 3:D:1347:TYR:CZ   | 3:D:1351:GLU:HG3  | 2.47                     | 0.50              |
| 2:C:1036:GLU:HG3  | 3:D:703:ASN:ND2   | 2.27                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:192:ALA:HB1   | 3:D:193:PRO:CD    | 2.33                     | 0.50              |
| 3:D:704:ARG:HD3   | 3:D:738:ALA:HB2   | 1.92                     | 0.50              |
| 2:C:1036:GLU:O    | 2:C:1039:ALA:HB3  | 2.11                     | 0.50              |
| 2:C:1083:GLU:O    | 2:C:1087:VAL:HB   | 2.12                     | 0.50              |
| 3:D:44:LEU:HB3    | 3:D:525:ARG:HH21  | 1.77                     | 0.50              |
| 3:D:206:ARG:HB2   | 3:D:392:SER:O     | 2.11                     | 0.50              |
| 2:C:285:LEU:HD23  | 2:C:285:LEU:H     | 1.76                     | 0.50              |
| 2:C:589:ARG:HA    | 2:C:596:TYR:HE1   | 1.75                     | 0.50              |
| 2:C:536:PRO:HB3   | 2:C:906:PHE:HB2   | 1.92                     | 0.50              |
| 2:C:754:ILE:N     | 2:C:754:ILE:HD12  | 2.27                     | 0.50              |
| 3:D:539:ASP:OD2   | 3:D:598:ARG:NH2   | 2.43                     | 0.50              |
| 3:D:939:PHE:O     | 3:D:940:THR:C     | 2.50                     | 0.50              |
| 3:D:1372:VAL:O    | 3:D:1375:MET:CB   | 2.60                     | 0.50              |
| 2:C:266:ARG:HH11  | 2:C:273:GLY:H     | 1.60                     | 0.49              |
| 2:C:881:ASN:ND2   | 2:C:881:ASN:N     | 2.36                     | 0.49              |
| 3:D:939:PHE:O     | 3:D:942:SER:N     | 2.45                     | 0.49              |
| 3:D:1481:VAL:O    | 3:D:1483:PHE:N    | 2.45                     | 0.49              |
| 5:F:79:ASP:HB3    | 5:F:83:GLN:HB2    | 1.93                     | 0.49              |
| 2:C:448:ASN:HA    | 2:C:451:LEU:HD12  | 1.94                     | 0.49              |
| 2:C:753:ASP:O     | 2:C:792:VAL:HG23  | 2.12                     | 0.49              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:CA    | 2.42                     | 0.49              |
| 3:D:1101:VAL:HG11 | 3:D:1424:VAL:HG12 | 1.94                     | 0.49              |
| 5:F:386:VAL:HG12  | 5:F:388:ALA:H     | 1.78                     | 0.49              |
| 3:D:543:LEU:HD23  | 3:D:546:ARG:HD3   | 1.95                     | 0.49              |
| 2:C:15:LEU:HD21   | 2:C:583:LEU:HD22  | 1.94                     | 0.49              |
| 2:C:196:LEU:HD23  | 2:C:238:LEU:HD22  | 1.93                     | 0.49              |
| 2:C:580:MET:SD    | 2:C:584:GLU:HG3   | 2.53                     | 0.49              |
| 3:D:158:TYR:CE1   | 3:D:454:ALA:HB3   | 2.44                     | 0.49              |
| 1:A:185:ARG:HB2   | 1:A:190:THR:HG22  | 1.94                     | 0.49              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:HB3   | 1.94                     | 0.49              |
| 2:C:545:ASN:HB3   | 2:C:583:LEU:CD1   | 2.42                     | 0.49              |
| 3:D:828:LYS:HB3   | 3:D:833:GLU:HG2   | 1.94                     | 0.49              |
| 3:D:853:VAL:HG12  | 3:D:858:VAL:HG13  | 1.93                     | 0.49              |
| 3:D:1463:LYS:O    | 3:D:1467:ILE:HG22 | 2.13                     | 0.49              |
| 3:D:1213:ARG:HB2  | 3:D:1214:PRO:CD   | 2.42                     | 0.49              |
| 2:C:486:MET:HE3   | 2:C:491:GLU:HA    | 1.92                     | 0.49              |
| 3:D:1167:SER:HB3  | 3:D:1170:ASP:OD2  | 2.12                     | 0.49              |
| 3:D:1320:GLU:O    | 3:D:1323:GLN:HB2  | 2.12                     | 0.49              |
| 5:F:393:THR:HG22  | 5:F:397:ILE:HD11  | 1.93                     | 0.49              |
| 2:C:713:ARG:HH11  | 2:C:713:ARG:HB2   | 1.78                     | 0.49              |
| 2:C:1101:THR:HB   | 3:D:5:VAL:HG21    | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:643:GLY:HA3   | 3:D:727:GLN:HB2   | 1.93                     | 0.49              |
| 3:D:1378:TYR:HE2  | 3:D:1394:VAL:HG22 | 1.75                     | 0.49              |
| 3:D:117:ASP:CB    | 3:D:495:ARG:HH12  | 2.23                     | 0.49              |
| 3:D:915:VAL:HG12  | 3:D:916:TYR:N     | 2.27                     | 0.49              |
| 2:C:657:ASP:CG    | 2:C:663:ASN:H     | 2.16                     | 0.48              |
| 2:C:1090:LYS:HE2  | 2:C:1112:PHE:CZ   | 2.48                     | 0.48              |
| 3:D:1434:TRP:HE1  | 3:D:1457:ASP:HB2  | 1.76                     | 0.48              |
| 1:B:11:PHE:HZ     | 1:B:211:LEU:HD21  | 1.78                     | 0.48              |
| 1:B:100:LEU:HB2   | 1:B:115:LEU:HD13  | 1.94                     | 0.48              |
| 2:C:881:ASN:OD1   | 2:C:884:GLN:NE2   | 2.46                     | 0.48              |
| 1:B:59:GLU:HB2    | 1:B:139:ASN:H     | 1.79                     | 0.48              |
| 3:D:605:ASP:HA    | 3:D:610:LYS:HB2   | 1.94                     | 0.48              |
| 2:C:595:LEU:HB2   | 2:C:639:GLN:HE21  | 1.79                     | 0.48              |
| 4:E:87:LYS:HE2    | 4:E:91:ARG:HH22   | 1.78                     | 0.48              |
| 5:F:152:ASP:H     | 5:F:153:PRO:HD3   | 1.79                     | 0.48              |
| 2:C:724:ARG:HG3   | 2:C:738:ASP:O     | 2.13                     | 0.48              |
| 3:D:1045:MET:O    | 3:D:1053:PHE:HD1  | 1.96                     | 0.48              |
| 3:D:1263:PHE:HD2  | 3:D:1375:MET:HE2  | 1.78                     | 0.48              |
| 3:D:1281:VAL:HG23 | 3:D:1317:ASP:O    | 2.14                     | 0.48              |
| 2:C:92:ALA:O      | 2:C:117:HIS:HB2   | 2.12                     | 0.48              |
| 2:C:759:THR:HA    | 2:C:786:LYS:O     | 2.13                     | 0.48              |
| 2:C:1085:PHE:O    | 2:C:1088:LEU:HB3  | 2.13                     | 0.48              |
| 3:D:444:VAL:O     | 3:D:444:VAL:HG23  | 2.14                     | 0.48              |
| 3:D:629:SER:OG    | 3:D:630:VAL:N     | 2.46                     | 0.48              |
| 3:D:695:ILE:O     | 3:D:696:HIS:C     | 2.51                     | 0.48              |
| 1:A:11:PHE:HB2    | 1:B:224:TYR:O     | 2.13                     | 0.48              |
| 2:C:603:VAL:HG21  | 2:C:643:VAL:CG1   | 2.44                     | 0.48              |
| 2:C:629:TYR:HD2   | 11:C:1330:HOH:O   | 1.96                     | 0.48              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:HG21  | 1.96                     | 0.48              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:H     | 1.79                     | 0.48              |
| 2:C:1051:GLU:O    | 2:C:1056:LYS:HD3  | 2.14                     | 0.48              |
| 2:C:1093:GLN:HB3  | 3:D:90:MET:CE     | 2.43                     | 0.48              |
| 3:D:233:LYS:HB2   | 3:D:236:TYR:HD1   | 1.79                     | 0.48              |
| 3:D:356:PRO:HB3   | 3:D:441:ARG:HG3   | 1.96                     | 0.48              |
| 3:D:785:ILE:HG23  | 3:D:935:LYS:HA    | 1.96                     | 0.48              |
| 3:D:1028:ALA:O    | 3:D:1029:ARG:HB2  | 2.12                     | 0.48              |
| 2:C:874:LEU:CD2   | 3:D:1023:MET:SD   | 3.02                     | 0.48              |
| 3:D:852:ALA:HB1   | 3:D:857:ILE:CG1   | 2.44                     | 0.48              |
| 3:D:1263:PHE:CE2  | 3:D:1371:VAL:HG11 | 2.49                     | 0.48              |
| 1:A:39:PRO:O      | 1:A:43:ILE:HG13   | 2.14                     | 0.48              |
| 2:C:267:TYR:CD2   | 2:C:271:GLU:HB2   | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:874:LEU:HD23 | 3:D:1023:MET:SD  | 2.54                     | 0.48              |
| 3:D:754:PHE:O    | 3:D:757:ALA:HB3  | 2.13                     | 0.48              |
| 3:D:798:GLU:O    | 3:D:825:ALA:HA   | 2.13                     | 0.48              |
| 3:D:853:VAL:HA   | 3:D:858:VAL:O    | 2.14                     | 0.48              |
| 3:D:860:LEU:HB3  | 3:D:878:GLY:CA   | 2.44                     | 0.48              |
| 3:D:1165:TYR:CZ  | 3:D:1214:PRO:HB3 | 2.49                     | 0.48              |
| 3:D:1404:ASN:OD1 | 3:D:1408:ILE:HB  | 2.14                     | 0.48              |
| 1:B:23:PHE:HE1   | 1:B:199:ILE:HD12 | 1.79                     | 0.48              |
| 2:C:343:GLN:OE1  | 2:C:343:GLN:HA   | 2.13                     | 0.48              |
| 3:D:131:LYS:HD3  | 3:D:152:LEU:HD12 | 1.95                     | 0.48              |
| 3:D:947:ILE:CG1  | 3:D:948:THR:N    | 2.73                     | 0.48              |
| 3:D:1140:ILE:O   | 3:D:1141:GLU:C   | 2.52                     | 0.48              |
| 2:C:272:ALA:O    | 2:C:275:TYR:HB3  | 2.13                     | 0.47              |
| 2:C:672:VAL:CG2  | 2:C:868:ASP:HB3  | 2.44                     | 0.47              |
| 2:C:1005:MET:HG2 | 3:D:629:SER:HB2  | 1.96                     | 0.47              |
| 3:D:233:LYS:HB2  | 3:D:236:TYR:CD1  | 2.49                     | 0.47              |
| 3:D:883:ALA:HA   | 3:D:900:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:38:ASN:HB3   | 1:A:39:PRO:CD    | 2.44                     | 0.47              |
| 2:C:3:ILE:HA     | 2:C:900:ARG:O    | 2.13                     | 0.47              |
| 2:C:154:ARG:HH21 | 2:C:156:GLY:HA3  | 1.79                     | 0.47              |
| 2:C:946:ARG:O    | 2:C:950:LEU:HG   | 2.14                     | 0.47              |
| 3:D:42:ASP:HB2   | 11:D:1731:HOH:O  | 2.14                     | 0.47              |
| 3:D:48:ARG:HB3   | 3:D:48:ARG:CZ    | 2.44                     | 0.47              |
| 3:D:406:ASP:HB2  | 3:D:423:ASP:HA   | 1.95                     | 0.47              |
| 3:D:1021:TYR:CE1 | 3:D:1025:GLN:HG3 | 2.49                     | 0.47              |
| 3:D:1231:GLU:N   | 3:D:1232:PRO:CD  | 2.77                     | 0.47              |
| 4:E:37:ASN:H     | 4:E:37:ASN:ND2   | 2.13                     | 0.47              |
| 5:F:384:GLU:HA   | 5:F:397:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:55:SER:HB2   | 1:A:158:ILE:HG21 | 1.95                     | 0.47              |
| 1:B:59:GLU:HB3   | 1:B:138:LEU:HG   | 1.96                     | 0.47              |
| 2:C:1112:PHE:O   | 2:C:1113:GLU:C   | 2.52                     | 0.47              |
| 3:D:834:THR:HG23 | 3:D:838:ARG:HB2  | 1.96                     | 0.47              |
| 3:D:1042:ARG:NH1 | 3:D:1045:MET:CE  | 2.77                     | 0.47              |
| 1:A:39:PRO:HG3   | 1:B:39:PRO:CG    | 2.44                     | 0.47              |
| 1:A:151:VAL:HA   | 1:A:152:PRO:HD3  | 1.80                     | 0.47              |
| 1:B:161:ARG:H    | 1:B:164:ALA:HB3  | 1.79                     | 0.47              |
| 1:B:175:ARG:HE   | 1:B:202:ASP:HA   | 1.79                     | 0.47              |
| 2:C:700:TYR:CB   | 2:C:833:LEU:HD13 | 2.44                     | 0.47              |
| 2:C:953:VAL:HG13 | 2:C:966:LEU:HD13 | 1.96                     | 0.47              |
| 3:D:889:ALA:O    | 3:D:929:ARG:NH1  | 2.47                     | 0.47              |
| 2:C:944:LEU:HD22 | 2:C:962:GLN:HB3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1007:ALA:HB2  | 3:D:648:MET:HG2   | 1.97                     | 0.47              |
| 3:D:1158:VAL:HG11 | 3:D:1173:LEU:HD21 | 1.96                     | 0.47              |
| 2:C:144:PRO:CB    | 2:C:266:ARG:HB3   | 2.45                     | 0.47              |
| 2:C:191:PHE:HZ    | 2:C:196:LEU:HD11  | 1.80                     | 0.47              |
| 2:C:575:GLN:HE22  | 2:C:671:ASN:H     | 1.56                     | 0.47              |
| 2:C:1001:VAL:O    | 2:C:1004:LYS:HB3  | 2.14                     | 0.47              |
| 3:D:339:TRP:CZ3   | 3:D:341:GLU:HB2   | 2.50                     | 0.47              |
| 3:D:835:SER:H     | 3:D:838:ARG:NE    | 2.12                     | 0.47              |
| 1:A:62:LEU:HB2    | 1:A:63:HIS:HD2    | 1.80                     | 0.47              |
| 2:C:889:HIS:CE1   | 3:D:951:ILE:H     | 2.13                     | 0.47              |
| 3:D:324:ALA:HA    | 3:D:331:VAL:HG13  | 1.97                     | 0.47              |
| 3:D:917:GLN:O     | 3:D:919:PHE:N     | 2.48                     | 0.47              |
| 3:D:989:TYR:CZ    | 3:D:993:LEU:HD11  | 2.49                     | 0.47              |
| 5:F:256:ARG:NH2   | 5:F:310:ILE:O     | 2.48                     | 0.47              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:CE1   | 2.50                     | 0.47              |
| 1:B:2:LEU:H       | 1:B:3:ASP:HA      | 1.76                     | 0.47              |
| 2:C:563:ASN:O     | 2:C:566:THR:HB    | 2.15                     | 0.47              |
| 2:C:679:PHE:CE2   | 2:C:853:LEU:HD11  | 2.49                     | 0.47              |
| 2:C:707:ARG:HD2   | 2:C:824:ARG:HH11  | 1.79                     | 0.47              |
| 3:D:601:ARG:HB2   | 5:F:318:GLU:HG2   | 1.97                     | 0.47              |
| 1:A:177:VAL:HG22  | 1:A:199:ILE:HG12  | 1.97                     | 0.47              |
| 2:C:689:VAL:HG22  | 2:C:870:ILE:HB    | 1.97                     | 0.47              |
| 2:C:897:LEU:HG    | 2:C:921:ALA:HB2   | 1.96                     | 0.47              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:N     | 2.29                     | 0.47              |
| 3:D:1098:LEU:O    | 3:D:1102:THR:HG23 | 2.15                     | 0.47              |
| 2:C:676:ILE:O     | 3:D:948:THR:CG2   | 2.53                     | 0.47              |
| 3:D:158:TYR:C     | 3:D:160:GLU:H     | 2.18                     | 0.47              |
| 3:D:478:LEU:HD12  | 3:D:478:LEU:HA    | 1.80                     | 0.47              |
| 3:D:705:ALA:HA    | 3:D:706:PRO:HA    | 1.59                     | 0.47              |
| 3:D:1058:ARG:N    | 3:D:1069:GLU:OE2  | 2.48                     | 0.47              |
| 5:F:234:LYS:HD2   | 5:F:236:SER:HB3   | 1.96                     | 0.47              |
| 2:C:265:ARG:HG2   | 2:C:288:ARG:HD2   | 1.97                     | 0.46              |
| 2:C:644:VAL:HG12  | 2:C:645:VAL:H     | 1.80                     | 0.46              |
| 3:D:538:SER:OG    | 3:D:539:ASP:N     | 2.47                     | 0.46              |
| 3:D:567:ILE:O     | 3:D:571:LYS:HG3   | 2.15                     | 0.46              |
| 1:A:224:TYR:CD1   | 1:B:9:PRO:HG2     | 2.49                     | 0.46              |
| 3:D:1232:PRO:HG2  | 3:D:1356:TYR:CE2  | 2.47                     | 0.46              |
| 5:F:392:VAL:HG11  | 5:F:396:ARG:HH11  | 1.80                     | 0.46              |
| 1:B:47:SER:O      | 1:B:148:VAL:HG11  | 2.16                     | 0.46              |
| 3:D:134:VAL:HA    | 3:D:454:ALA:HA    | 1.97                     | 0.46              |
| 3:D:505:SER:HB3   | 3:D:1453:ALA:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:643:GLY:N    | 3:D:727:GLN:O     | 2.46                     | 0.46              |
| 3:D:651:GLU:HA   | 3:D:651:GLU:OE1   | 2.15                     | 0.46              |
| 3:D:654:LYS:CB   | 3:D:655:PRO:HD3   | 2.40                     | 0.46              |
| 2:C:683:ASN:HB2  | 2:C:687:ALA:O     | 2.16                     | 0.46              |
| 2:C:1008:ARG:NH1 | 2:C:1011:GLY:N    | 2.63                     | 0.46              |
| 3:D:212:ARG:HD3  | 3:D:342:PRO:HB3   | 1.97                     | 0.46              |
| 3:D:885:ILE:HG12 | 3:D:937:TYR:CE1   | 2.51                     | 0.46              |
| 5:F:329:TYR:HE1  | 5:F:333:ILE:HD11  | 1.81                     | 0.46              |
| 2:C:34:VAL:H     | 2:C:35:PRO:HD2    | 1.78                     | 0.46              |
| 2:C:1014:SER:O   | 2:C:1018:GLN:HA   | 2.15                     | 0.46              |
| 3:D:1378:TYR:CE2 | 3:D:1394:VAL:HG22 | 2.50                     | 0.46              |
| 3:D:813:LEU:O    | 3:D:817:GLU:HG2   | 2.15                     | 0.46              |
| 3:D:1222:GLY:O   | 3:D:1225:ALA:HB3  | 2.16                     | 0.46              |
| 3:D:1366:LYS:O   | 3:D:1369:GLU:HB2  | 2.16                     | 0.46              |
| 2:C:52:PHE:CD2   | 2:C:68:PHE:HB2    | 2.51                     | 0.46              |
| 2:C:841:ASN:ND2  | 2:C:845:ASN:HB2   | 2.31                     | 0.46              |
| 3:D:1411:GLY:O   | 3:D:1412:LYS:HB2  | 2.16                     | 0.46              |
| 5:F:261:PRO:O    | 5:F:265:VAL:HG23  | 2.15                     | 0.46              |
| 5:F:401:GLU:O    | 5:F:405:LEU:HB2   | 2.15                     | 0.46              |
| 1:A:39:PRO:HG3   | 1:B:39:PRO:HG3    | 1.98                     | 0.46              |
| 1:B:80:LEU:HD23  | 1:B:83:LYS:HD2    | 1.98                     | 0.46              |
| 1:B:211:LEU:O    | 1:B:215:VAL:HG13  | 2.16                     | 0.46              |
| 2:C:139:GLN:HG2  | 2:C:339:LEU:HD21  | 1.98                     | 0.46              |
| 2:C:627:ARG:HA   | 2:C:638:ASP:HB2   | 1.97                     | 0.46              |
| 2:C:684:PHE:HB3  | 3:D:633:VAL:HG21  | 1.97                     | 0.46              |
| 2:C:710:ILE:HD11 | 2:C:758:ARG:CZ    | 2.46                     | 0.46              |
| 2:C:771:GLU:HA   | 2:C:774:LEU:HB3   | 1.96                     | 0.46              |
| 3:D:239:GLY:HA2  | 3:D:313:MET:HB3   | 1.98                     | 0.46              |
| 3:D:575:GLN:NE2  | 11:D:1705:HOH:O   | 2.48                     | 0.46              |
| 3:D:701:LEU:O    | 3:D:747:VAL:HG23  | 2.15                     | 0.46              |
| 3:D:1436:SER:O   | 3:D:1438:ALA:N    | 2.49                     | 0.46              |
| 5:F:299:TRP:CE3  | 5:F:303:ARG:HD3   | 2.51                     | 0.46              |
| 5:F:394:ARG:HB3  | 5:F:395:GLU:H     | 1.61                     | 0.46              |
| 1:A:24:VAL:HA    | 1:A:195:LEU:O     | 2.16                     | 0.46              |
| 2:C:189:ARG:HD2  | 2:C:241:LEU:HD22  | 1.97                     | 0.46              |
| 2:C:317:VAL:H    | 2:C:318:PRO:HD3   | 1.78                     | 0.46              |
| 2:C:923:GLU:O    | 2:C:924:VAL:C     | 2.54                     | 0.46              |
| 3:D:115:LEU:HD11 | 3:D:499:VAL:HG22  | 1.97                     | 0.46              |
| 3:D:1479:ASP:OD1 | 3:D:1479:ASP:N    | 2.49                     | 0.46              |
| 1:A:41:ARG:HD2   | 1:A:177:VAL:HG12  | 1.98                     | 0.46              |
| 2:C:23:VAL:HG12  | 2:C:121:MET:HE1   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:520:LEU:HD12  | 3:D:521:PRO:HD2  | 1.97                     | 0.46              |
| 3:D:1112:CYS:HB3  | 3:D:1201:CYS:HB3 | 1.58                     | 0.46              |
| 3:D:1350:GLU:O    | 3:D:1352:ILE:N   | 2.49                     | 0.46              |
| 5:F:123:ASP:OD2   | 5:F:123:ASP:N    | 2.48                     | 0.46              |
| 1:A:25:LEU:HD23   | 1:A:28:LEU:HD11  | 1.98                     | 0.45              |
| 1:B:212:ASN:O     | 1:B:215:VAL:HG22 | 2.16                     | 0.45              |
| 2:C:62:GLY:HA2    | 2:C:103:LYS:HG2  | 1.98                     | 0.45              |
| 2:C:126:SER:HB2   | 2:C:134:ARG:O    | 2.16                     | 0.45              |
| 2:C:266:ARG:NH1   | 2:C:271:GLU:O    | 2.49                     | 0.45              |
| 2:C:376:ARG:HH12  | 5:F:276:ARG:HG2  | 1.80                     | 0.45              |
| 2:C:860:HIS:NE2   | 2:C:975:TYR:HB2  | 2.32                     | 0.45              |
| 2:C:972:VAL:HG23  | 2:C:973:VAL:N    | 2.31                     | 0.45              |
| 3:D:95:LEU:HA     | 3:D:551:ASN:HD21 | 1.81                     | 0.45              |
| 3:D:237:LYS:HB2   | 3:D:240:GLU:HG3  | 1.98                     | 0.45              |
| 3:D:297:ILE:HG23  | 3:D:298:VAL:HG23 | 1.98                     | 0.45              |
| 1:A:20:TYR:CD1    | 1:A:21:GLY:N     | 2.85                     | 0.45              |
| 1:B:58:ILE:HG21   | 1:B:61:VAL:HG12  | 1.99                     | 0.45              |
| 2:C:385:PHE:HD2   | 2:C:386:PHE:CD1  | 2.34                     | 0.45              |
| 3:D:8:VAL:CG1     | 3:D:1434:TRP:CZ2 | 2.96                     | 0.45              |
| 3:D:539:ASP:HB3   | 3:D:600:LEU:HD22 | 1.97                     | 0.45              |
| 3:D:1459:LEU:CA   | 3:D:1464:GLU:HG3 | 2.44                     | 0.45              |
| 3:D:536:ALA:HA    | 5:F:315:VAL:O    | 2.16                     | 0.45              |
| 3:D:675:ARG:HH12  | 5:F:423:ASP:HB2  | 1.80                     | 0.45              |
| 3:D:1194:CYS:SG   | 3:D:1200:VAL:HA  | 2.56                     | 0.45              |
| 3:D:1350:GLU:O    | 3:D:1353:GLN:N   | 2.49                     | 0.45              |
| 5:F:104:ARG:HG3   | 5:F:229:TYR:CZ   | 2.51                     | 0.45              |
| 1:A:79:ILE:CG2    | 1:A:167:VAL:HG11 | 2.47                     | 0.45              |
| 2:C:54:ILE:HG23   | 2:C:66:LEU:HB3   | 1.99                     | 0.45              |
| 2:C:144:PRO:HB3   | 2:C:266:ARG:HB3  | 1.99                     | 0.45              |
| 2:C:428:ARG:HH21  | 2:C:451:LEU:HD11 | 1.81                     | 0.45              |
| 2:C:751:PRO:HA    | 2:C:792:VAL:CG1  | 2.46                     | 0.45              |
| 3:D:131:LYS:HB3   | 3:D:152:LEU:HB2  | 1.99                     | 0.45              |
| 3:D:729:HIS:CD2   | 3:D:730:PRO:CD   | 2.99                     | 0.45              |
| 1:A:64:GLU:HG2    | 1:A:76:VAL:HG22  | 1.99                     | 0.45              |
| 1:A:173:PRO:O     | 1:A:201:THR:HB   | 2.16                     | 0.45              |
| 2:C:23:VAL:HG23   | 2:C:24:GLU:N     | 2.30                     | 0.45              |
| 2:C:560:MET:O     | 2:C:564:MET:HG3  | 2.17                     | 0.45              |
| 3:D:880:ILE:O     | 3:D:884:ARG:N    | 2.49                     | 0.45              |
| 3:D:1217:ILE:HD12 | 3:D:1217:ILE:H   | 1.82                     | 0.45              |
| 3:D:1394:VAL:HB   | 3:D:1397:LYS:HE2 | 1.97                     | 0.45              |
| 1:B:57:TYR:HD1    | 1:B:161:ARG:HG3  | 1.82                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:72:ARG:O      | 2:C:95:TYR:N     | 2.40                     | 0.45              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:HD3  | 1.99                     | 0.45              |
| 2:C:627:ARG:HA    | 2:C:627:ARG:HD3  | 1.85                     | 0.45              |
| 3:D:95:LEU:HB2    | 3:D:515:GLU:O    | 2.17                     | 0.45              |
| 3:D:270:LEU:HB3   | 3:D:284:LEU:HD11 | 1.99                     | 0.45              |
| 3:D:368:VAL:HG23  | 3:D:377:VAL:HG11 | 1.98                     | 0.45              |
| 3:D:643:GLY:O     | 3:D:726:ILE:HG23 | 2.17                     | 0.45              |
| 3:D:1478:SER:O    | 3:D:1480:PHE:N   | 2.50                     | 0.45              |
| 1:A:22:GLU:C      | 1:A:23:PHE:CD1   | 2.90                     | 0.45              |
| 1:A:42:ARG:O      | 1:A:43:ILE:C     | 2.54                     | 0.45              |
| 1:A:206:THR:HG22  | 1:A:208:LEU:N    | 2.30                     | 0.45              |
| 2:C:694:LEU:O     | 2:C:699:PHE:HB2  | 2.17                     | 0.45              |
| 2:C:1009:SER:O    | 3:D:624:ASP:O    | 2.34                     | 0.45              |
| 3:D:134:VAL:HG12  | 3:D:135:LEU:N    | 2.32                     | 0.45              |
| 3:D:659:LYS:HG3   | 3:D:663:GLU:OE2  | 2.16                     | 0.45              |
| 3:D:662:GLU:OE1   | 3:D:670:VAL:HG23 | 2.16                     | 0.45              |
| 3:D:959:GLU:HB3   | 3:D:963:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:55:SER:HB2    | 1:A:158:ILE:CG2  | 2.47                     | 0.45              |
| 1:B:100:LEU:O     | 1:B:114:PHE:HA   | 2.17                     | 0.45              |
| 2:C:846:LYS:CE    | 3:D:741:ASP:O    | 2.63                     | 0.45              |
| 2:C:872:ASN:OD1   | 2:C:874:LEU:HG   | 2.17                     | 0.45              |
| 3:D:542:ASP:O     | 3:D:546:ARG:HG2  | 2.17                     | 0.45              |
| 2:C:551:GLU:HB3   | 2:C:906:PHE:CE2  | 2.52                     | 0.45              |
| 3:D:95:LEU:HD21   | 3:D:517:VAL:CG2  | 2.46                     | 0.45              |
| 3:D:783:ARG:HB3   | 3:D:784:ASP:H    | 1.42                     | 0.45              |
| 3:D:854:ALA:C     | 3:D:856:GLY:H    | 2.20                     | 0.45              |
| 3:D:864:VAL:HG13  | 3:D:865:THR:N    | 2.32                     | 0.45              |
| 3:D:1208:ASP:O    | 3:D:1209:LEU:CB  | 2.60                     | 0.45              |
| 3:D:1481:VAL:HG13 | 4:E:18:ARG:HG3   | 1.99                     | 0.45              |
| 3:D:1484:THR:HG21 | 4:E:18:ARG:HG2   | 1.98                     | 0.45              |
| 1:A:28:LEU:O      | 1:A:193:ASP:N    | 2.50                     | 0.45              |
| 1:B:19:GLU:O      | 1:B:200:TRP:HA   | 2.17                     | 0.45              |
| 2:C:324:ASP:HB3   | 2:C:327:HIS:HB2  | 1.99                     | 0.45              |
| 2:C:668:LEU:HD23  | 2:C:668:LEU:HA   | 1.73                     | 0.45              |
| 2:C:848:VAL:HG12  | 3:D:632:VAL:HG23 | 1.99                     | 0.45              |
| 3:D:116:LEU:HD21  | 3:D:465:LEU:HD23 | 1.99                     | 0.45              |
| 3:D:411:THR:O     | 5:F:178:ARG:HD2  | 2.17                     | 0.45              |
| 3:D:539:ASP:N     | 3:D:539:ASP:OD1  | 2.50                     | 0.45              |
| 3:D:1023:MET:HA   | 3:D:1028:ALA:HB3 | 1.97                     | 0.45              |
| 1:A:222:LEU:HD21  | 1:B:218:LEU:HD23 | 1.97                     | 0.44              |
| 1:B:38:ASN:HB2    | 1:B:39:PRO:HD3   | 1.98                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:154:ARG:HE    | 2:C:156:GLY:HA3  | 1.82                     | 0.44              |
| 2:C:265:ARG:H     | 2:C:265:ARG:HG3  | 1.64                     | 0.44              |
| 2:C:713:ARG:HB2   | 2:C:713:ARG:NH1  | 2.32                     | 0.44              |
| 3:D:566:ILE:O     | 3:D:566:ILE:HG13 | 2.16                     | 0.44              |
| 3:D:675:ARG:NH2   | 5:F:420:ASP:O    | 2.50                     | 0.44              |
| 3:D:1305:LEU:HA   | 3:D:1306:PRO:HD2 | 1.79                     | 0.44              |
| 2:C:435:TYR:HA    | 3:D:1071:PHE:CE2 | 2.49                     | 0.44              |
| 2:C:860:HIS:HA    | 2:C:866:PRO:HA   | 1.98                     | 0.44              |
| 2:C:915:LYS:O     | 2:C:968:LEU:HD22 | 2.17                     | 0.44              |
| 3:D:171:LEU:HD21  | 3:D:192:ALA:HB1  | 2.00                     | 0.44              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:HE1 | 1.98                     | 0.44              |
| 4:E:11:GLY:HA3    | 11:E:103:HOH:O   | 2.18                     | 0.44              |
| 1:A:70:GLY:CA     | 1:A:133:GLU:HG2  | 2.47                     | 0.44              |
| 2:C:266:ARG:HD2   | 2:C:273:GLY:HA3  | 1.99                     | 0.44              |
| 2:C:833:LEU:HA    | 2:C:837:ASP:OD2  | 2.17                     | 0.44              |
| 3:D:661:MET:HE1   | 3:D:677:LEU:HD21 | 1.99                     | 0.44              |
| 3:D:1378:TYR:O    | 3:D:1420:LEU:HB2 | 2.17                     | 0.44              |
| 1:A:40:LEU:HD23   | 1:A:43:ILE:HD12  | 2.00                     | 0.44              |
| 2:C:283:ILE:HG22  | 2:C:284:ARG:HG2  | 1.98                     | 0.44              |
| 2:C:397:GLU:HG3   | 2:C:631:SER:HB2  | 1.97                     | 0.44              |
| 2:C:971:LYS:HA    | 2:C:988:VAL:CA   | 2.43                     | 0.44              |
| 3:D:191:LEU:HD12  | 3:D:195:VAL:HB   | 1.99                     | 0.44              |
| 3:D:523:ASP:O     | 3:D:526:PRO:HD3  | 2.17                     | 0.44              |
| 3:D:643:GLY:O     | 3:D:726:ILE:HA   | 2.18                     | 0.44              |
| 2:C:468:ARG:HE    | 2:C:487:THR:CG2  | 2.29                     | 0.44              |
| 3:D:1213:ARG:HB2  | 3:D:1214:PRO:HD2 | 1.99                     | 0.44              |
| 3:D:1440:PHE:HE2  | 3:D:1463:LYS:NZ  | 2.15                     | 0.44              |
| 1:A:206:THR:O     | 1:A:207:PRO:C    | 2.55                     | 0.44              |
| 1:A:225:PHE:CD2   | 1:B:11:PHE:HE1   | 2.35                     | 0.44              |
| 1:B:23:PHE:CE1    | 1:B:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:B:167:VAL:CG1   | 1:B:168:ASP:H    | 2.23                     | 0.44              |
| 3:D:186:VAL:O     | 3:D:189:GLN:HB2  | 2.16                     | 0.44              |
| 3:D:659:LYS:O     | 3:D:662:GLU:N    | 2.50                     | 0.44              |
| 3:D:1472:ILE:HG23 | 3:D:1474:ALA:H   | 1.83                     | 0.44              |
| 1:A:215:VAL:HG13  | 1:B:222:LEU:HD22 | 1.99                     | 0.44              |
| 1:A:226:SER:O     | 1:A:227:ASN:HB3  | 2.18                     | 0.44              |
| 2:C:599:GLU:HG3   | 2:C:600:ASP:H    | 1.82                     | 0.44              |
| 3:D:787:LEU:HD13  | 3:D:1023:MET:HG2 | 2.00                     | 0.44              |
| 2:C:13:ILE:HD12   | 2:C:14:PRO:CD    | 2.42                     | 0.44              |
| 2:C:292:ARG:HD3   | 2:C:299:LYS:HB3  | 1.99                     | 0.44              |
| 2:C:462:ASP:HB3   | 2:C:468:ARG:HD2  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:834:THR:HA    | 3:D:838:ARG:HE   | 1.83                     | 0.44              |
| 2:C:605:LYS:O     | 2:C:611:ILE:HG23 | 2.18                     | 0.44              |
| 2:C:721:ARG:O     | 2:C:758:ARG:HG3  | 2.18                     | 0.44              |
| 3:D:16:GLU:O      | 3:D:20:SER:N     | 2.51                     | 0.44              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:N    | 2.25                     | 0.44              |
| 3:D:496:LEU:HD11  | 3:D:500:ARG:HH12 | 1.83                     | 0.44              |
| 3:D:947:ILE:O     | 3:D:948:THR:HG23 | 2.17                     | 0.44              |
| 2:C:69:LEU:HD13   | 2:C:97:ARG:HB3   | 2.00                     | 0.43              |
| 2:C:393:GLN:HG3   | 2:C:406:HIS:HE2  | 1.82                     | 0.43              |
| 3:D:493:ARG:NH1   | 3:D:1389:LEU:HB3 | 2.33                     | 0.43              |
| 3:D:631:ILE:HG12  | 3:D:743:ASP:O    | 2.17                     | 0.43              |
| 3:D:786:ILE:HG21  | 3:D:1026:SER:O   | 2.18                     | 0.43              |
| 3:D:1104:GLU:HA   | 3:D:1461:GLY:HA2 | 1.99                     | 0.43              |
| 5:F:91:VAL:HA     | 5:F:92:PRO:HD3   | 1.80                     | 0.43              |
| 5:F:132:ARG:HH21  | 5:F:184:ARG:NE   | 2.16                     | 0.43              |
| 2:C:159:ILE:HG23  | 2:C:175:GLU:HB2  | 1.99                     | 0.43              |
| 2:C:540:PHE:CE1   | 2:C:906:PHE:HE1  | 2.36                     | 0.43              |
| 2:C:728:HIS:CG    | 2:C:729:LEU:N    | 2.85                     | 0.43              |
| 3:D:885:ILE:HG21  | 3:D:937:TYR:CD1  | 2.40                     | 0.43              |
| 3:D:1443:THR:O    | 3:D:1444:THR:C   | 2.57                     | 0.43              |
| 3:D:1481:VAL:HG13 | 4:E:18:ARG:HA    | 1.99                     | 0.43              |
| 5:F:79:ASP:N      | 5:F:80:PRO:CD    | 2.82                     | 0.43              |
| 5:F:379:ARG:HD2   | 5:F:383:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:216:GLU:CD    | 1:A:219:ARG:HH21 | 2.22                     | 0.43              |
| 1:B:44:LEU:HA     | 1:B:48:ILE:HD13  | 2.00                     | 0.43              |
| 2:C:561:GLY:O     | 2:C:562:SER:C    | 2.55                     | 0.43              |
| 3:D:841:TYR:HB2   | 3:D:864:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:83:LYS:HE3    | 1:A:168:ASP:O    | 2.18                     | 0.43              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:HG11 | 2.01                     | 0.43              |
| 2:C:713:ARG:HA    | 2:C:819:VAL:HA   | 2.00                     | 0.43              |
| 3:D:156:GLU:CD    | 3:D:156:GLU:H    | 2.22                     | 0.43              |
| 3:D:493:ARG:NH1   | 3:D:1390:LEU:H   | 2.01                     | 0.43              |
| 2:C:434:HIS:O     | 2:C:435:TYR:C    | 2.56                     | 0.43              |
| 2:C:683:ASN:CG    | 2:C:872:ASN:HB2  | 2.38                     | 0.43              |
| 2:C:876:VAL:O     | 2:C:877:PRO:C    | 2.55                     | 0.43              |
| 4:E:9:LEU:O       | 4:E:19:LEU:HD13  | 2.19                     | 0.43              |
| 1:B:112:ARG:NH1   | 1:B:112:ARG:HB3  | 2.33                     | 0.43              |
| 2:C:537:LYS:O     | 2:C:539:VAL:N    | 2.51                     | 0.43              |
| 2:C:690:ILE:HD13  | 2:C:690:ILE:HA   | 1.72                     | 0.43              |
| 3:D:114:THR:HG21  | 3:D:498:VAL:HG21 | 2.00                     | 0.43              |
| 3:D:986:ARG:HG3   | 3:D:990:ASP:OD1  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1190:SER:OG   | 3:D:1191:PRO:CD   | 2.66                     | 0.43              |
| 3:D:1400:VAL:HG12 | 3:D:1404:ASN:ND2  | 2.32                     | 0.43              |
| 5:F:201:LYS:HA    | 5:F:201:LYS:HD2   | 1.86                     | 0.43              |
| 1:A:51:THR:HG22   | 1:A:146:ARG:HA    | 2.01                     | 0.43              |
| 1:A:73:GLU:CB     | 1:A:78:ILE:HG12   | 2.48                     | 0.43              |
| 2:C:52:PHE:HD2    | 2:C:68:PHE:HB2    | 1.84                     | 0.43              |
| 2:C:141:HIS:HE1   | 2:C:332:ARG:HH12  | 1.65                     | 0.43              |
| 2:C:274:ARG:HA    | 2:C:277:ALA:HB3   | 2.01                     | 0.43              |
| 2:C:724:ARG:HE    | 2:C:738:ASP:CA    | 2.19                     | 0.43              |
| 3:D:757:ALA:O     | 3:D:758:GLU:C     | 2.56                     | 0.43              |
| 3:D:836:VAL:N     | 3:D:837:GLY:CA    | 2.73                     | 0.43              |
| 3:D:1219:GLU:O    | 3:D:1221:VAL:N    | 2.49                     | 0.43              |
| 1:A:149:GLY:O     | 1:A:171:PHE:HB2   | 2.19                     | 0.43              |
| 2:C:195:LEU:HB3   | 2:C:238:LEU:CD2   | 2.49                     | 0.43              |
| 2:C:589:ARG:NH2   | 2:C:596:TYR:CD2   | 2.87                     | 0.43              |
| 2:C:751:PRO:HB2   | 3:D:680:GLN:HG3   | 2.00                     | 0.43              |
| 3:D:508:ARG:C     | 3:D:510:GLU:H     | 2.21                     | 0.43              |
| 3:D:948:THR:O     | 3:D:949:ILE:HG13  | 2.19                     | 0.43              |
| 5:F:222:ARG:HG2   | 5:F:242:TRP:CE3   | 2.54                     | 0.43              |
| 2:C:266:ARG:H     | 2:C:266:ARG:NE    | 2.16                     | 0.43              |
| 2:C:683:ASN:HA    | 2:C:687:ALA:HB3   | 2.00                     | 0.43              |
| 2:C:997:LEU:HD23  | 2:C:997:LEU:HA    | 1.77                     | 0.43              |
| 3:D:126:VAL:HG21  | 3:D:461:ILE:HD11  | 2.01                     | 0.43              |
| 3:D:372:ASP:O     | 3:D:374:GLU:N     | 2.52                     | 0.43              |
| 3:D:1107:VAL:HA   | 3:D:1200:VAL:O    | 2.18                     | 0.43              |
| 1:A:68:ILE:HA     | 1:A:69:PRO:HD2    | 1.83                     | 0.43              |
| 2:C:238:LEU:C     | 2:C:240:THR:H     | 2.21                     | 0.43              |
| 2:C:437:ARG:NH2   | 2:C:487:THR:O     | 2.52                     | 0.43              |
| 2:C:1095:LEU:HD13 | 3:D:103:TRP:CH2   | 2.53                     | 0.43              |
| 3:D:117:ASP:HB2   | 3:D:495:ARG:NH1   | 2.26                     | 0.43              |
| 3:D:272:LEU:HG    | 3:D:282:TYR:CE1   | 2.52                     | 0.43              |
| 3:D:953:ASP:HB3   | 3:D:1019:PRO:HG2  | 2.01                     | 0.43              |
| 3:D:969:ARG:HA    | 3:D:972:LEU:HD23  | 2.00                     | 0.43              |
| 3:D:1042:ARG:HD3  | 3:D:1057:VAL:HG11 | 2.01                     | 0.43              |
| 5:F:320:PRO:HA    | 5:F:328:PHE:HA    | 2.00                     | 0.43              |
| 5:F:397:ILE:HA    | 5:F:400:ILE:HB    | 1.99                     | 0.43              |
| 1:A:49:PRO:HB3    | 1:A:148:VAL:HG22  | 2.00                     | 0.42              |
| 1:A:177:VAL:HG12  | 1:A:177:VAL:O     | 2.19                     | 0.42              |
| 1:B:58:ILE:HD13   | 1:B:59:GLU:N      | 2.33                     | 0.42              |
| 1:B:176:ARG:HB3   | 1:B:200:TRP:CE3   | 2.54                     | 0.42              |
| 2:C:698:ASP:OD1   | 2:C:701:THR:OG1   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1008:ARG:HH11 | 2:C:1011:GLY:N    | 2.17                     | 0.42              |
| 3:D:116:LEU:HB3   | 3:D:118:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:806:PHE:H     | 3:D:829:VAL:HG12  | 1.84                     | 0.42              |
| 1:A:58:ILE:HB     | 1:A:61:VAL:CG2    | 2.48                     | 0.42              |
| 2:C:231:PRO:HA    | 2:C:234:ALA:HB3   | 2.01                     | 0.42              |
| 2:C:317:VAL:N     | 2:C:318:PRO:CD    | 2.82                     | 0.42              |
| 2:C:341:THR:HG22  | 2:C:345:ARG:HE    | 1.84                     | 0.42              |
| 2:C:414:GLY:HA3   | 2:C:415:PRO:HD3   | 1.86                     | 0.42              |
| 2:C:1107:ASN:O    | 2:C:1108:PRO:C    | 2.58                     | 0.42              |
| 3:D:272:LEU:HB3   | 3:D:274:ARG:NH1   | 2.34                     | 0.42              |
| 3:D:594:PRO:HB2   | 3:D:595:GLY:H     | 1.63                     | 0.42              |
| 5:F:292:ALA:C     | 5:F:294:ALA:H     | 2.22                     | 0.42              |
| 1:A:80:LEU:HD23   | 1:A:83:LYS:HG3    | 2.01                     | 0.42              |
| 1:A:84:GLU:O      | 1:A:85:LEU:C      | 2.58                     | 0.42              |
| 2:C:121:MET:HG3   | 2:C:127:PHE:CE1   | 2.54                     | 0.42              |
| 2:C:360:LEU:HG    | 2:C:361:MET:H     | 1.83                     | 0.42              |
| 2:C:569:VAL:HA    | 2:C:570:PRO:HD2   | 1.87                     | 0.42              |
| 2:C:724:ARG:HB2   | 2:C:741:GLY:H     | 1.84                     | 0.42              |
| 3:D:207:PHE:HB2   | 3:D:391:ALA:HB3   | 2.01                     | 0.42              |
| 3:D:1087:ARG:HB3  | 3:D:1091:SER:HB2  | 2.01                     | 0.42              |
| 3:D:1150:ALA:C    | 3:D:1151:ARG:HG2  | 2.39                     | 0.42              |
| 3:D:1341:PRO:O    | 3:D:1344:VAL:HG12 | 2.19                     | 0.42              |
| 4:E:31:LEU:HD12   | 4:E:60:ALA:HB2    | 2.00                     | 0.42              |
| 1:A:40:LEU:O      | 1:A:44:LEU:HB2    | 2.19                     | 0.42              |
| 1:B:216:GLU:OE2   | 1:B:220:GLU:HB2   | 2.19                     | 0.42              |
| 2:C:575:GLN:HE21  | 2:C:670:GLN:HA    | 1.85                     | 0.42              |
| 3:D:650:LEU:HB2   | 3:D:691:LEU:HD22  | 2.02                     | 0.42              |
| 3:D:996:TRP:HA    | 3:D:999:THR:HB    | 2.02                     | 0.42              |
| 3:D:1486:VAL:HG11 | 4:E:26:ARG:HB2    | 2.01                     | 0.42              |
| 1:B:104:GLU:HA    | 1:B:132:LEU:HD22  | 2.01                     | 0.42              |
| 2:C:182:VAL:HG13  | 2:C:220:GLY:HA3   | 2.01                     | 0.42              |
| 2:C:263:ASP:N     | 2:C:264:PRO:CD    | 2.62                     | 0.42              |
| 2:C:964:LYS:O     | 2:C:968:LEU:HG    | 2.19                     | 0.42              |
| 2:C:1037:VAL:O    | 2:C:1041:GLU:HG3  | 2.19                     | 0.42              |
| 3:D:256:GLU:OE1   | 3:D:302:GLN:HB3   | 2.19                     | 0.42              |
| 3:D:835:SER:HB2   | 3:D:838:ARG:HG3   | 2.02                     | 0.42              |
| 3:D:938:GLY:O     | 3:D:939:PHE:O     | 2.37                     | 0.42              |
| 3:D:1119:SER:HA   | 3:D:1186:VAL:O    | 2.20                     | 0.42              |
| 3:D:1314:LYS:HB3  | 3:D:1314:LYS:HE2  | 1.88                     | 0.42              |
| 4:E:25:LYS:O      | 4:E:28:GLN:HB2    | 2.19                     | 0.42              |
| 2:C:136:ILE:HB    | 2:C:336:VAL:HG22  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:948:THR:HB   | 3:D:949:ILE:H    | 1.49                     | 0.42              |
| 3:D:1375:MET:HE3 | 3:D:1375:MET:HB2 | 1.78                     | 0.42              |
| 3:D:1378:TYR:HD2 | 3:D:1394:VAL:HA  | 1.85                     | 0.42              |
| 1:A:41:ARG:NH1   | 1:A:45:LEU:HD11  | 2.35                     | 0.42              |
| 1:A:152:PRO:O    | 1:A:153:ALA:C    | 2.57                     | 0.42              |
| 1:A:154:GLU:H    | 1:A:154:GLU:CD   | 2.22                     | 0.42              |
| 1:B:29:GLU:O     | 1:B:30:ARG:C     | 2.58                     | 0.42              |
| 2:C:472:ARG:HA   | 2:C:483:VAL:HA   | 2.02                     | 0.42              |
| 2:C:1054:THR:HB  | 2:C:1059:ASP:HB2 | 2.02                     | 0.42              |
| 3:D:141:ILE:C    | 3:D:143:ASN:H    | 2.23                     | 0.42              |
| 3:D:374:GLU:HG3  | 3:D:375:GLU:N    | 2.34                     | 0.42              |
| 1:A:8:ALA:HA     | 1:A:9:PRO:HD3    | 1.72                     | 0.42              |
| 1:B:144:VAL:HG12 | 1:B:145:ASP:H    | 1.84                     | 0.42              |
| 2:C:139:GLN:O    | 2:C:333:ILE:HA   | 2.20                     | 0.42              |
| 2:C:173:ASP:HB2  | 2:C:185:LYS:HB3  | 2.01                     | 0.42              |
| 2:C:589:ARG:HA   | 2:C:596:TYR:CE1  | 2.53                     | 0.42              |
| 3:D:567:ILE:HG22 | 3:D:571:LYS:NZ   | 2.35                     | 0.42              |
| 1:A:34:VAL:HA    | 1:A:179:PHE:HE1  | 1.84                     | 0.42              |
| 1:A:225:PHE:CD2  | 1:B:11:PHE:CE1   | 3.06                     | 0.42              |
| 1:B:37:GLY:HA3   | 1:B:179:PHE:CE1  | 2.55                     | 0.42              |
| 2:C:15:LEU:HD12  | 2:C:15:LEU:N     | 2.30                     | 0.42              |
| 2:C:297:GLU:HB3  | 2:C:298:PHE:H    | 1.68                     | 0.42              |
| 2:C:540:PHE:HE1  | 2:C:906:PHE:HE1  | 1.68                     | 0.42              |
| 5:F:125:ASP:HA   | 5:F:128:ARG:NH2  | 2.35                     | 0.42              |
| 2:C:260:LEU:HD12 | 2:C:288:ARG:HG2  | 2.02                     | 0.42              |
| 3:D:226:PRO:HA   | 3:D:330:THR:HG22 | 2.02                     | 0.42              |
| 3:D:714:GLN:HE21 | 3:D:765:SER:CB   | 2.32                     | 0.42              |
| 3:D:913:ASP:O    | 3:D:914:LEU:C    | 2.58                     | 0.42              |
| 3:D:1372:VAL:HA  | 3:D:1375:MET:CE  | 2.50                     | 0.42              |
| 5:F:369:LEU:O    | 5:F:374:GLY:N    | 2.50                     | 0.42              |
| 1:A:132:LEU:HD11 | 1:A:138:LEU:HB3  | 2.02                     | 0.41              |
| 2:C:309:TYR:HE1  | 2:C:319:GLY:HA3  | 1.85                     | 0.41              |
| 2:C:700:TYR:HB3  | 2:C:833:LEU:HD13 | 2.01                     | 0.41              |
| 2:C:910:LYS:C    | 2:C:912:PRO:HD2  | 2.40                     | 0.41              |
| 2:C:1009:SER:N   | 3:D:651:GLU:HG3  | 2.35                     | 0.41              |
| 3:D:700:VAL:HG13 | 3:D:718:PRO:HG3  | 2.01                     | 0.41              |
| 3:D:835:SER:O    | 3:D:836:VAL:HG23 | 2.20                     | 0.41              |
| 3:D:911:LEU:O    | 3:D:912:LYS:C    | 2.59                     | 0.41              |
| 3:D:1161:GLU:OE2 | 3:D:1164:ARG:HG3 | 2.18                     | 0.41              |
| 3:D:1242:HIS:CE1 | 3:D:1245:GLY:HA3 | 2.55                     | 0.41              |
| 1:A:37:GLY:HA3   | 1:A:195:LEU:HD11 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:38:ASN:O      | 1:B:42:ARG:HG2    | 2.21                     | 0.41              |
| 2:C:408:ARG:NH2   | 2:C:455:LEU:HD23  | 2.35                     | 0.41              |
| 2:C:1107:ASN:HA   | 2:C:1108:PRO:HD2  | 1.91                     | 0.41              |
| 3:D:463:GLN:NE2   | 3:D:467:GLU:HG3   | 2.34                     | 0.41              |
| 3:D:493:ARG:HH21  | 3:D:494:LYS:HZ3   | 1.66                     | 0.41              |
| 3:D:662:GLU:OE2   | 3:D:669:ASN:HA    | 2.20                     | 0.41              |
| 3:D:760:ARG:NH2   | 4:E:62:THR:OG1    | 2.53                     | 0.41              |
| 3:D:916:TYR:O     | 3:D:919:PHE:HB3   | 2.20                     | 0.41              |
| 3:D:1042:ARG:NH1  | 3:D:1045:MET:HE1  | 2.35                     | 0.41              |
| 3:D:1046:GLN:HA   | 3:D:1052:THR:HA   | 2.01                     | 0.41              |
| 3:D:1459:LEU:HD11 | 3:D:1468:LEU:HD13 | 2.02                     | 0.41              |
| 4:E:30:LEU:HD21   | 4:E:63:TRP:HB3    | 2.02                     | 0.41              |
| 1:B:12:THR:HB     | 1:B:24:VAL:HB     | 2.01                     | 0.41              |
| 2:C:121:MET:HG3   | 2:C:127:PHE:CZ    | 2.55                     | 0.41              |
| 2:C:707:ARG:HD2   | 2:C:824:ARG:NH1   | 2.35                     | 0.41              |
| 2:C:850:ALA:CA    | 3:D:632:VAL:HG22  | 2.48                     | 0.41              |
| 2:C:1032:PHE:CD1  | 2:C:1052:MET:HG2  | 2.54                     | 0.41              |
| 2:C:1040:LEU:HA   | 2:C:1043:TYR:HB2  | 2.01                     | 0.41              |
| 3:D:539:ASP:HB3   | 3:D:600:LEU:HB3   | 2.02                     | 0.41              |
| 3:D:1377:LYS:HD2  | 3:D:1378:TYR:HE2  | 1.78                     | 0.41              |
| 5:F:88:ILE:HD13   | 5:F:88:ILE:HA     | 1.70                     | 0.41              |
| 5:F:291:ILE:HG23  | 5:F:304:VAL:HG21  | 2.02                     | 0.41              |
| 1:A:11:PHE:HA     | 1:A:25:LEU:HD12   | 2.01                     | 0.41              |
| 2:C:1060:ILE:O    | 2:C:1064:ASN:ND2  | 2.53                     | 0.41              |
| 3:D:727:GLN:HB2   | 3:D:727:GLN:HE21  | 1.54                     | 0.41              |
| 3:D:756:GLN:HE21  | 3:D:756:GLN:HB3   | 1.68                     | 0.41              |
| 3:D:1225:ALA:HA   | 3:D:1367:HIS:ND1  | 2.34                     | 0.41              |
| 3:D:1254:GLN:O    | 3:D:1257:PRO:HG2  | 2.19                     | 0.41              |
| 1:B:64:GLU:HB2    | 1:B:75:VAL:HG11   | 2.02                     | 0.41              |
| 2:C:284:ARG:HA    | 2:C:284:ARG:HH11  | 1.85                     | 0.41              |
| 2:C:338:GLU:HG2   | 2:C:342:ASP:OD2   | 2.21                     | 0.41              |
| 2:C:439:CYS:HB2   | 2:C:541:SER:H     | 1.85                     | 0.41              |
| 2:C:842:ARG:NH2   | 2:C:887:GLU:OE2   | 2.52                     | 0.41              |
| 2:C:1059:ASP:OD1  | 2:C:1062:GLY:CA   | 2.68                     | 0.41              |
| 3:D:108:VAL:HA    | 3:D:110:SER:N     | 2.35                     | 0.41              |
| 3:D:653:PHE:N     | 3:D:653:PHE:CD1   | 2.89                     | 0.41              |
| 3:D:1431:THR:HG21 | 11:D:1713:HOH:O   | 2.20                     | 0.41              |
| 2:C:264:PRO:HB2   | 2:C:289:THR:HG21  | 2.02                     | 0.41              |
| 2:C:839:LEU:HA    | 2:C:839:LEU:HD23  | 1.62                     | 0.41              |
| 2:C:926:PHE:C     | 2:C:928:LYS:H     | 2.23                     | 0.41              |
| 3:D:53:ILE:HG22   | 3:D:54:LYS:HG3    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:226:PRO:HG3   | 3:D:249:TYR:HB2   | 2.02                     | 0.41              |
| 3:D:257:GLY:H     | 3:D:272:LEU:HD22  | 1.85                     | 0.41              |
| 3:D:304:LEU:O     | 3:D:305:ALA:HB3   | 2.21                     | 0.41              |
| 3:D:387:LEU:H     | 3:D:387:LEU:HD12  | 1.86                     | 0.41              |
| 3:D:473:LEU:HD11  | 3:D:495:ARG:HH21  | 1.85                     | 0.41              |
| 3:D:772:PRO:O     | 3:D:1209:LEU:HD23 | 2.21                     | 0.41              |
| 3:D:984:THR:HG23  | 3:D:987:GLU:H     | 1.86                     | 0.41              |
| 3:D:1031:ASN:HB2  | 3:D:1032:PRO:HD2  | 2.00                     | 0.41              |
| 3:D:1383:ASP:HA   | 3:D:1384:PRO:HD3  | 1.90                     | 0.41              |
| 4:E:81:PRO:HB2    | 4:E:84:ARG:HB2    | 2.02                     | 0.41              |
| 5:F:208:SER:HB3   | 5:F:211:ASP:HB2   | 2.01                     | 0.41              |
| 1:A:101:LEU:HB3   | 1:A:140:MET:HG2   | 2.02                     | 0.41              |
| 2:C:405:ARG:HB2   | 2:C:543:ASN:HD21  | 1.85                     | 0.41              |
| 2:C:471:TYR:CE2   | 2:C:496:ILE:HG21  | 2.56                     | 0.41              |
| 2:C:949:LYS:HD2   | 3:D:796:ARG:HH21  | 1.81                     | 0.41              |
| 3:D:211:VAL:HG12  | 3:D:387:LEU:HA    | 2.02                     | 0.41              |
| 3:D:1364:HIS:ND1  | 3:D:1366:LYS:HG2  | 2.35                     | 0.41              |
| 2:C:418:LEU:O     | 2:C:420:ARG:N     | 2.48                     | 0.41              |
| 2:C:776:SER:CA    | 2:C:780:GLU:HB2   | 2.44                     | 0.41              |
| 3:D:356:PRO:HB2   | 3:D:359:ALA:HB2   | 2.02                     | 0.41              |
| 3:D:539:ASP:CG    | 3:D:598:ARG:HH21  | 2.23                     | 0.41              |
| 3:D:786:ILE:O     | 3:D:787:LEU:C     | 2.58                     | 0.41              |
| 2:C:95:TYR:CG     | 2:C:114:PHE:HB3   | 2.56                     | 0.41              |
| 2:C:1056:LYS:HB3  | 3:D:624:ASP:H     | 1.86                     | 0.41              |
| 3:D:731:LEU:HA    | 3:D:731:LEU:HD23  | 1.91                     | 0.41              |
| 3:D:1135:ARG:O    | 3:D:1136:LYS:C    | 2.58                     | 0.41              |
| 3:D:1397:LYS:C    | 3:D:1398:TRP:CE3  | 2.90                     | 0.41              |
| 3:D:1459:LEU:HD22 | 3:D:1464:GLU:HB2  | 2.03                     | 0.41              |
| 3:D:1495:ILE:O    | 3:D:1499:ARG:HB2  | 2.21                     | 0.41              |
| 1:A:115:LEU:HA    | 1:A:116:PRO:HD2   | 1.84                     | 0.41              |
| 2:C:137:VAL:O     | 2:C:391:LEU:HG    | 2.21                     | 0.41              |
| 2:C:286:SER:OG    | 2:C:301:GLU:HB2   | 2.21                     | 0.41              |
| 2:C:421:GLU:O     | 2:C:423:ALA:N     | 2.49                     | 0.41              |
| 2:C:1095:LEU:HD12 | 3:D:607:LEU:HD12  | 2.03                     | 0.41              |
| 3:D:177:ALA:O     | 3:D:178:LEU:HB2   | 2.20                     | 0.41              |
| 3:D:1264:GLU:CB   | 3:D:1266:ARG:HH21 | 2.33                     | 0.41              |
| 2:C:154:ARG:NE    | 2:C:157:ARG:H     | 2.18                     | 0.40              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:HG21  | 2.02                     | 0.40              |
| 3:D:912:LYS:HB3   | 3:D:912:LYS:HE2   | 1.73                     | 0.40              |
| 3:D:1267:ARG:HD2  | 3:D:1271:LYS:NZ   | 2.36                     | 0.40              |
| 1:A:23:PHE:CD2    | 1:A:211:LEU:HD23  | 2.57                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:63:HIS:CE1   | 2:C:801:VAL:HG12  | 2.56                     | 0.40              |
| 1:A:158:ILE:H    | 1:A:159:LYS:NZ    | 2.18                     | 0.40              |
| 1:B:74:ASP:OD2   | 1:B:75:VAL:N      | 2.54                     | 0.40              |
| 2:C:1059:ASP:OD2 | 2:C:1080:SER:N    | 2.54                     | 0.40              |
| 3:D:217:LYS:HD2  | 3:D:339:TRP:CZ2   | 2.55                     | 0.40              |
| 3:D:935:LYS:HB3  | 3:D:935:LYS:HE2   | 1.76                     | 0.40              |
| 3:D:1271:LYS:HD2 | 3:D:1334:GLN:OE1  | 2.21                     | 0.40              |
| 3:D:1413:THR:HA  | 3:D:1414:PRO:HD3  | 1.79                     | 0.40              |
| 5:F:88:ILE:HG23  | 5:F:193:ARG:HG2   | 2.03                     | 0.40              |
| 6:Z:30:UNK:HA    | 6:Z:31:UNK:HA     | 1.61                     | 0.40              |
| 1:B:91:ASN:HA    | 1:B:92:PRO:HD3    | 1.85                     | 0.40              |
| 2:C:224:GLU:HB3  | 2:C:227:PHE:HB2   | 2.04                     | 0.40              |
| 3:D:410:SER:OG   | 3:D:411:THR:N     | 2.55                     | 0.40              |
| 3:D:450:TYR:HB2  | 3:D:452:ILE:HD11  | 2.03                     | 0.40              |
| 3:D:774:SER:HB3  | 3:D:1362:LYS:O    | 2.21                     | 0.40              |
| 3:D:1103:HIS:CE1 | 3:D:1463:LYS:HB2  | 2.56                     | 0.40              |
| 3:D:1141:GLU:HA  | 3:D:1171:VAL:HG11 | 2.02                     | 0.40              |
| 3:D:1350:GLU:O   | 3:D:1351:GLU:C    | 2.60                     | 0.40              |
| 1:A:7:LYS:HE2    | 1:A:7:LYS:HB3     | 1.98                     | 0.40              |
| 1:A:101:LEU:HD21 | 1:A:109:VAL:CG1   | 2.52                     | 0.40              |
| 1:A:115:LEU:HD13 | 1:A:116:PRO:HD2   | 2.04                     | 0.40              |
| 1:A:179:PHE:CG   | 1:A:179:PHE:O     | 2.75                     | 0.40              |
| 1:B:213:GLN:O    | 1:B:217:ILE:HG13  | 2.21                     | 0.40              |
| 2:C:271:GLU:O    | 2:C:273:GLY:N     | 2.54                     | 0.40              |
| 2:C:948:GLU:HB3  | 2:C:953:VAL:HG23  | 2.02                     | 0.40              |
| 3:D:206:ARG:H    | 3:D:390:PRO:HB3   | 1.86                     | 0.40              |
| 3:D:879:ARG:HB3  | 3:D:902:LEU:HD12  | 2.03                     | 0.40              |
| 3:D:906:GLN:HA   | 3:D:910:SER:OG    | 2.22                     | 0.40              |
| 3:D:1364:HIS:O   | 3:D:1365:ASP:C    | 2.60                     | 0.40              |
| 2:C:807:ARG:HA   | 2:C:821:GLU:CB    | 2.51                     | 0.40              |
| 3:D:341:GLU:HA   | 3:D:342:PRO:HD3   | 1.88                     | 0.40              |
| 3:D:1011:PHE:O   | 3:D:1016:PRO:HA   | 2.21                     | 0.40              |
| 3:D:1037:GLN:HG2 | 3:D:1042:ARG:HA   | 2.03                     | 0.40              |
| 3:D:1066:THR:HB  | 3:D:1069:GLU:HB2  | 2.04                     | 0.40              |
| 3:D:1255:GLY:O   | 3:D:1258:ARG:N    | 2.51                     | 0.40              |
| 3:D:1365:ASP:HA  | 3:D:1368:ILE:HD13 | 2.03                     | 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     | 229/315 (73%)    | 175 (76%)  | 40 (18%)  | 14 (6%)  | 1           | 2  |
| 1   | B     | 236/315 (75%)    | 186 (79%)  | 45 (19%)  | 5 (2%)   | 5           | 14 |
| 2   | C     | 1117/1119 (100%) | 877 (78%)  | 187 (17%) | 53 (5%)  | 2           | 3  |
| 3   | D     | 1502/1524 (99%)  | 1160 (77%) | 260 (17%) | 82 (6%)  | 1           | 2  |
| 4   | E     | 93/99 (94%)      | 76 (82%)   | 14 (15%)  | 3 (3%)   | 3           | 7  |
| 5   | F     | 349/423 (82%)    | 286 (82%)  | 54 (16%)  | 9 (3%)   | 4           | 10 |
| All | All   | 3526/3795 (93%)  | 2760 (78%) | 600 (17%) | 166 (5%) | 2           | 3  |

All (166) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 229  | GLN  |
| 2   | C     | 42   | VAL  |
| 2   | C     | 263  | ASP  |
| 2   | C     | 272  | ALA  |
| 2   | C     | 738  | ASP  |
| 2   | C     | 739  | GLU  |
| 2   | C     | 1115 | LEU  |
| 3   | D     | 137  | PRO  |
| 3   | D     | 587  | ARG  |
| 3   | D     | 593  | ASN  |
| 3   | D     | 594  | PRO  |
| 3   | D     | 809  | PRO  |
| 3   | D     | 939  | PHE  |
| 3   | D     | 940  | THR  |
| 3   | D     | 1128 | VAL  |
| 3   | D     | 1386 | ASP  |
| 3   | D     | 1391 | GLU  |
| 3   | D     | 1437 | ALA  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1482 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | E     | 82   | GLU  |
| 1   | A     | 14   | ARG  |
| 1   | A     | 105  | GLY  |
| 1   | A     | 153  | ALA  |
| 1   | A     | 158  | ILE  |
| 1   | A     | 159  | LYS  |
| 1   | B     | 233  | VAL  |
| 2   | C     | 60   | GLY  |
| 2   | C     | 80   | GLN  |
| 2   | C     | 105  | THR  |
| 2   | C     | 223  | ASP  |
| 2   | C     | 262  | ALA  |
| 2   | C     | 316  | GLY  |
| 2   | C     | 369  | PRO  |
| 2   | C     | 419  | THR  |
| 2   | C     | 1016 | ILE  |
| 3   | D     | 110  | SER  |
| 3   | D     | 178  | LEU  |
| 3   | D     | 192  | ALA  |
| 3   | D     | 196  | VAL  |
| 3   | D     | 409  | VAL  |
| 3   | D     | 525  | ARG  |
| 3   | D     | 549  | ASN  |
| 3   | D     | 595  | GLY  |
| 3   | D     | 822  | ALA  |
| 3   | D     | 823  | LEU  |
| 3   | D     | 830  | ALA  |
| 3   | D     | 918  | ALA  |
| 3   | D     | 949  | ILE  |
| 3   | D     | 1209 | LEU  |
| 3   | D     | 1220 | ALA  |
| 3   | D     | 1266 | ARG  |
| 3   | D     | 1297 | GLU  |
| 3   | D     | 1341 | PRO  |
| 3   | D     | 1412 | LYS  |
| 3   | D     | 1444 | THR  |
| 5   | F     | 141  | VAL  |
| 5   | F     | 153  | PRO  |
| 1   | A     | 38   | ASN  |
| 1   | B     | 125  | PRO  |
| 1   | B     | 158  | ILE  |
| 2   | C     | 208  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 288  | ARG  |
| 2   | C     | 422  | ARG  |
| 2   | C     | 541  | SER  |
| 2   | C     | 626  | ARG  |
| 2   | C     | 728  | HIS  |
| 2   | C     | 876  | VAL  |
| 2   | C     | 908  | GLY  |
| 2   | C     | 1042 | ALA  |
| 2   | C     | 1108 | PRO  |
| 2   | C     | 1113 | GLU  |
| 3   | D     | 82   | LYS  |
| 3   | D     | 119  | SER  |
| 3   | D     | 230  | TRP  |
| 3   | D     | 287  | GLY  |
| 3   | D     | 483  | HIS  |
| 3   | D     | 603  | LEU  |
| 3   | D     | 652  | LEU  |
| 3   | D     | 835  | SER  |
| 3   | D     | 1166 | LEU  |
| 3   | D     | 1245 | GLY  |
| 3   | D     | 1269 | LYS  |
| 3   | D     | 1348 | LEU  |
| 3   | D     | 1389 | LEU  |
| 3   | D     | 1390 | LEU  |
| 3   | D     | 1442 | ASN  |
| 5   | F     | 255  | ALA  |
| 1   | A     | 59   | GLU  |
| 1   | A     | 160  | ASP  |
| 2   | C     | 31   | GLN  |
| 2   | C     | 261  | ILE  |
| 2   | C     | 482  | GLU  |
| 2   | C     | 638  | ASP  |
| 2   | C     | 735  | ARG  |
| 2   | C     | 880  | MET  |
| 2   | C     | 1079 | PRO  |
| 3   | D     | 117  | ASP  |
| 3   | D     | 248  | PRO  |
| 3   | D     | 255  | GLU  |
| 3   | D     | 316  | GLN  |
| 3   | D     | 373  | PRO  |
| 3   | D     | 437  | VAL  |
| 3   | D     | 509  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 601  | ARG  |
| 3   | D     | 654  | LYS  |
| 3   | D     | 801  | GLY  |
| 3   | D     | 836  | VAL  |
| 3   | D     | 1040 | GLY  |
| 3   | D     | 1238 | MET  |
| 3   | D     | 1248 | GLY  |
| 3   | D     | 1349 | VAL  |
| 5   | F     | 394  | ARG  |
| 1   | A     | 227  | ASN  |
| 2   | C     | 36   | PRO  |
| 2   | C     | 37   | GLU  |
| 2   | C     | 99   | GLN  |
| 2   | C     | 111  | ASP  |
| 2   | C     | 195  | LEU  |
| 2   | C     | 820  | ARG  |
| 2   | C     | 835  | VAL  |
| 2   | C     | 907  | ASP  |
| 2   | C     | 945  | ARG  |
| 3   | D     | 245  | LEU  |
| 3   | D     | 303  | PRO  |
| 3   | D     | 440  | VAL  |
| 3   | D     | 485  | SER  |
| 3   | D     | 869  | MET  |
| 3   | D     | 883  | ALA  |
| 3   | D     | 1365 | ASP  |
| 3   | D     | 1408 | ILE  |
| 4   | E     | 86   | GLN  |
| 5   | F     | 389  | PHE  |
| 5   | F     | 395  | GLU  |
| 1   | A     | 4    | SER  |
| 1   | A     | 228  | PRO  |
| 1   | B     | 49   | PRO  |
| 2   | C     | 289  | THR  |
| 2   | C     | 570  | PRO  |
| 2   | C     | 784  | ASP  |
| 2   | C     | 796  | GLU  |
| 2   | C     | 808  | ARG  |
| 3   | D     | 227  | LEU  |
| 3   | D     | 305  | ALA  |
| 3   | D     | 1023 | MET  |
| 3   | D     | 1072 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1410 | GLU  |
| 4   | E     | 39   | VAL  |
| 5   | F     | 80   | PRO  |
| 5   | F     | 152  | ASP  |
| 1   | A     | 17   | GLY  |
| 2   | C     | 427  | VAL  |
| 3   | D     | 328  | GLY  |
| 3   | D     | 457  | GLY  |
| 3   | D     | 530  | VAL  |
| 3   | D     | 1067 | VAL  |
| 1   | A     | 157  | GLY  |
| 2   | C     | 318  | PRO  |
| 2   | C     | 924  | VAL  |
| 2   | C     | 1020 | PRO  |
| 2   | C     | 226  | VAL  |
| 1   | B     | 120  | VAL  |
| 2   | C     | 155  | PRO  |
| 3   | D     | 612  | GLY  |
| 5   | F     | 314  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 202/273 (74%)   | 171 (85%)  | 31 (15%)  | 2           | 5  |
| 1   | B     | 206/273 (76%)   | 183 (89%)  | 23 (11%)  | 5           | 11 |
| 2   | C     | 941/941 (100%)  | 816 (87%)  | 125 (13%) | 3           | 7  |
| 3   | D     | 1264/1279 (99%) | 1111 (88%) | 153 (12%) | 4           | 9  |
| 4   | E     | 83/87 (95%)     | 75 (90%)   | 8 (10%)   | 7           | 16 |
| 5   | F     | 306/370 (83%)   | 283 (92%)  | 23 (8%)   | 11          | 26 |
| All | All   | 3002/3223 (93%) | 2639 (88%) | 363 (12%) | 4           | 9  |

All (363) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | LEU  |
| 1   | A     | 7   | LYS  |
| 1   | A     | 12  | THR  |
| 1   | A     | 15  | THR  |
| 1   | A     | 19  | GLU  |
| 1   | A     | 24  | VAL  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 34  | VAL  |
| 1   | A     | 42  | ARG  |
| 1   | A     | 44  | LEU  |
| 1   | A     | 45  | LEU  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 88  | ARG  |
| 1   | A     | 90  | LEU  |
| 1   | A     | 96  | THR  |
| 1   | A     | 112 | ARG  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 127 | LEU  |
| 1   | A     | 131 | THR  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 154 | GLU  |
| 1   | A     | 159 | LYS  |
| 1   | A     | 182 | GLU  |
| 1   | A     | 184 | THR  |
| 1   | A     | 196 | THR  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 200 | TRP  |
| 1   | A     | 202 | ASP  |
| 1   | A     | 221 | HIS  |
| 1   | A     | 224 | TYR  |
| 1   | B     | 5   | LYS  |
| 1   | B     | 7   | LYS  |
| 1   | B     | 10  | VAL  |
| 1   | B     | 22  | GLU  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 42  | ARG  |
| 1   | B     | 54  | THR  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 60  | ASP  |
| 1   | B     | 61  | VAL  |
| 1   | B     | 64  | GLU  |
| 1   | B     | 87  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 100 | LEU  |
| 1   | B     | 104 | GLU  |
| 1   | B     | 119 | ASP  |
| 1   | B     | 140 | MET  |
| 1   | B     | 146 | ARG  |
| 1   | B     | 176 | ARG  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 184 | THR  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 233 | VAL  |
| 2   | C     | 1   | MET  |
| 2   | C     | 2   | GLU  |
| 2   | C     | 8   | ARG  |
| 2   | C     | 15  | LEU  |
| 2   | C     | 26  | TYR  |
| 2   | C     | 39  | ARG  |
| 2   | C     | 54  | ILE  |
| 2   | C     | 73  | LEU  |
| 2   | C     | 81  | ASP  |
| 2   | C     | 99  | GLN  |
| 2   | C     | 103 | LYS  |
| 2   | C     | 113 | VAL  |
| 2   | C     | 114 | PHE  |
| 2   | C     | 122 | THR  |
| 2   | C     | 138 | SER  |
| 2   | C     | 143 | SER  |
| 2   | C     | 154 | ARG  |
| 2   | C     | 157 | ARG  |
| 2   | C     | 159 | ILE  |
| 2   | C     | 165 | LEU  |
| 2   | C     | 184 | MET  |
| 2   | C     | 186 | VAL  |
| 2   | C     | 189 | ARG  |
| 2   | C     | 206 | THR  |
| 2   | C     | 209 | ARG  |
| 2   | C     | 214 | TYR  |
| 2   | C     | 216 | GLU  |
| 2   | C     | 232 | GLU  |
| 2   | C     | 239 | PHE  |
| 2   | C     | 242 | LEU  |
| 2   | C     | 250 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 256 | TYR  |
| 2   | C     | 265 | ARG  |
| 2   | C     | 266 | ARG  |
| 2   | C     | 289 | THR  |
| 2   | C     | 290 | LEU  |
| 2   | C     | 297 | GLU  |
| 2   | C     | 307 | LEU  |
| 2   | C     | 308 | ARG  |
| 2   | C     | 317 | VAL  |
| 2   | C     | 321 | GLU  |
| 2   | C     | 325 | ILE  |
| 2   | C     | 335 | THR  |
| 2   | C     | 353 | ARG  |
| 2   | C     | 358 | ARG  |
| 2   | C     | 360 | LEU  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 371 | LYS  |
| 2   | C     | 372 | LEU  |
| 2   | C     | 379 | GLU  |
| 2   | C     | 387 | SER  |
| 2   | C     | 388 | ARG  |
| 2   | C     | 393 | GLN  |
| 2   | C     | 394 | PHE  |
| 2   | C     | 398 | THR  |
| 2   | C     | 402 | SER  |
| 2   | C     | 421 | GLU  |
| 2   | C     | 425 | PHE  |
| 2   | C     | 434 | HIS  |
| 2   | C     | 441 | VAL  |
| 2   | C     | 443 | THR  |
| 2   | C     | 455 | LEU  |
| 2   | C     | 489 | THR  |
| 2   | C     | 491 | GLU  |
| 2   | C     | 512 | ARG  |
| 2   | C     | 514 | VAL  |
| 2   | C     | 522 | VAL  |
| 2   | C     | 539 | VAL  |
| 2   | C     | 554 | ASP  |
| 2   | C     | 600 | ASP  |
| 2   | C     | 610 | ARG  |
| 2   | C     | 616 | GLU  |
| 2   | C     | 625 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 627 | ARG  |
| 2   | C     | 637 | LEU  |
| 2   | C     | 640 | ARG  |
| 2   | C     | 657 | ASP  |
| 2   | C     | 661 | SER  |
| 2   | C     | 672 | VAL  |
| 2   | C     | 673 | LEU  |
| 2   | C     | 676 | ILE  |
| 2   | C     | 680 | ASP  |
| 2   | C     | 683 | ASN  |
| 2   | C     | 685 | GLU  |
| 2   | C     | 689 | VAL  |
| 2   | C     | 698 | ASP  |
| 2   | C     | 699 | PHE  |
| 2   | C     | 714 | ASP  |
| 2   | C     | 715 | THR  |
| 2   | C     | 717 | LEU  |
| 2   | C     | 720 | GLU  |
| 2   | C     | 722 | ILE  |
| 2   | C     | 723 | THR  |
| 2   | C     | 728 | HIS  |
| 2   | C     | 729 | LEU  |
| 2   | C     | 739 | GLU  |
| 2   | C     | 740 | GLU  |
| 2   | C     | 750 | LYS  |
| 2   | C     | 799 | ILE  |
| 2   | C     | 807 | ARG  |
| 2   | C     | 822 | VAL  |
| 2   | C     | 829 | GLN  |
| 2   | C     | 837 | ASP  |
| 2   | C     | 838 | LYS  |
| 2   | C     | 855 | VAL  |
| 2   | C     | 856 | GLU  |
| 2   | C     | 869 | VAL  |
| 2   | C     | 871 | LEU  |
| 2   | C     | 879 | ARG  |
| 2   | C     | 881 | ASN  |
| 2   | C     | 900 | ARG  |
| 2   | C     | 913 | GLU  |
| 2   | C     | 937 | ASP  |
| 2   | C     | 969 | GLN  |
| 2   | C     | 981 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 999  | HIS  |
| 2   | C     | 1000 | MET  |
| 2   | C     | 1008 | ARG  |
| 2   | C     | 1009 | SER  |
| 2   | C     | 1016 | ILE  |
| 2   | C     | 1043 | TYR  |
| 2   | C     | 1055 | LEU  |
| 2   | C     | 1078 | GLU  |
| 2   | C     | 1081 | VAL  |
| 2   | C     | 1113 | GLU  |
| 3   | D     | 12   | LEU  |
| 3   | D     | 17   | LYS  |
| 3   | D     | 32   | ILE  |
| 3   | D     | 38   | LYS  |
| 3   | D     | 40   | GLU  |
| 3   | D     | 48   | ARG  |
| 3   | D     | 68   | PHE  |
| 3   | D     | 85   | VAL  |
| 3   | D     | 97   | THR  |
| 3   | D     | 108  | VAL  |
| 3   | D     | 142  | LEU  |
| 3   | D     | 152  | LEU  |
| 3   | D     | 153  | LEU  |
| 3   | D     | 184  | GLU  |
| 3   | D     | 185  | VAL  |
| 3   | D     | 190  | GLU  |
| 3   | D     | 191  | LEU  |
| 3   | D     | 236  | TYR  |
| 3   | D     | 241  | ILE  |
| 3   | D     | 251  | PHE  |
| 3   | D     | 252  | ARG  |
| 3   | D     | 317  | VAL  |
| 3   | D     | 323  | GLU  |
| 3   | D     | 333  | LEU  |
| 3   | D     | 344  | ASP  |
| 3   | D     | 346  | ARG  |
| 3   | D     | 360  | ARG  |
| 3   | D     | 371  | ILE  |
| 3   | D     | 376  | GLU  |
| 3   | D     | 380  | GLU  |
| 3   | D     | 389  | GLU  |
| 3   | D     | 399  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 411 | THR  |
| 3   | D     | 431 | VAL  |
| 3   | D     | 434 | ARG  |
| 3   | D     | 448 | GLU  |
| 3   | D     | 478 | LEU  |
| 3   | D     | 493 | ARG  |
| 3   | D     | 500 | ARG  |
| 3   | D     | 502 | PHE  |
| 3   | D     | 510 | GLU  |
| 3   | D     | 523 | ASP  |
| 3   | D     | 524 | LEU  |
| 3   | D     | 539 | ASP  |
| 3   | D     | 560 | GLN  |
| 3   | D     | 564 | GLU  |
| 3   | D     | 565 | ILE  |
| 3   | D     | 566 | ILE  |
| 3   | D     | 587 | ARG  |
| 3   | D     | 624 | ASP  |
| 3   | D     | 632 | VAL  |
| 3   | D     | 636 | GLN  |
| 3   | D     | 648 | MET  |
| 3   | D     | 650 | LEU  |
| 3   | D     | 676 | MET  |
| 3   | D     | 678 | GLU  |
| 3   | D     | 680 | GLN  |
| 3   | D     | 686 | GLU  |
| 3   | D     | 703 | ASN  |
| 3   | D     | 708 | LEU  |
| 3   | D     | 709 | HIS  |
| 3   | D     | 711 | LEU  |
| 3   | D     | 734 | GLU  |
| 3   | D     | 754 | PHE  |
| 3   | D     | 756 | GLN  |
| 3   | D     | 771 | SER  |
| 3   | D     | 780 | LYS  |
| 3   | D     | 782 | SER  |
| 3   | D     | 818 | ARG  |
| 3   | D     | 827 | ILE  |
| 3   | D     | 836 | VAL  |
| 3   | D     | 842 | VAL  |
| 3   | D     | 860 | LEU  |
| 3   | D     | 864 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 876  | SER  |
| 3   | D     | 894  | LYS  |
| 3   | D     | 903  | ASP  |
| 3   | D     | 907  | GLU  |
| 3   | D     | 911  | LEU  |
| 3   | D     | 915  | VAL  |
| 3   | D     | 920  | LEU  |
| 3   | D     | 922  | LEU  |
| 3   | D     | 947  | ILE  |
| 3   | D     | 948  | THR  |
| 3   | D     | 952  | ASP  |
| 3   | D     | 964  | LEU  |
| 3   | D     | 968  | ASP  |
| 3   | D     | 971  | LEU  |
| 3   | D     | 983  | LEU  |
| 3   | D     | 985  | ASP  |
| 3   | D     | 994  | GLN  |
| 3   | D     | 1020 | LEU  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1041 | LEU  |
| 3   | D     | 1055 | VAL  |
| 3   | D     | 1086 | LEU  |
| 3   | D     | 1096 | ARG  |
| 3   | D     | 1116 | ASN  |
| 3   | D     | 1119 | SER  |
| 3   | D     | 1124 | GLN  |
| 3   | D     | 1133 | ARG  |
| 3   | D     | 1155 | VAL  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1162 | GLU  |
| 3   | D     | 1170 | ASP  |
| 3   | D     | 1188 | VAL  |
| 3   | D     | 1192 | LEU  |
| 3   | D     | 1202 | GLN  |
| 3   | D     | 1204 | CYS  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1213 | ARG  |
| 3   | D     | 1216 | SER  |
| 3   | D     | 1234 | THR  |
| 3   | D     | 1238 | MET  |
| 3   | D     | 1239 | ARG  |
| 3   | D     | 1241 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1253 | THR  |
| 3   | D     | 1266 | ARG  |
| 3   | D     | 1276 | GLU  |
| 3   | D     | 1277 | ILE  |
| 3   | D     | 1286 | THR  |
| 3   | D     | 1287 | GLU  |
| 3   | D     | 1288 | GLU  |
| 3   | D     | 1297 | GLU  |
| 3   | D     | 1301 | LYS  |
| 3   | D     | 1305 | LEU  |
| 3   | D     | 1307 | LYS  |
| 3   | D     | 1313 | VAL  |
| 3   | D     | 1314 | LYS  |
| 3   | D     | 1319 | VAL  |
| 3   | D     | 1331 | ASP  |
| 3   | D     | 1344 | VAL  |
| 3   | D     | 1346 | ARG  |
| 3   | D     | 1348 | LEU  |
| 3   | D     | 1350 | GLU  |
| 3   | D     | 1359 | GLN  |
| 3   | D     | 1363 | LEU  |
| 3   | D     | 1368 | ILE  |
| 3   | D     | 1388 | ARG  |
| 3   | D     | 1390 | LEU  |
| 3   | D     | 1396 | GLU  |
| 3   | D     | 1398 | TRP  |
| 3   | D     | 1415 | VAL  |
| 3   | D     | 1422 | MET  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1430 | SER  |
| 3   | D     | 1431 | THR  |
| 3   | D     | 1467 | ILE  |
| 3   | D     | 1468 | LEU  |
| 3   | D     | 1479 | ASP  |
| 3   | D     | 1482 | ARG  |
| 3   | D     | 1487 | VAL  |
| 3   | D     | 1496 | GLU  |
| 4   | E     | 10   | PHE  |
| 4   | E     | 19   | LEU  |
| 4   | E     | 31   | LEU  |
| 4   | E     | 37   | ASN  |
| 4   | E     | 39   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 43  | GLU  |
| 4   | E     | 68  | LEU  |
| 4   | E     | 80  | VAL  |
| 5   | F     | 81  | VAL  |
| 5   | F     | 88  | ILE  |
| 5   | F     | 123 | ASP  |
| 5   | F     | 141 | VAL  |
| 5   | F     | 150 | THR  |
| 5   | F     | 179 | GLU  |
| 5   | F     | 205 | ARG  |
| 5   | F     | 208 | SER  |
| 5   | F     | 228 | GLU  |
| 5   | F     | 230 | LYS  |
| 5   | F     | 237 | THR  |
| 5   | F     | 249 | ARG  |
| 5   | F     | 256 | ARG  |
| 5   | F     | 264 | MET  |
| 5   | F     | 290 | GLU  |
| 5   | F     | 304 | VAL  |
| 5   | F     | 307 | THR  |
| 5   | F     | 319 | THR  |
| 5   | F     | 336 | GLU  |
| 5   | F     | 358 | LEU  |
| 5   | F     | 361 | LEU  |
| 5   | F     | 382 | THR  |
| 5   | F     | 394 | ARG  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | HIS  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 128 | HIS  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 212 | ASN  |
| 1   | B     | 38  | ASN  |
| 2   | C     | 22  | GLN  |
| 2   | C     | 179 | ASN  |
| 2   | C     | 187 | ASN  |
| 2   | C     | 393 | GLN  |
| 2   | C     | 406 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 498  | GLN  |
| 2   | C     | 552  | HIS  |
| 2   | C     | 575  | GLN  |
| 2   | C     | 639  | GLN  |
| 2   | C     | 683  | ASN  |
| 2   | C     | 829  | GLN  |
| 2   | C     | 843  | HIS  |
| 2   | C     | 845  | ASN  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 884  | GLN  |
| 2   | C     | 889  | HIS  |
| 2   | C     | 920  | GLN  |
| 3   | D     | 33   | ASN  |
| 3   | D     | 294  | HIS  |
| 3   | D     | 302  | GLN  |
| 3   | D     | 442  | ASN  |
| 3   | D     | 463  | GLN  |
| 3   | D     | 507  | ASN  |
| 3   | D     | 636  | GLN  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 703  | ASN  |
| 3   | D     | 714  | GLN  |
| 3   | D     | 727  | GLN  |
| 3   | D     | 729  | HIS  |
| 3   | D     | 901  | GLN  |
| 3   | D     | 906  | GLN  |
| 3   | D     | 1034 | GLN  |
| 3   | D     | 1075 | HIS  |
| 3   | D     | 1172 | HIS  |
| 3   | D     | 1195 | GLN  |
| 3   | D     | 1242 | HIS  |
| 3   | D     | 1353 | GLN  |
| 3   | D     | 1442 | ASN  |
| 4   | E     | 33   | HIS  |
| 4   | E     | 37   | ASN  |
| 5   | F     | 175  | HIS  |
| 5   | F     | 248  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 7   | PO4  | A     | 401  | -    | 4,4,4        | 1.05 | 0           | 6,6,6       | 0.43 | 0           |
| 10  | G4P  | D     | 1605 | 8    | 32,38,38     | 1.37 | 2 (6%)      | 42,61,61    | 1.16 | 4 (9%)      |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 10  | G4P  | D     | 1605 | 8    | -       | 6/23/43/43 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 10  | D     | 1605 | G4P  | O6-C6  | 5.78 | 1.36        | 1.23     |
| 10  | D     | 1605 | G4P  | PC-O3C | 2.04 | 1.61        | 1.59     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 10  | D     | 1605 | G4P  | C8-N7-C5 | 3.00 | 107.66      | 102.55   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10  | D     | 1605 | G4P  | C2-N1-C6   | -2.47 | 120.58      | 125.11   |
| 10  | D     | 1605 | G4P  | C5-C6-N1   | 2.30  | 118.45      | 114.07   |
| 10  | D     | 1605 | G4P  | O4'-C1'-N9 | 2.08  | 111.50      | 108.75   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

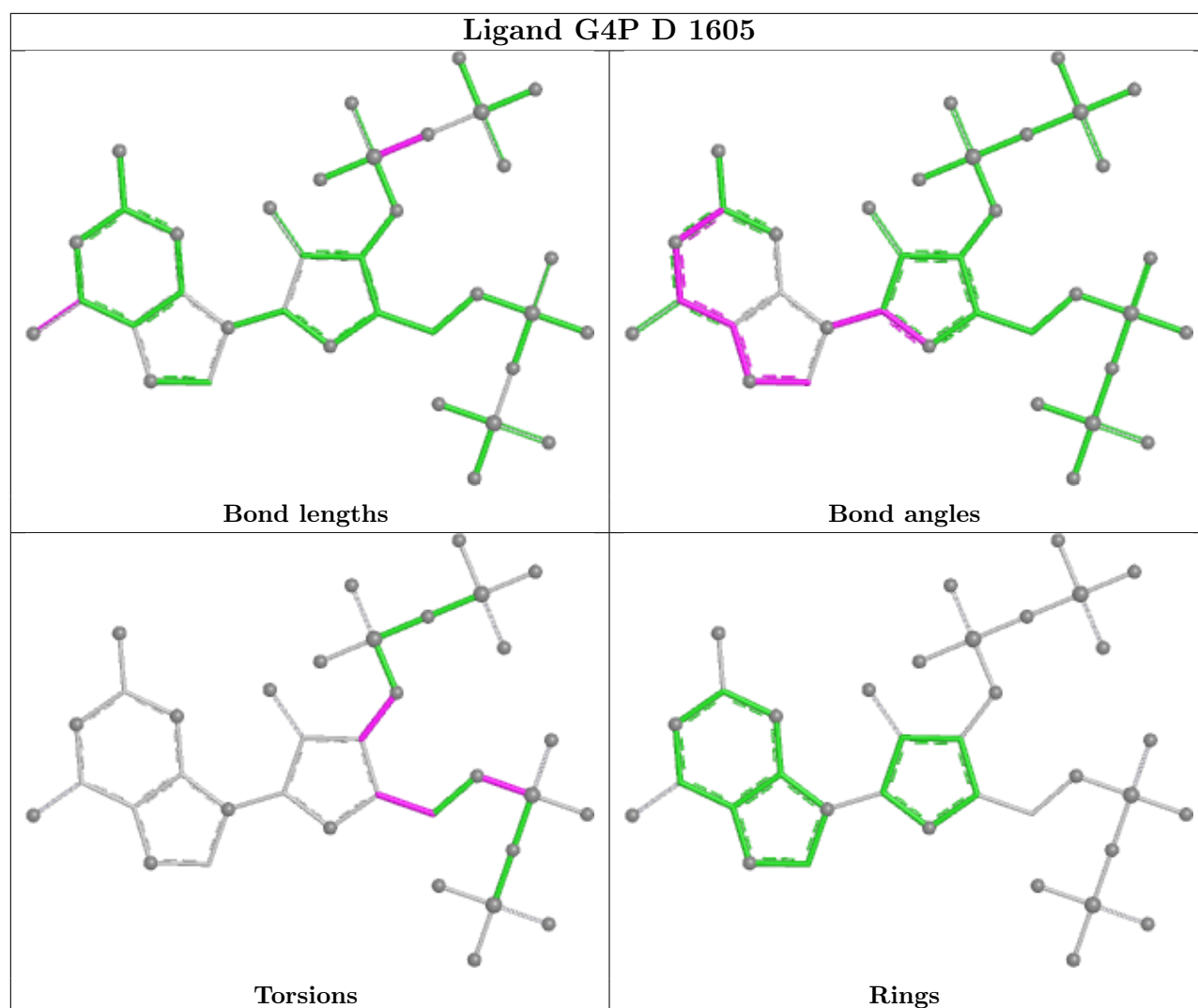
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | D     | 1605 | G4P  | C5'-O5'-PA-O3A  |
| 10  | D     | 1605 | G4P  | C5'-O5'-PA-O1A  |
| 10  | D     | 1605 | G4P  | C5'-O5'-PA-O2A  |
| 10  | D     | 1605 | G4P  | O4'-C4'-C5'-O5' |
| 10  | D     | 1605 | G4P  | C4'-C3'-O3'-PC  |
| 10  | D     | 1605 | G4P  | C3'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | D     | 1605 | G4P  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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     | 231/315 (73%)    | 0.50   | 20 (8%) 17 17 | 51, 78, 162, 212      | 1 (0%) |
| 1   | B     | 238/315 (75%)    | 1.56   | 67 (28%) 1 2  | 70, 149, 236, 260     | 0      |
| 2   | C     | 1119/1119 (100%) | 0.97   | 195 (17%) 5 5 | 49, 97, 222, 263      | 2 (0%) |
| 3   | D     | 1504/1524 (98%)  | 0.99   | 308 (20%) 3 4 | 49, 95, 245, 296      | 4 (0%) |
| 4   | E     | 95/99 (95%)      | 0.71   | 14 (14%) 7 7  | 58, 104, 192, 203     | 0      |
| 5   | F     | 351/423 (82%)    | 1.54   | 114 (32%) 1 1 | 68, 124, 245, 277     | 2 (0%) |
| 6   | Z     | 0/48             | -      | -             | -                     | -      |
| All | All   | 3538/3843 (92%)  | 1.04   | 718 (20%) 3 4 | 49, 102, 232, 296     | 9 (0%) |

All (718) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 3    | ASP  | 12.9 |
| 3   | D     | 428  | LYS  | 12.3 |
| 1   | A     | 4    | SER  | 11.2 |
| 1   | B     | 158  | ILE  | 10.9 |
| 5   | F     | 144  | ILE  | 10.2 |
| 3   | D     | 328  | GLY  | 9.9  |
| 1   | A     | 1    | MET  | 9.7  |
| 3   | D     | 326  | GLU  | 9.3  |
| 3   | D     | 418  | GLY  | 9.1  |
| 1   | B     | 238  | GLU  | 8.7  |
| 5   | F     | 147  | LEU  | 8.6  |
| 1   | B     | 96   | THR  | 8.6  |
| 1   | B     | 157  | GLY  | 8.6  |
| 3   | D     | 235  | ALA  | 8.4  |
| 3   | D     | 1247 | ALA  | 8.3  |
| 1   | A     | 2    | LEU  | 8.3  |
| 5   | F     | 236  | SER  | 8.3  |
| 3   | D     | 616  | GLN  | 8.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 5    | LYS  | 8.1  |
| 3   | D     | 417  | PRO  | 7.8  |
| 5   | F     | 148  | LYS  | 7.7  |
| 3   | D     | 236  | TYR  | 7.6  |
| 2   | C     | 269  | LEU  | 7.5  |
| 3   | D     | 613  | ARG  | 7.5  |
| 3   | D     | 375  | GLU  | 7.5  |
| 3   | D     | 1089 | ALA  | 7.4  |
| 1   | B     | 98   | THR  | 7.3  |
| 1   | B     | 62   | LEU  | 7.3  |
| 2   | C     | 254  | VAL  | 7.3  |
| 2   | C     | 275  | TYR  | 7.3  |
| 1   | B     | 160  | ASP  | 7.3  |
| 2   | C     | 221  | LEU  | 7.1  |
| 3   | D     | 895  | VAL  | 7.0  |
| 3   | D     | 229  | ALA  | 6.9  |
| 3   | D     | 595  | GLY  | 6.8  |
| 3   | D     | 227  | LEU  | 6.8  |
| 2   | C     | 42   | VAL  | 6.6  |
| 2   | C     | 360  | LEU  | 6.6  |
| 3   | D     | 230  | TRP  | 6.4  |
| 3   | D     | 420  | VAL  | 6.4  |
| 1   | B     | 97   | VAL  | 6.4  |
| 1   | B     | 162  | ILE  | 6.3  |
| 1   | B     | 93   | SER  | 6.3  |
| 3   | D     | 1249 | ALA  | 6.2  |
| 1   | A     | 6    | LEU  | 6.2  |
| 2   | C     | 763  | GLY  | 6.1  |
| 2   | C     | 1031 | ARG  | 6.1  |
| 5   | F     | 355  | GLU  | 6.0  |
| 1   | B     | 2    | LEU  | 6.0  |
| 3   | D     | 228  | ALA  | 5.9  |
| 3   | D     | 1245 | GLY  | 5.9  |
| 5   | F     | 321  | ILE  | 5.9  |
| 3   | D     | 394  | LEU  | 5.9  |
| 5   | F     | 237  | THR  | 5.8  |
| 2   | C     | 39   | ARG  | 5.8  |
| 3   | D     | 324  | ALA  | 5.8  |
| 2   | C     | 272  | ALA  | 5.8  |
| 3   | D     | 1246 | VAL  | 5.7  |
| 2   | C     | 268  | ASP  | 5.6  |
| 2   | C     | 762  | LYS  | 5.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 773  | LEU  | 5.5  |
| 5   | F     | 324  | GLU  | 5.5  |
| 1   | B     | 141  | GLU  | 5.4  |
| 1   | A     | 188  | GLN  | 5.4  |
| 5   | F     | 73   | PRO  | 5.3  |
| 1   | B     | 155  | LYS  | 5.2  |
| 2   | C     | 214  | TYR  | 5.2  |
| 3   | D     | 245  | LEU  | 5.2  |
| 3   | D     | 425  | GLY  | 5.2  |
| 5   | F     | 391  | GLY  | 5.1  |
| 3   | D     | 1250 | ALA  | 5.1  |
| 5   | F     | 383  | LEU  | 5.1  |
| 3   | D     | 241  | ILE  | 5.0  |
| 3   | D     | 73   | CYS  | 5.0  |
| 3   | D     | 416  | ALA  | 5.0  |
| 1   | B     | 236  | PRO  | 5.0  |
| 2   | C     | 165  | LEU  | 4.9  |
| 2   | C     | 267  | TYR  | 4.9  |
| 2   | C     | 293  | PHE  | 4.9  |
| 2   | C     | 1027 | PHE  | 4.9  |
| 2   | C     | 261  | ILE  | 4.9  |
| 3   | D     | 1241 | PHE  | 4.9  |
| 3   | D     | 594  | PRO  | 4.9  |
| 5   | F     | 423  | ASP  | 4.9  |
| 3   | D     | 391  | ALA  | 4.9  |
| 2   | C     | 729  | LEU  | 4.8  |
| 5   | F     | 143  | HIS  | 4.8  |
| 2   | C     | 1002 | GLU  | 4.7  |
| 2   | C     | 34   | VAL  | 4.7  |
| 2   | C     | 420  | ARG  | 4.7  |
| 3   | D     | 432  | TYR  | 4.7  |
| 3   | D     | 1408 | ILE  | 4.7  |
| 3   | D     | 1243 | THR  | 4.7  |
| 3   | D     | 237  | LYS  | 4.7  |
| 3   | D     | 76   | CYS  | 4.7  |
| 3   | D     | 1248 | GLY  | 4.6  |
| 2   | C     | 217  | LEU  | 4.6  |
| 3   | D     | 108  | VAL  | 4.6  |
| 3   | D     | 1244 | GLY  | 4.6  |
| 5   | F     | 354  | LEU  | 4.6  |
| 2   | C     | 228  | ALA  | 4.6  |
| 2   | C     | 418  | LEU  | 4.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 331  | VAL  | 4.5  |
| 3   | D     | 353  | VAL  | 4.5  |
| 3   | D     | 330  | THR  | 4.4  |
| 3   | D     | 430  | ASP  | 4.4  |
| 3   | D     | 364  | GLY  | 4.4  |
| 2   | C     | 419  | THR  | 4.4  |
| 5   | F     | 202  | TYR  | 4.4  |
| 5   | F     | 203  | THR  | 4.4  |
| 5   | F     | 142  | ARG  | 4.4  |
| 3   | D     | 1090 | ASP  | 4.4  |
| 3   | D     | 205  | TYR  | 4.3  |
| 5   | F     | 96   | LEU  | 4.3  |
| 2   | C     | 422  | ARG  | 4.3  |
| 3   | D     | 921  | ARG  | 4.3  |
| 3   | D     | 371  | ILE  | 4.3  |
| 2   | C     | 194  | VAL  | 4.3  |
| 3   | D     | 1197 | ARG  | 4.3  |
| 1   | A     | 186  | LEU  | 4.3  |
| 1   | B     | 57   | TYR  | 4.3  |
| 5   | F     | 240  | THR  | 4.3  |
| 2   | C     | 153  | ALA  | 4.2  |
| 3   | D     | 900  | ILE  | 4.2  |
| 5   | F     | 408  | LEU  | 4.2  |
| 3   | D     | 1198 | TYR  | 4.2  |
| 5   | F     | 139  | ALA  | 4.2  |
| 2   | C     | 108  | ILE  | 4.2  |
| 3   | D     | 102  | ILE  | 4.2  |
| 2   | C     | 287  | GLY  | 4.2  |
| 5   | F     | 75   | ILE  | 4.2  |
| 1   | B     | 115  | LEU  | 4.2  |
| 3   | D     | 427  | VAL  | 4.2  |
| 3   | D     | 77   | GLY  | 4.2  |
| 3   | D     | 1440 | PHE  | 4.2  |
| 2   | C     | 262  | ALA  | 4.2  |
| 3   | D     | 381  | ALA  | 4.2  |
| 3   | D     | 60   | CYS  | 4.2  |
| 3   | D     | 329  | GLU  | 4.2  |
| 5   | F     | 103  | ALA  | 4.1  |
| 5   | F     | 146  | GLY  | 4.1  |
| 3   | D     | 225  | LEU  | 4.1  |
| 3   | D     | 240  | GLU  | 4.1  |
| 5   | F     | 141  | VAL  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 208  | ALA  | 4.1  |
| 2   | C     | 258  | TYR  | 4.1  |
| 1   | B     | 159  | LYS  | 4.1  |
| 3   | D     | 223  | LEU  | 4.1  |
| 2   | C     | 40   | GLU  | 4.1  |
| 2   | C     | 421  | GLU  | 4.1  |
| 2   | C     | 370  | ALA  | 4.0  |
| 4   | E     | 2    | ALA  | 4.0  |
| 3   | D     | 75   | ARG  | 4.0  |
| 3   | D     | 355  | VAL  | 4.0  |
| 3   | D     | 614  | PHE  | 4.0  |
| 3   | D     | 1399 | ASP  | 4.0  |
| 4   | E     | 85   | LEU  | 4.0  |
| 2   | C     | 152  | PRO  | 4.0  |
| 2   | C     | 361  | MET  | 4.0  |
| 3   | D     | 810  | GLU  | 4.0  |
| 1   | B     | 143  | ARG  | 4.0  |
| 2   | C     | 523  | ILE  | 4.0  |
| 3   | D     | 901  | GLN  | 3.9  |
| 2   | C     | 774  | LEU  | 3.9  |
| 1   | B     | 58   | ILE  | 3.9  |
| 2   | C     | 814  | GLU  | 3.9  |
| 3   | D     | 327  | GLU  | 3.9  |
| 3   | D     | 812  | ALA  | 3.9  |
| 3   | D     | 168  | THR  | 3.9  |
| 5   | F     | 349  | LEU  | 3.9  |
| 3   | D     | 439  | LEU  | 3.9  |
| 1   | B     | 1    | MET  | 3.9  |
| 3   | D     | 242  | LEU  | 3.9  |
| 3   | D     | 261  | LEU  | 3.9  |
| 3   | D     | 615  | ARG  | 3.9  |
| 2   | C     | 242  | LEU  | 3.8  |
| 3   | D     | 402  | PRO  | 3.8  |
| 3   | D     | 144  | GLY  | 3.8  |
| 5   | F     | 198  | ILE  | 3.8  |
| 3   | D     | 79   | GLU  | 3.8  |
| 3   | D     | 147  | VAL  | 3.8  |
| 3   | D     | 400  | VAL  | 3.8  |
| 5   | F     | 418  | LEU  | 3.8  |
| 3   | D     | 1091 | SER  | 3.8  |
| 3   | D     | 419  | ASP  | 3.8  |
| 3   | D     | 109  | PRO  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | F     | 244  | ARG  | 3.8  |
| 2   | C     | 67   | ASP  | 3.7  |
| 2   | C     | 113  | VAL  | 3.7  |
| 3   | D     | 345  | TYR  | 3.7  |
| 2   | C     | 197  | LEU  | 3.7  |
| 2   | C     | 167  | LYS  | 3.7  |
| 3   | D     | 72   | VAL  | 3.7  |
| 3   | D     | 179  | VAL  | 3.7  |
| 3   | D     | 808  | THR  | 3.7  |
| 1   | B     | 95   | GLN  | 3.7  |
| 5   | F     | 329  | TYR  | 3.7  |
| 2   | C     | 218  | VAL  | 3.7  |
| 2   | C     | 118  | ILE  | 3.7  |
| 1   | B     | 109  | VAL  | 3.6  |
| 2   | C     | 176  | VAL  | 3.6  |
| 3   | D     | 1128 | VAL  | 3.6  |
| 2   | C     | 768  | THR  | 3.6  |
| 5   | F     | 74   | LYS  | 3.6  |
| 5   | F     | 358  | LEU  | 3.6  |
| 2   | C     | 315  | ALA  | 3.6  |
| 2   | C     | 719  | PRO  | 3.6  |
| 3   | D     | 78   | VAL  | 3.6  |
| 3   | D     | 378  | ILE  | 3.6  |
| 3   | D     | 360  | ARG  | 3.6  |
| 3   | D     | 1388 | ARG  | 3.6  |
| 5   | F     | 394  | ARG  | 3.6  |
| 3   | D     | 56   | TYR  | 3.6  |
| 3   | D     | 1237 | THR  | 3.6  |
| 2   | C     | 33   | ASP  | 3.6  |
| 2   | C     | 344  | PHE  | 3.6  |
| 5   | F     | 234  | LYS  | 3.6  |
| 1   | B     | 144  | VAL  | 3.6  |
| 2   | C     | 1028 | GLY  | 3.6  |
| 3   | D     | 138  | LYS  | 3.6  |
| 5   | F     | 390  | PHE  | 3.6  |
| 2   | C     | 196  | LEU  | 3.5  |
| 3   | D     | 617  | ASN  | 3.5  |
| 2   | C     | 512  | ARG  | 3.5  |
| 2   | C     | 811  | PRO  | 3.5  |
| 5   | F     | 278  | LEU  | 3.5  |
| 5   | F     | 313  | GLU  | 3.5  |
| 3   | D     | 806  | PHE  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | F     | 376  | ILE  | 3.5  |
| 1   | B     | 156  | HIS  | 3.5  |
| 2   | C     | 290  | LEU  | 3.5  |
| 5   | F     | 151  | LEU  | 3.5  |
| 3   | D     | 269  | PHE  | 3.5  |
| 5   | F     | 389  | PHE  | 3.5  |
| 1   | A     | 231  | ALA  | 3.4  |
| 2   | C     | 423  | ALA  | 3.4  |
| 5   | F     | 199  | ALA  | 3.4  |
| 2   | C     | 209  | ARG  | 3.4  |
| 3   | D     | 292  | VAL  | 3.4  |
| 1   | B     | 100  | LEU  | 3.4  |
| 2   | C     | 211  | LEU  | 3.4  |
| 5   | F     | 201  | LYS  | 3.4  |
| 5   | F     | 325  | LYS  | 3.4  |
| 2   | C     | 253  | ALA  | 3.4  |
| 3   | D     | 59   | ALA  | 3.4  |
| 3   | D     | 387  | LEU  | 3.4  |
| 1   | A     | 7    | LYS  | 3.4  |
| 5   | F     | 356  | LYS  | 3.4  |
| 3   | D     | 170  | PRO  | 3.4  |
| 3   | D     | 373  | PRO  | 3.3  |
| 1   | A     | 230  | ALA  | 3.3  |
| 2   | C     | 115  | LEU  | 3.3  |
| 3   | D     | 1113 | GLY  | 3.3  |
| 5   | F     | 371  | LEU  | 3.3  |
| 3   | D     | 429  | SER  | 3.3  |
| 5   | F     | 77   | THR  | 3.3  |
| 2   | C     | 769  | PRO  | 3.3  |
| 1   | B     | 61   | VAL  | 3.3  |
| 3   | D     | 107  | ASP  | 3.3  |
| 1   | B     | 132  | LEU  | 3.3  |
| 3   | D     | 311  | LEU  | 3.3  |
| 2   | C     | 388  | ARG  | 3.3  |
| 3   | D     | 318  | ARG  | 3.3  |
| 5   | F     | 150  | THR  | 3.3  |
| 3   | D     | 376  | GLU  | 3.3  |
| 2   | C     | 171  | TRP  | 3.3  |
| 5   | F     | 392  | VAL  | 3.3  |
| 2   | C     | 204  | GLN  | 3.3  |
| 2   | C     | 66   | LEU  | 3.3  |
| 3   | D     | 310  | LEU  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 239  | PHE  | 3.3  |
| 2   | C     | 716  | LYS  | 3.3  |
| 3   | D     | 180  | LYS  | 3.3  |
| 3   | D     | 486  | ARG  | 3.3  |
| 2   | C     | 279  | GLU  | 3.3  |
| 2   | C     | 257  | VAL  | 3.3  |
| 3   | D     | 350  | HIS  | 3.3  |
| 3   | D     | 354  | VAL  | 3.3  |
| 2   | C     | 898  | GLY  | 3.3  |
| 3   | D     | 141  | ILE  | 3.2  |
| 3   | D     | 320  | ALA  | 3.2  |
| 5   | F     | 344  | ALA  | 3.2  |
| 3   | D     | 829  | VAL  | 3.2  |
| 5   | F     | 386  | VAL  | 3.2  |
| 2   | C     | 284  | ARG  | 3.2  |
| 5   | F     | 412  | GLU  | 3.2  |
| 1   | B     | 117  | VAL  | 3.2  |
| 2   | C     | 302  | VAL  | 3.2  |
| 2   | C     | 373  | VAL  | 3.2  |
| 2   | C     | 816  | LYS  | 3.2  |
| 3   | D     | 385  | VAL  | 3.2  |
| 5   | F     | 368  | VAL  | 3.2  |
| 2   | C     | 241  | LEU  | 3.2  |
| 5   | F     | 209  | PHE  | 3.2  |
| 2   | C     | 277  | ALA  | 3.2  |
| 3   | D     | 101  | HIS  | 3.2  |
| 3   | D     | 67   | ARG  | 3.2  |
| 5   | F     | 145  | PRO  | 3.2  |
| 2   | C     | 195  | LEU  | 3.2  |
| 2   | C     | 924  | VAL  | 3.2  |
| 3   | D     | 282  | TYR  | 3.2  |
| 3   | D     | 434  | ARG  | 3.2  |
| 3   | D     | 457  | GLY  | 3.2  |
| 3   | D     | 968  | ASP  | 3.2  |
| 3   | D     | 183  | GLU  | 3.1  |
| 3   | D     | 1391 | GLU  | 3.1  |
| 2   | C     | 731  | GLU  | 3.1  |
| 5   | F     | 415  | THR  | 3.1  |
| 1   | B     | 99   | LEU  | 3.1  |
| 5   | F     | 205  | ARG  | 3.1  |
| 2   | C     | 417  | GLY  | 3.1  |
| 1   | B     | 131  | THR  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 281  | THR  | 3.1  |
| 5   | F     | 332  | PHE  | 3.1  |
| 3   | D     | 169  | TYR  | 3.1  |
| 2   | C     | 2    | GLU  | 3.1  |
| 3   | D     | 1130 | ARG  | 3.1  |
| 3   | D     | 222  | GLY  | 3.1  |
| 3   | D     | 358  | GLY  | 3.1  |
| 3   | D     | 401  | TYR  | 3.1  |
| 1   | B     | 6    | LEU  | 3.0  |
| 3   | D     | 297  | ILE  | 3.0  |
| 5   | F     | 194  | LEU  | 3.0  |
| 3   | D     | 1503 | VAL  | 3.0  |
| 2   | C     | 114  | PHE  | 3.0  |
| 5   | F     | 421  | PHE  | 3.0  |
| 2   | C     | 256  | TYR  | 3.0  |
| 2   | C     | 283  | ILE  | 3.0  |
| 2   | C     | 348  | LEU  | 3.0  |
| 3   | D     | 393  | ILE  | 3.0  |
| 5   | F     | 319  | THR  | 3.0  |
| 1   | B     | 130  | ALA  | 3.0  |
| 3   | D     | 407  | VAL  | 3.0  |
| 3   | D     | 415  | VAL  | 3.0  |
| 3   | D     | 487  | ALA  | 3.0  |
| 2   | C     | 26   | TYR  | 3.0  |
| 3   | D     | 404  | GLU  | 3.0  |
| 2   | C     | 717  | LEU  | 3.0  |
| 2   | C     | 186  | VAL  | 3.0  |
| 3   | D     | 379  | ALA  | 3.0  |
| 3   | D     | 883  | ALA  | 3.0  |
| 2   | C     | 225  | SER  | 3.0  |
| 4   | E     | 3    | GLU  | 3.0  |
| 3   | D     | 333  | LEU  | 3.0  |
| 2   | C     | 266  | ARG  | 3.0  |
| 3   | D     | 312  | ARG  | 3.0  |
| 3   | D     | 896  | ALA  | 3.0  |
| 2   | C     | 38   | LYS  | 3.0  |
| 1   | B     | 111  | ALA  | 2.9  |
| 2   | C     | 155  | PRO  | 2.9  |
| 3   | D     | 103  | TRP  | 2.9  |
| 1   | B     | 161  | ARG  | 2.9  |
| 3   | D     | 233  | LYS  | 2.9  |
| 1   | B     | 170  | VAL  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 830  | ALA  | 2.9  |
| 3   | D     | 1409 | ALA  | 2.9  |
| 5   | F     | 152  | ASP  | 2.9  |
| 3   | D     | 104  | PHE  | 2.9  |
| 3   | D     | 619  | LEU  | 2.9  |
| 3   | D     | 1389 | LEU  | 2.9  |
| 1   | B     | 165  | ILE  | 2.9  |
| 2   | C     | 123  | GLU  | 2.9  |
| 5   | F     | 149  | GLU  | 2.9  |
| 5   | F     | 359  | SER  | 2.9  |
| 5   | F     | 413  | SER  | 2.9  |
| 1   | B     | 118  | ALA  | 2.9  |
| 2   | C     | 29   | ALA  | 2.9  |
| 2   | C     | 317  | VAL  | 2.9  |
| 2   | C     | 813  | VAL  | 2.9  |
| 3   | D     | 319  | ALA  | 2.9  |
| 2   | C     | 68   | PHE  | 2.9  |
| 3   | D     | 182  | GLY  | 2.9  |
| 5   | F     | 400  | ILE  | 2.9  |
| 3   | D     | 298  | VAL  | 2.9  |
| 3   | D     | 361  | VAL  | 2.9  |
| 3   | D     | 221  | ALA  | 2.9  |
| 5   | F     | 357  | ALA  | 2.9  |
| 1   | A     | 189  | ARG  | 2.8  |
| 5   | F     | 91   | VAL  | 2.8  |
| 5   | F     | 382  | THR  | 2.8  |
| 2   | C     | 227  | PHE  | 2.8  |
| 4   | E     | 4    | PRO  | 2.8  |
| 2   | C     | 59   | LYS  | 2.8  |
| 3   | D     | 998  | GLU  | 2.8  |
| 3   | D     | 271  | VAL  | 2.8  |
| 3   | D     | 314  | PRO  | 2.8  |
| 2   | C     | 637  | LEU  | 2.8  |
| 1   | B     | 163  | ASN  | 2.8  |
| 2   | C     | 289  | THR  | 2.8  |
| 3   | D     | 918  | ALA  | 2.8  |
| 2   | C     | 207  | LEU  | 2.8  |
| 2   | C     | 260  | LEU  | 2.8  |
| 3   | D     | 612  | GLY  | 2.8  |
| 3   | D     | 175  | VAL  | 2.8  |
| 2   | C     | 351  | LEU  | 2.8  |
| 5   | F     | 322  | GLY  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 315  | ARG  | 2.8  |
| 5   | F     | 140  | ARG  | 2.8  |
| 1   | B     | 235  | ALA  | 2.7  |
| 2   | C     | 443  | THR  | 2.7  |
| 2   | C     | 35   | PRO  | 2.7  |
| 2   | C     | 48   | PHE  | 2.7  |
| 3   | D     | 283  | PHE  | 2.7  |
| 5   | F     | 241  | TRP  | 2.7  |
| 2   | C     | 220  | GLY  | 2.7  |
| 3   | D     | 383  | GLY  | 2.7  |
| 1   | A     | 158  | ILE  | 2.7  |
| 2   | C     | 738  | ASP  | 2.7  |
| 2   | C     | 226  | VAL  | 2.7  |
| 2   | C     | 899  | GLN  | 2.7  |
| 5   | F     | 245  | GLN  | 2.7  |
| 1   | B     | 89   | PHE  | 2.7  |
| 2   | C     | 369  | PRO  | 2.7  |
| 3   | D     | 251  | PHE  | 2.7  |
| 3   | D     | 349  | PRO  | 2.7  |
| 3   | D     | 894  | LYS  | 2.7  |
| 1   | B     | 101  | LEU  | 2.7  |
| 5   | F     | 102  | LEU  | 2.7  |
| 1   | B     | 56   | VAL  | 2.7  |
| 1   | B     | 87   | VAL  | 2.7  |
| 3   | D     | 253  | ALA  | 2.7  |
| 3   | D     | 1505 | ALA  | 2.7  |
| 1   | B     | 65   | PHE  | 2.7  |
| 1   | B     | 127  | LEU  | 2.7  |
| 3   | D     | 367  | ILE  | 2.7  |
| 4   | E     | 96   | GLU  | 2.7  |
| 3   | D     | 216  | VAL  | 2.7  |
| 5   | F     | 195  | VAL  | 2.7  |
| 1   | B     | 90   | LEU  | 2.7  |
| 2   | C     | 96   | ALA  | 2.7  |
| 2   | C     | 100  | LEU  | 2.7  |
| 3   | D     | 390  | PRO  | 2.7  |
| 3   | D     | 399  | ARG  | 2.7  |
| 3   | D     | 441  | ARG  | 2.7  |
| 3   | D     | 622  | ARG  | 2.7  |
| 3   | D     | 294  | HIS  | 2.7  |
| 3   | D     | 897  | TRP  | 2.7  |
| 4   | E     | 91   | ARG  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | F     | 197  | SER  | 2.7  |
| 5   | F     | 232  | ARG  | 2.7  |
| 1   | A     | 157  | GLY  | 2.7  |
| 2   | C     | 131  | GLY  | 2.7  |
| 5   | F     | 283  | GLY  | 2.7  |
| 1   | B     | 122  | ILE  | 2.7  |
| 3   | D     | 163  | TYR  | 2.6  |
| 3   | D     | 1251 | ASP  | 2.6  |
| 2   | C     | 1    | MET  | 2.6  |
| 3   | D     | 1393 | GLN  | 2.6  |
| 3   | D     | 1502 | ALA  | 2.6  |
| 4   | E     | 51   | LEU  | 2.6  |
| 3   | D     | 224  | ARG  | 2.6  |
| 3   | D     | 1129 | THR  | 2.6  |
| 5   | F     | 414  | ARG  | 2.6  |
| 1   | B     | 4    | SER  | 2.6  |
| 3   | D     | 467  | GLU  | 2.6  |
| 3   | D     | 804  | LEU  | 2.6  |
| 2   | C     | 356  | ARG  | 2.6  |
| 5   | F     | 260  | ILE  | 2.6  |
| 3   | D     | 184  | GLU  | 2.6  |
| 2   | C     | 322  | VAL  | 2.6  |
| 2   | C     | 783  | ARG  | 2.6  |
| 3   | D     | 882  | PHE  | 2.6  |
| 5   | F     | 417  | LYS  | 2.6  |
| 2   | C     | 663  | ASN  | 2.6  |
| 5   | F     | 248  | ASN  | 2.6  |
| 3   | D     | 268  | ALA  | 2.6  |
| 5   | F     | 307  | THR  | 2.6  |
| 2   | C     | 316  | GLY  | 2.6  |
| 2   | C     | 281  | LEU  | 2.5  |
| 1   | B     | 60   | ASP  | 2.5  |
| 3   | D     | 1381 | VAL  | 2.5  |
| 1   | A     | 185  | ARG  | 2.5  |
| 1   | B     | 88   | ARG  | 2.5  |
| 3   | D     | 336  | PHE  | 2.5  |
| 5   | F     | 186  | HIS  | 2.5  |
| 2   | C     | 172  | ILE  | 2.5  |
| 3   | D     | 61   | GLY  | 2.5  |
| 3   | D     | 426  | LYS  | 2.5  |
| 3   | D     | 392  | SER  | 2.5  |
| 5   | F     | 78   | SER  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 145  | ASP  | 2.5  |
| 3   | D     | 200  | ASP  | 2.5  |
| 3   | D     | 577  | ALA  | 2.5  |
| 3   | D     | 1242 | HIS  | 2.5  |
| 3   | D     | 571  | LYS  | 2.5  |
| 3   | D     | 1413 | THR  | 2.5  |
| 4   | E     | 95   | GLY  | 2.5  |
| 3   | D     | 197  | SER  | 2.5  |
| 3   | D     | 596  | SER  | 2.5  |
| 3   | D     | 270  | LEU  | 2.5  |
| 3   | D     | 316  | GLN  | 2.5  |
| 2   | C     | 303  | PHE  | 2.5  |
| 3   | D     | 289  | THR  | 2.5  |
| 3   | D     | 234  | GLU  | 2.5  |
| 3   | D     | 975  | GLU  | 2.5  |
| 3   | D     | 142  | LEU  | 2.5  |
| 3   | D     | 208  | PRO  | 2.5  |
| 2   | C     | 1001 | VAL  | 2.5  |
| 2   | C     | 312  | ALA  | 2.5  |
| 2   | C     | 43   | GLY  | 2.5  |
| 2   | C     | 463  | GLU  | 2.4  |
| 2   | C     | 98   | LEU  | 2.4  |
| 3   | D     | 899  | LEU  | 2.4  |
| 3   | D     | 238  | PRO  | 2.4  |
| 3   | D     | 446  | VAL  | 2.4  |
| 3   | D     | 66   | GLN  | 2.4  |
| 2   | C     | 311  | PHE  | 2.4  |
| 5   | F     | 154  | LYS  | 2.4  |
| 5   | F     | 388  | ALA  | 2.4  |
| 3   | D     | 405  | ASP  | 2.4  |
| 5   | F     | 323  | ASP  | 2.4  |
| 2   | C     | 145  | GLY  | 2.4  |
| 2   | C     | 416  | GLY  | 2.4  |
| 2   | C     | 766  | GLU  | 2.4  |
| 3   | D     | 1305 | LEU  | 2.4  |
| 5   | F     | 163  | LEU  | 2.4  |
| 2   | C     | 767  | PRO  | 2.4  |
| 3   | D     | 248  | PRO  | 2.4  |
| 3   | D     | 1307 | LYS  | 2.4  |
| 5   | F     | 403  | LYS  | 2.4  |
| 3   | D     | 249  | TYR  | 2.4  |
| 3   | D     | 332  | TYR  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 282  | GLY  | 2.4  |
| 2   | C     | 464  | LEU  | 2.4  |
| 3   | D     | 304  | LEU  | 2.4  |
| 3   | D     | 652  | LEU  | 2.4  |
| 2   | C     | 308  | ARG  | 2.4  |
| 5   | F     | 80   | PRO  | 2.4  |
| 5   | F     | 370  | LYS  | 2.4  |
| 2   | C     | 389  | SER  | 2.4  |
| 3   | D     | 317  | VAL  | 2.4  |
| 3   | D     | 611  | GLN  | 2.4  |
| 3   | D     | 363  | ALA  | 2.4  |
| 3   | D     | 845  | ASN  | 2.4  |
| 5   | F     | 269  | ASN  | 2.4  |
| 5   | F     | 326  | ASP  | 2.4  |
| 4   | E     | 50   | THR  | 2.4  |
| 2   | C     | 815  | LEU  | 2.4  |
| 3   | D     | 971  | LEU  | 2.4  |
| 3   | D     | 1086 | LEU  | 2.4  |
| 3   | D     | 226  | PRO  | 2.4  |
| 3   | D     | 484  | PRO  | 2.4  |
| 2   | C     | 182  | VAL  | 2.4  |
| 3   | D     | 195  | VAL  | 2.4  |
| 2   | C     | 730  | SER  | 2.4  |
| 2   | C     | 765  | SER  | 2.4  |
| 2   | C     | 349  | ALA  | 2.4  |
| 2   | C     | 629  | TYR  | 2.4  |
| 2   | C     | 263  | ASP  | 2.4  |
| 3   | D     | 58   | CYS  | 2.4  |
| 3   | D     | 665  | GLY  | 2.4  |
| 3   | D     | 1240 | THR  | 2.3  |
| 2   | C     | 37   | GLU  | 2.3  |
| 2   | C     | 168  | ARG  | 2.3  |
| 2   | C     | 244  | PRO  | 2.3  |
| 3   | D     | 213  | VAL  | 2.3  |
| 5   | F     | 263  | HIS  | 2.3  |
| 1   | A     | 11   | PHE  | 2.3  |
| 1   | B     | 232  | ALA  | 2.3  |
| 3   | D     | 63   | TYR  | 2.3  |
| 2   | C     | 307  | LEU  | 2.3  |
| 5   | F     | 274  | THR  | 2.3  |
| 2   | C     | 75   | GLU  | 2.3  |
| 3   | D     | 445  | ARG  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 125  | PRO  | 2.3  |
| 1   | B     | 53   | VAL  | 2.3  |
| 5   | F     | 275  | ALA  | 2.3  |
| 2   | C     | 30   | LEU  | 2.3  |
| 5   | F     | 94   | LEU  | 2.3  |
| 2   | C     | 86   | LYS  | 2.3  |
| 2   | C     | 715  | THR  | 2.3  |
| 2   | C     | 764  | GLU  | 2.3  |
| 3   | D     | 80   | VAL  | 2.3  |
| 3   | D     | 444  | VAL  | 2.3  |
| 3   | D     | 821  | VAL  | 2.3  |
| 1   | A     | 23   | PHE  | 2.3  |
| 1   | A     | 225  | PHE  | 2.3  |
| 2   | C     | 1080 | SER  | 2.3  |
| 3   | D     | 171  | LEU  | 2.3  |
| 3   | D     | 264  | LEU  | 2.3  |
| 1   | B     | 3    | ASP  | 2.3  |
| 1   | B     | 64   | GLU  | 2.3  |
| 2   | C     | 807  | ARG  | 2.3  |
| 3   | D     | 325  | GLU  | 2.3  |
| 3   | D     | 592  | THR  | 2.3  |
| 2   | C     | 166  | PRO  | 2.3  |
| 3   | D     | 322  | VAL  | 2.3  |
| 5   | F     | 235  | PHE  | 2.3  |
| 3   | D     | 1417 | TRP  | 2.3  |
| 3   | D     | 494  | LYS  | 2.2  |
| 5   | F     | 282  | LEU  | 2.3  |
| 3   | D     | 220  | ARG  | 2.2  |
| 5   | F     | 222  | ARG  | 2.2  |
| 3   | D     | 265  | GLU  | 2.2  |
| 3   | D     | 408  | GLU  | 2.2  |
| 5   | F     | 153  | PRO  | 2.2  |
| 1   | B     | 142  | VAL  | 2.2  |
| 1   | B     | 167  | VAL  | 2.2  |
| 3   | D     | 105  | VAL  | 2.2  |
| 3   | D     | 145  | VAL  | 2.2  |
| 3   | D     | 1441 | GLN  | 2.2  |
| 3   | D     | 1252 | ILE  | 2.2  |
| 5   | F     | 233  | PHE  | 2.2  |
| 5   | F     | 291  | ILE  | 2.2  |
| 2   | C     | 238  | LEU  | 2.2  |
| 3   | D     | 161  | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 986  | ARG  | 2.2  |
| 3   | D     | 497  | GLU  | 2.2  |
| 1   | A     | 224  | TYR  | 2.2  |
| 1   | B     | 139  | ASN  | 2.2  |
| 3   | D     | 193  | PRO  | 2.2  |
| 3   | D     | 1088 | THR  | 2.2  |
| 2   | C     | 78   | PHE  | 2.2  |
| 3   | D     | 636  | GLN  | 2.2  |
| 2   | C     | 188  | LYS  | 2.2  |
| 2   | C     | 193  | LEU  | 2.2  |
| 3   | D     | 1407 | LEU  | 2.2  |
| 5   | F     | 369  | LEU  | 2.2  |
| 1   | B     | 14   | ARG  | 2.2  |
| 3   | D     | 1239 | ARG  | 2.2  |
| 2   | C     | 631  | SER  | 2.2  |
| 5   | F     | 76   | SER  | 2.2  |
| 2   | C     | 445  | GLU  | 2.2  |
| 3   | D     | 69   | GLU  | 2.2  |
| 3   | D     | 1000 | THR  | 2.2  |
| 2   | C     | 158  | TYR  | 2.2  |
| 2   | C     | 781  | LYS  | 2.2  |
| 3   | D     | 62   | LYS  | 2.2  |
| 1   | A     | 8    | ALA  | 2.2  |
| 5   | F     | 366  | ALA  | 2.2  |
| 1   | B     | 80   | LEU  | 2.2  |
| 3   | D     | 1087 | ARG  | 2.2  |
| 5   | F     | 385  | GLU  | 2.2  |
| 2   | C     | 314  | THR  | 2.2  |
| 2   | C     | 341  | THR  | 2.2  |
| 3   | D     | 1084 | THR  | 2.2  |
| 5   | F     | 393  | THR  | 2.2  |
| 5   | F     | 288  | TYR  | 2.2  |
| 2   | C     | 101  | ILE  | 2.2  |
| 3   | D     | 403  | PHE  | 2.2  |
| 5   | F     | 312  | GLN  | 2.2  |
| 1   | B     | 102  | LYS  | 2.2  |
| 3   | D     | 262  | LYS  | 2.2  |
| 3   | D     | 335  | LEU  | 2.2  |
| 2   | C     | 318  | PRO  | 2.1  |
| 2   | C     | 511  | GLU  | 2.1  |
| 3   | D     | 4    | GLU  | 2.1  |
| 3   | D     | 263  | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 1308 | GLU  | 2.1  |
| 4   | E     | 94   | PRO  | 2.1  |
| 3   | D     | 110  | SER  | 2.1  |
| 1   | B     | 129  | ILE  | 2.1  |
| 3   | D     | 231  | VAL  | 2.1  |
| 3   | D     | 886  | VAL  | 2.1  |
| 3   | D     | 1400 | VAL  | 2.1  |
| 3   | D     | 902  | LEU  | 2.1  |
| 2   | C     | 255  | ALA  | 2.1  |
| 3   | D     | 832  | ARG  | 2.1  |
| 2   | C     | 414  | GLY  | 2.1  |
| 3   | D     | 70   | GLY  | 2.1  |
| 3   | D     | 898  | GLU  | 2.1  |
| 5   | F     | 290  | GLU  | 2.1  |
| 3   | D     | 1439 | SER  | 2.1  |
| 2   | C     | 276  | LYS  | 2.1  |
| 3   | D     | 482  | LYS  | 2.1  |
| 2   | C     | 355  | VAL  | 2.1  |
| 3   | D     | 207  | PHE  | 2.1  |
| 4   | E     | 93   | TYR  | 2.1  |
| 3   | D     | 359  | ALA  | 2.1  |
| 2   | C     | 927  | GLY  | 2.1  |
| 2   | C     | 231  | PRO  | 2.1  |
| 3   | D     | 1268 | PRO  | 2.1  |
| 5   | F     | 381  | HIS  | 2.1  |
| 3   | D     | 366  | LYS  | 2.1  |
| 2   | C     | 722  | ILE  | 2.1  |
| 3   | D     | 827  | ILE  | 2.1  |
| 3   | D     | 68   | PHE  | 2.1  |
| 2   | C     | 925  | TYR  | 2.1  |
| 2   | C     | 64   | LEU  | 2.1  |
| 2   | C     | 345  | ARG  | 2.1  |
| 4   | E     | 84   | ARG  | 2.1  |
| 3   | D     | 938  | GLY  | 2.1  |
| 2   | C     | 77   | PRO  | 2.1  |
| 2   | C     | 1074 | GLU  | 2.1  |
| 3   | D     | 244  | GLU  | 2.1  |
| 3   | D     | 382  | GLU  | 2.1  |
| 3   | D     | 491  | LYS  | 2.1  |
| 4   | E     | 89   | MET  | 2.1  |
| 2   | C     | 162  | ILE  | 2.1  |
| 3   | D     | 1495 | ILE  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 233  | VAL  | 2.1  |
| 3   | D     | 129  | PHE  | 2.1  |
| 3   | D     | 578  | VAL  | 2.1  |
| 2   | C     | 107  | LEU  | 2.1  |
| 3   | D     | 424  | GLY  | 2.1  |
| 3   | D     | 1092 | GLY  | 2.1  |
| 3   | D     | 374  | GLU  | 2.0  |
| 1   | B     | 107  | LYS  | 2.0  |
| 4   | E     | 87   | LYS  | 2.0  |
| 3   | D     | 944  | THR  | 2.0  |
| 2   | C     | 127  | PHE  | 2.0  |
| 5   | F     | 315  | VAL  | 2.0  |
| 3   | D     | 1390 | LEU  | 2.0  |
| 5   | F     | 308  | LEU  | 2.0  |
| 2   | C     | 1119 | ARG  | 2.0  |
| 3   | D     | 150  | ARG  | 2.0  |
| 3   | D     | 198  | ARG  | 2.0  |
| 3   | D     | 273  | ARG  | 2.0  |
| 2   | C     | 170  | PRO  | 2.0  |
| 1   | B     | 128  | HIS  | 2.0  |
| 1   | B     | 13   | VAL  | 2.0  |
| 2   | C     | 199  | VAL  | 2.0  |
| 3   | D     | 337  | LEU  | 2.0  |
| 3   | D     | 421  | LEU  | 2.0  |
| 3   | D     | 982  | PHE  | 2.0  |
| 2   | C     | 49   | ARG  | 2.0  |
| 3   | D     | 1318 | TYR  | 2.0  |
| 3   | D     | 1402 | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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,

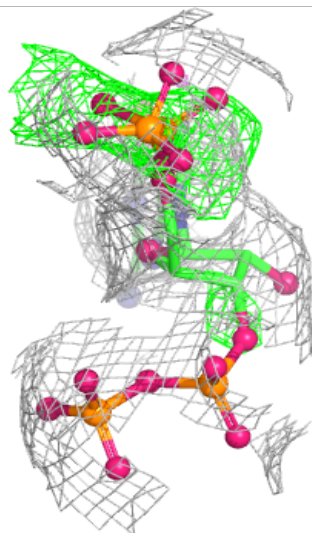
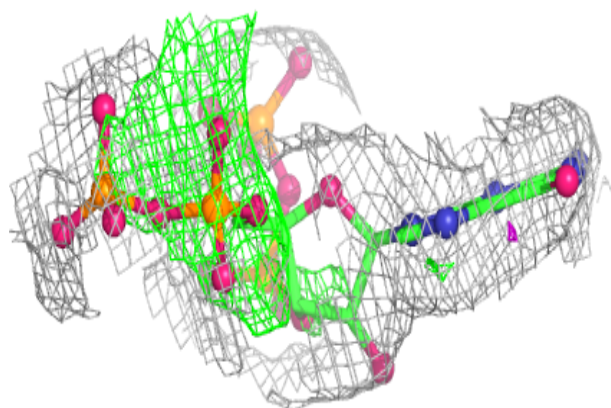
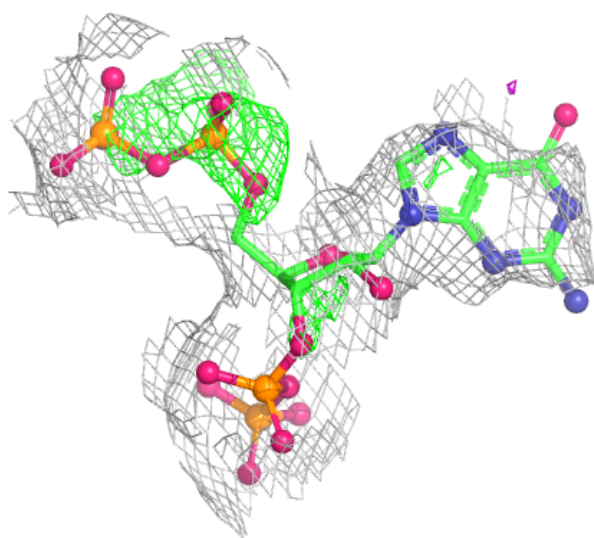
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 8   | MG   | C     | 1201 | 1/1   | 0.68 | 0.36 | 131,131,131,131            | 0     |
| 8   | MG   | D     | 1601 | 1/1   | 0.83 | 0.37 | 133,133,133,133            | 0     |
| 10  | G4P  | D     | 1605 | 36/36 | 0.90 | 0.20 | 183,197,222,224            | 0     |
| 8   | MG   | D     | 1606 | 1/1   | 0.94 | 0.07 | 155,155,155,155            | 0     |
| 8   | MG   | D     | 1604 | 1/1   | 0.95 | 0.14 | 86,86,86,86                | 0     |
| 9   | ZN   | D     | 1602 | 1/1   | 0.96 | 0.20 | 225,225,225,225            | 0     |
| 9   | ZN   | D     | 1603 | 1/1   | 0.98 | 0.07 | 168,168,168,168            | 0     |
| 7   | PO4  | A     | 401  | 5/5   | 0.98 | 0.15 | 143,144,148,149            | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around G4P D 1605:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.