



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:20 PM UTC

PDB ID : 3H0L / pdb\_00003h0l  
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus  
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.  
Deposited on : 2009-04-09  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

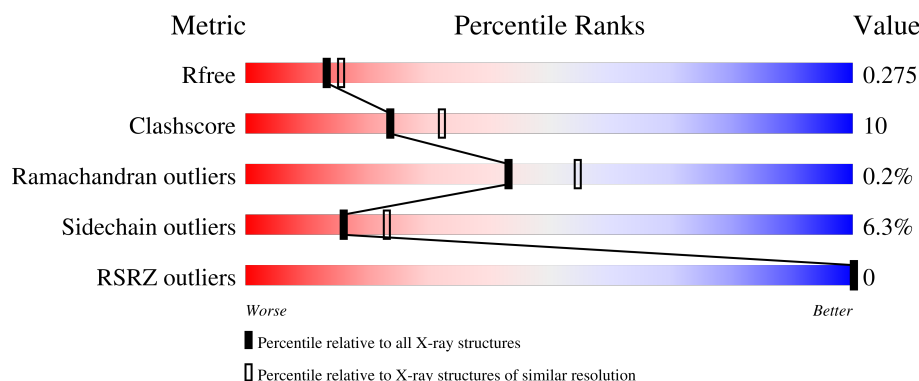
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



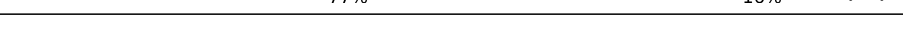
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

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     | 478    |  |
| 1   | D     | 478    |  |
| 1   | G     | 478    |  |
| 1   | J     | 478    |  |
| 1   | M     | 478    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | P     | 478    |    |
| 1   | S     | 478    |    |
| 1   | V     | 478    |    |
| 2   | B     | 478    |    |
| 2   | E     | 478    |    |
| 2   | H     | 478    |    |
| 2   | K     | 478    |    |
| 2   | N     | 478    |    |
| 2   | Q     | 478    |    |
| 2   | T     | 478    |    |
| 2   | W     | 478    |    |
| 3   | C     | 94     |    |
| 3   | F     | 94     |  |
| 3   | I     | 94     |  |
| 3   | L     | 94     |  |
| 3   | O     | 94     |  |
| 3   | R     | 94     |  |
| 3   | U     | 94     |  |
| 3   | X     | 94     |  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 63144 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | D     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | G     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | J     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | M     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | P     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | S     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |
| 1   | V     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3784  | 2450 | 615 | 712 | 7 |         |         |       |

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |
| 2   | E     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |
| 2   | H     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |
| 2   | K     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |
| 2   | N     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |
| 2   | Q     | 410      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2104 | 567 | 622 | 15 |         |         |       |

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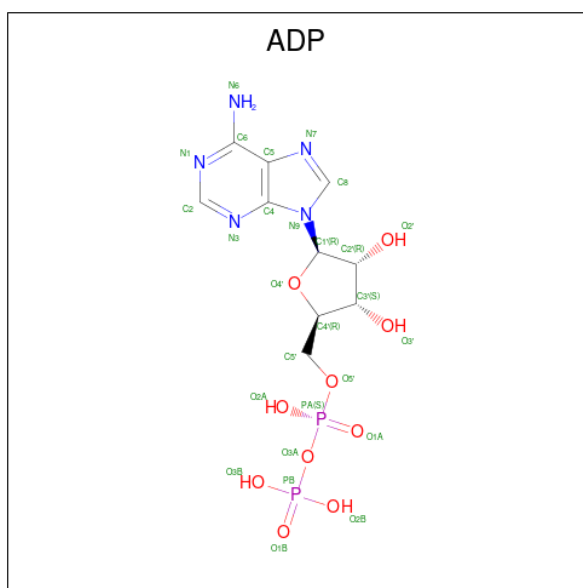
| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 2   | T     | 410      | Total<br>3308 | C<br>2104 | N<br>567 | O<br>622 | S<br>15 | 0       | 0       | 0     |
| 2   | W     | 410      | Total<br>3308 | C<br>2104 | N<br>567 | O<br>622 | S<br>15 | 0       | 0       | 0     |

- | Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 3   | C     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | F     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | I     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | L     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | O     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | R     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | U     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |
| 3   | X     | 91       | Total<br>764 | C<br>487 | N<br>125 | O<br>150 | S<br>2 | 0       | 0       | 0     |

- ASN
- 
- The diagram illustrates the chemical structure of Asparagine (ASN). The central carbon atom is labeled CA(S). It is bonded to a hydrogen atom (H) and an amino group (NH<sub>2</sub>, with N labeled). The amino group is shown with a blue arrow pointing to the nitrogen atom. The central carbon is also bonded to a carboxyl group (COO<sup>-</sup>, with O labeled) and an amide group (CONH<sub>2</sub>, with N labeled). The amide group is shown with a blue arrow pointing to the nitrogen atom. The carboxyl group is shown with a red arrow pointing to the oxygen atom. The amide group is shown with a red arrow pointing to the nitrogen atom. The central carbon is also bonded to a carbon atom (C) which is part of a side chain. This side chain consists of a methylene group (CH<sub>2</sub>, with C labeled) and a carboxyl group (COO<sup>-</sup>, with O labeled). The side chain is shown with a red arrow pointing to the oxygen atom. The central carbon is also bonded to a carbon atom (C) which is part of a side chain. This side chain consists of a methylene group (CH<sub>2</sub>, with C labeled) and a carboxyl group (COO<sup>-</sup>, with O labeled). The side chain is shown with a red arrow pointing to the oxygen atom.

| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | M     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | S     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 4   | V     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | K     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | N     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | Q     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | T     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | W     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | N     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | Q     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | T     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | W     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | E     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | H     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | K     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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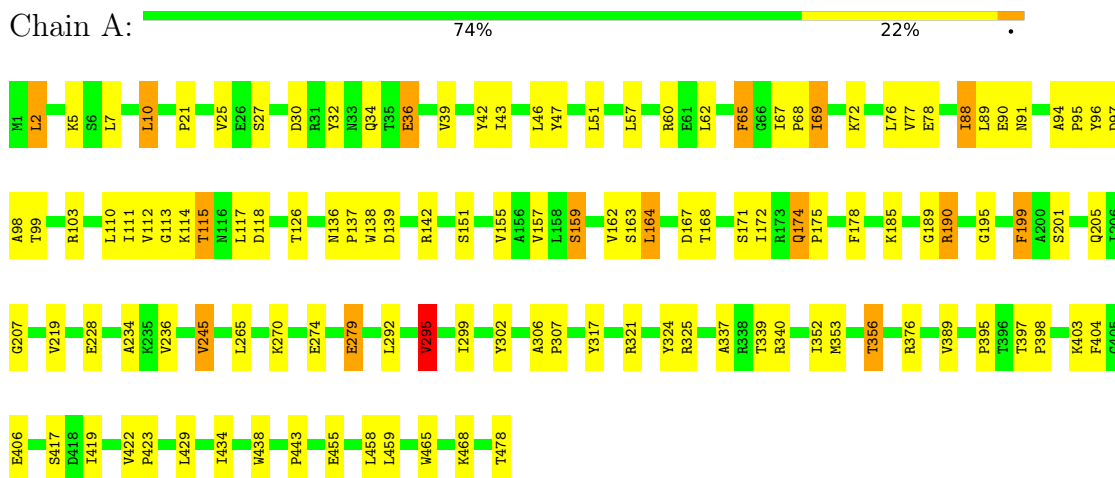
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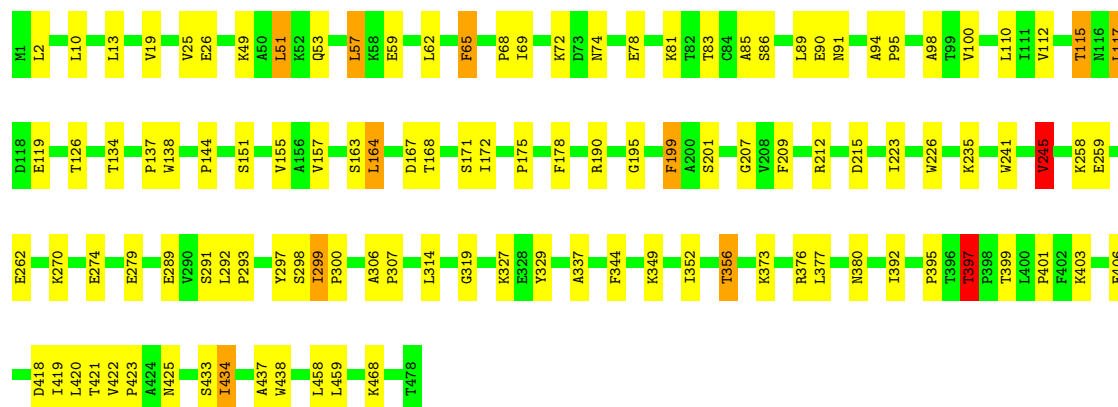
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 7   | Q     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 7   | T     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 7   | W     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

### 3 Residue-property plots [i](#)

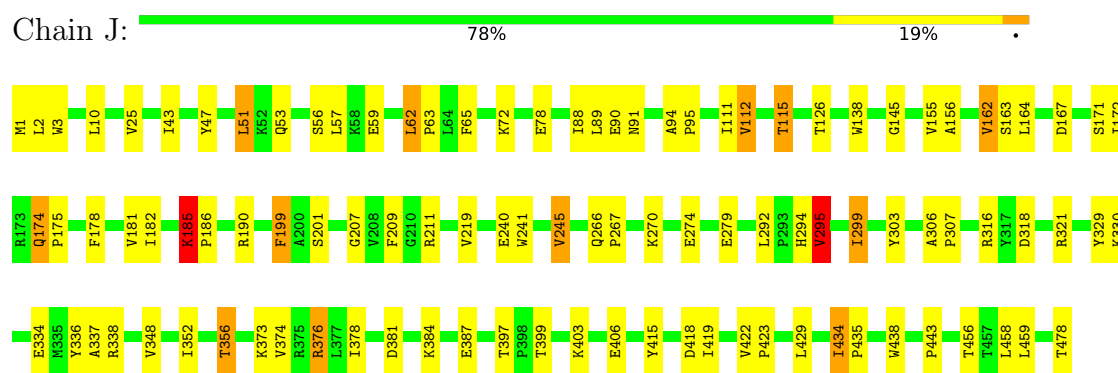
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

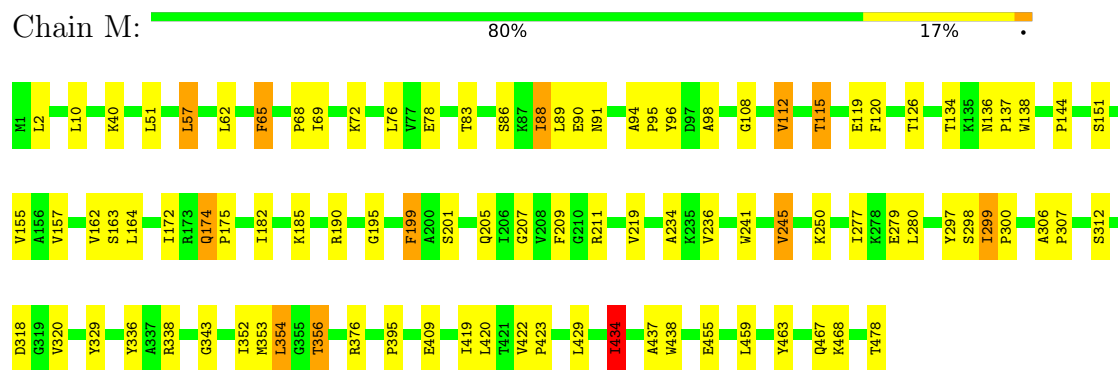




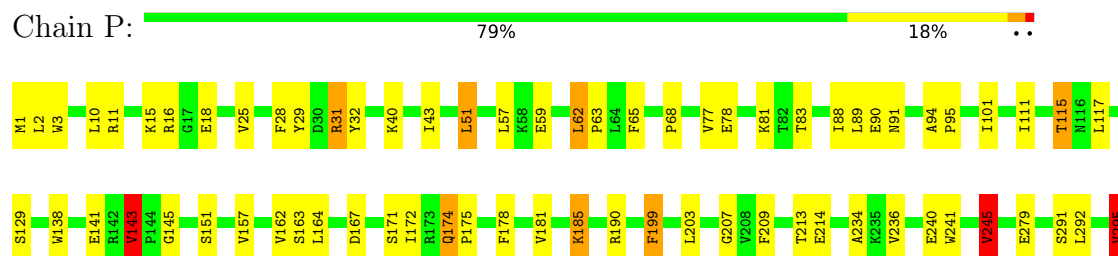
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

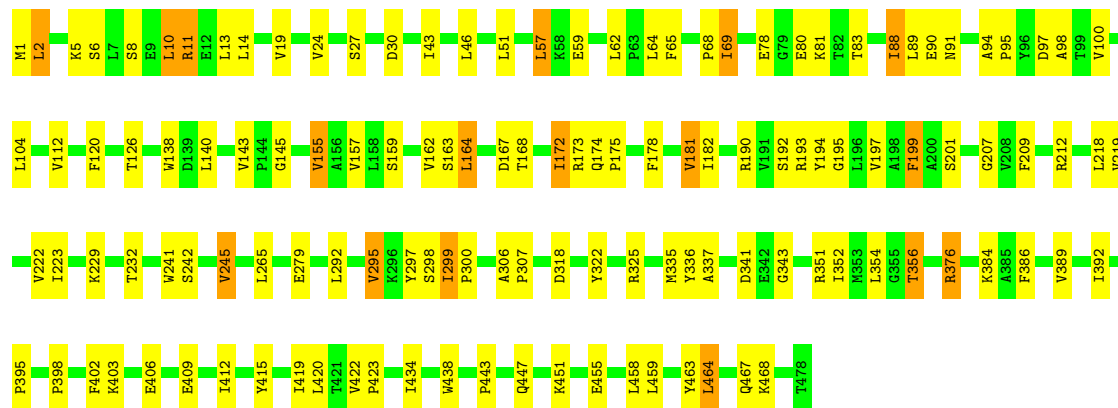


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

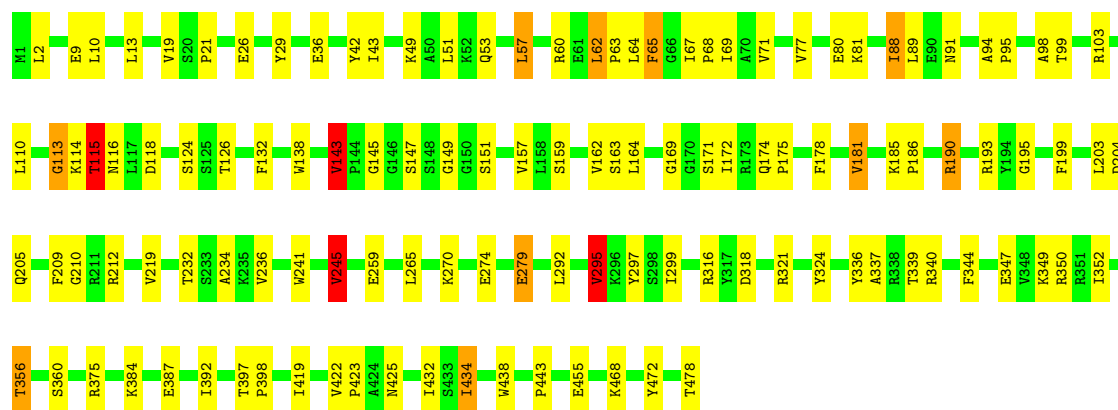




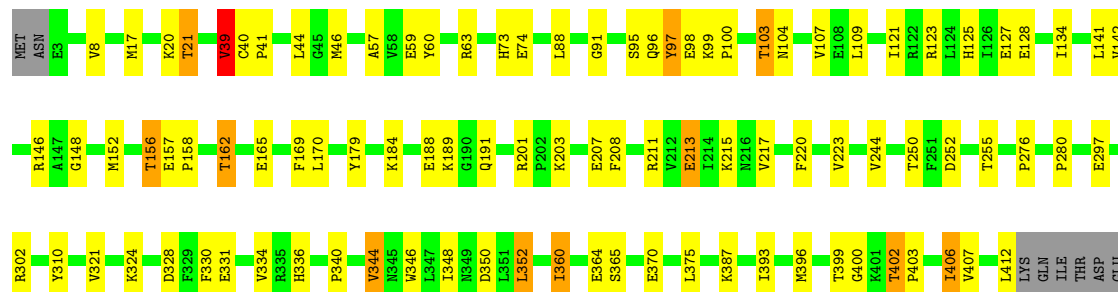
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



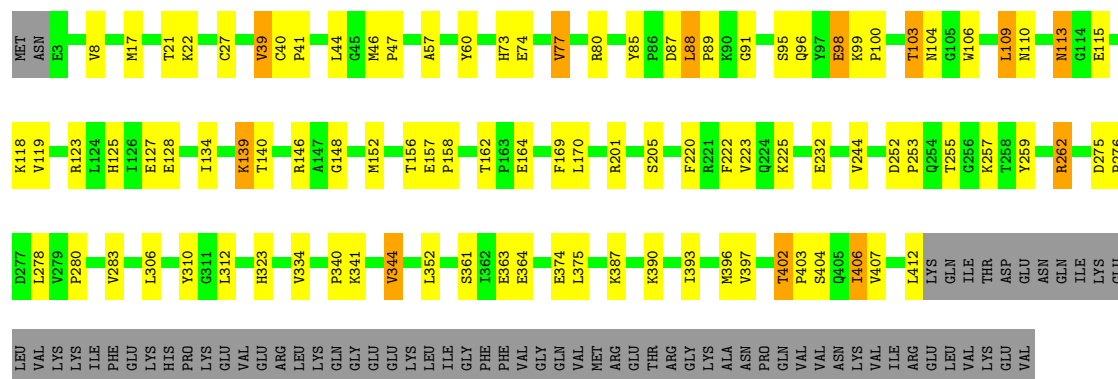
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



ASN  
GLN  
ILE  
LYS  
GLU  
LEU  
VAL  
LYS  
LYS  
PHE  
ILE  
GLY  
LYS  
HIS  
PRO  
LYS  
GLU  
VAL  
GLU  
ARG  
LEU  
LYS  
GLN  
GLY  
GLY  
GLU  
ILE  
LYS  
PHE  
PHE  
VAL  
GLY  
GLN  
VAL  
MET  
ARG  
GLU  
THR  
ARG  
GLY  
LYS  
ALA  
ASN  
PRO  
GLN  
VAL  
VAL  
ASN  
LYS  
VAL  
ILE  
ARG  
GLU  
LEU  
VAL  
LYS  
GLU  
VAL

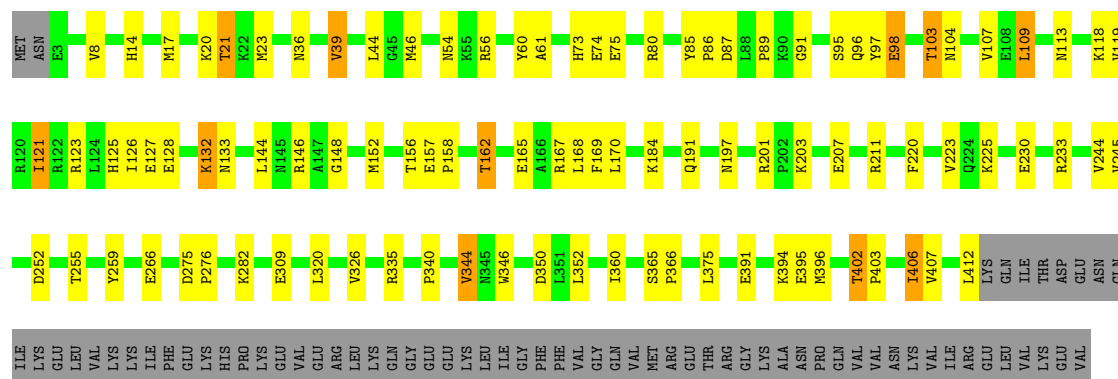
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain E: 65% 18% 14%



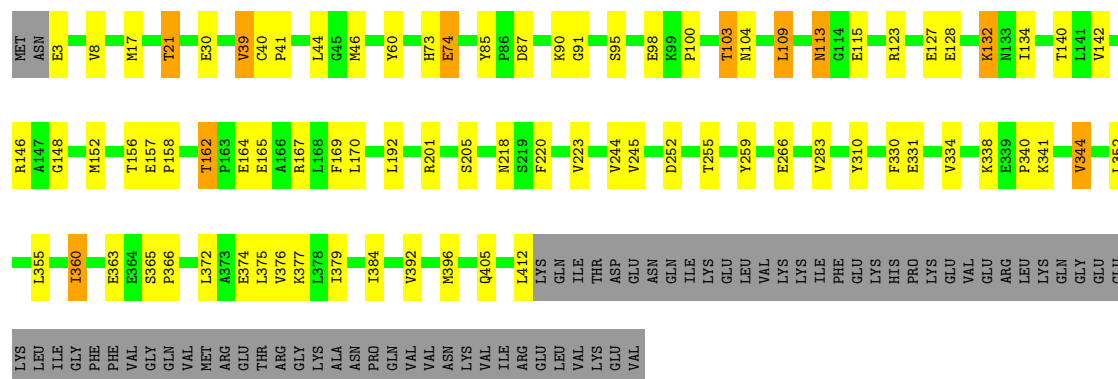
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain H: 65% 18% 14%



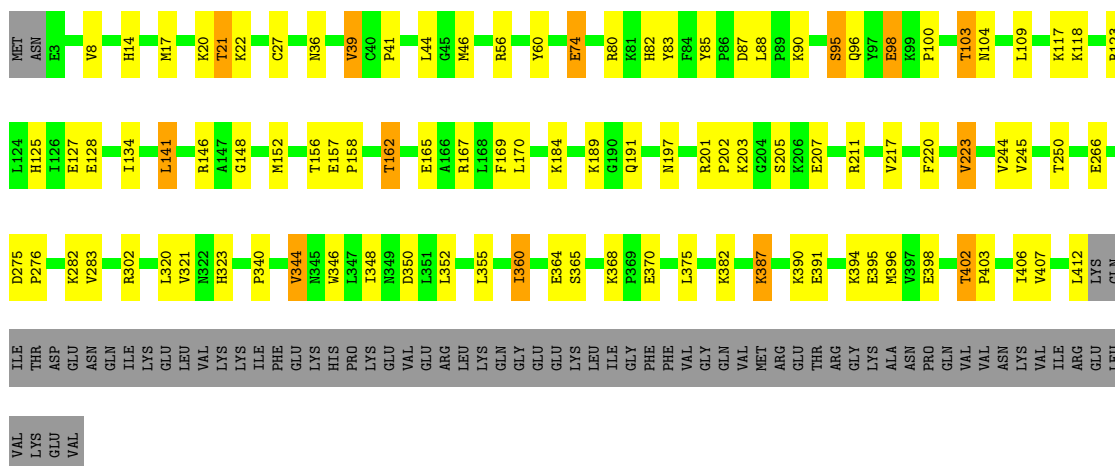
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain K: 69% 15% 14%



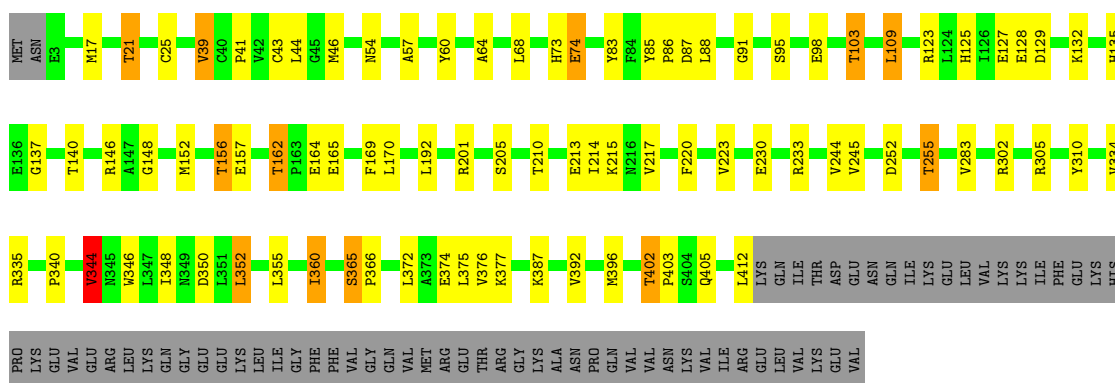
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain N:  65% 18% . 14%



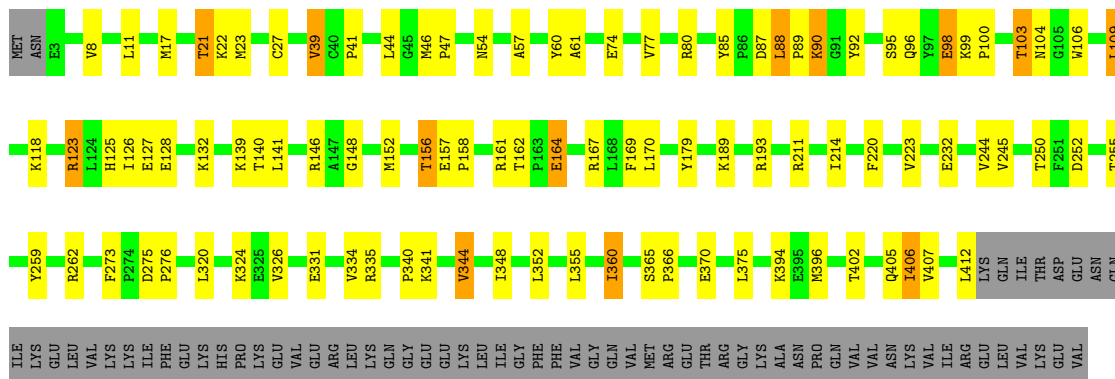
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain Q:  67% 16% • 14%

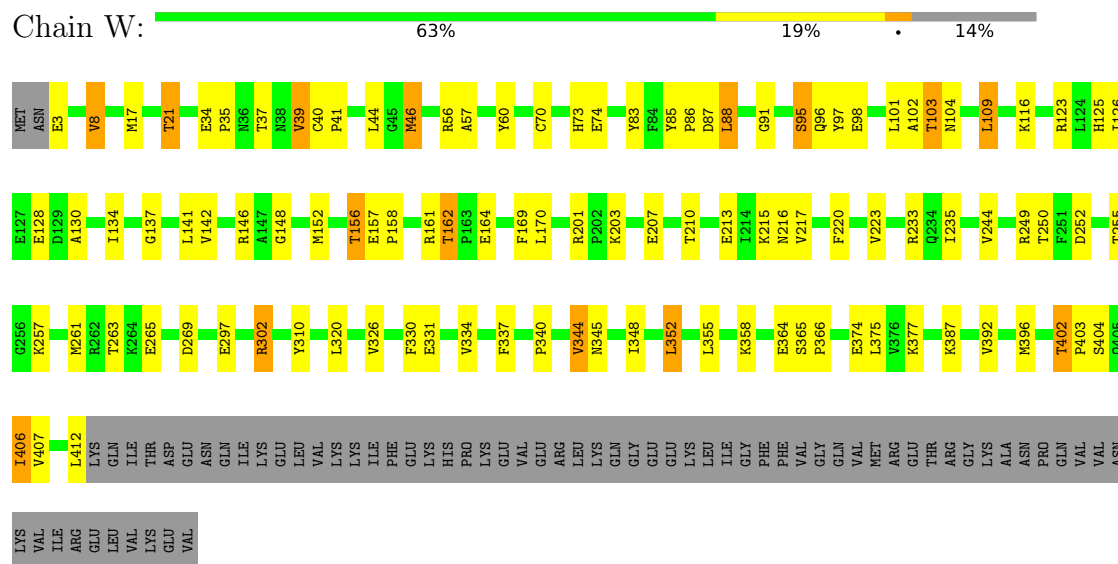


- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

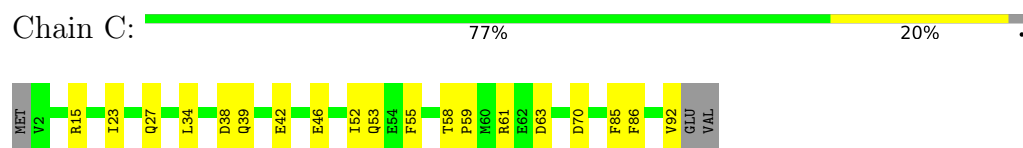
Chain T:  65% 18% • 14%



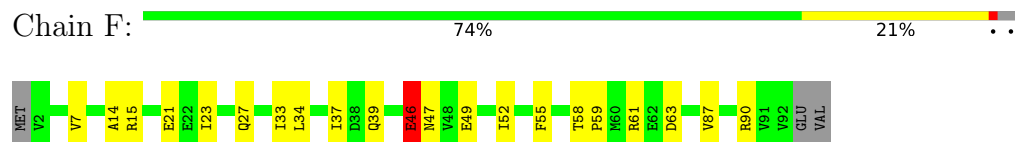
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



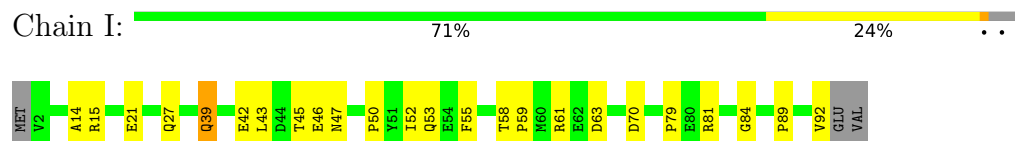
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



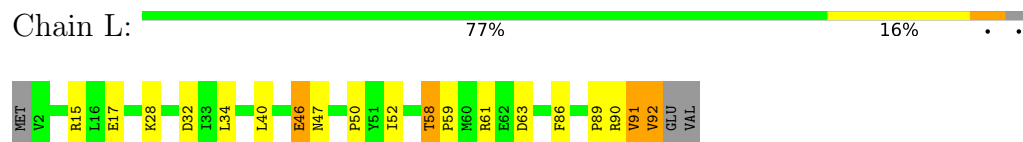
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

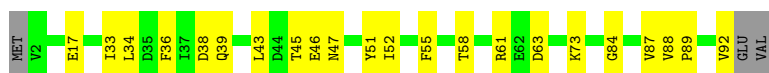


• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

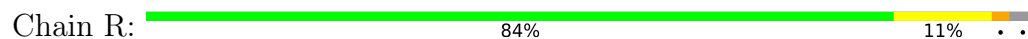


• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

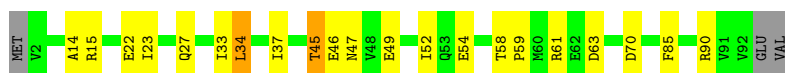




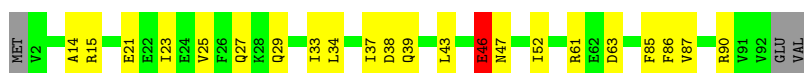
- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                                                         | Source           |
|-------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                                                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 127.48Å 131.01Å 154.67Å<br>90.02° 90.00° 89.91°                                                                                               | Depositor        |
| Resolution (Å)                                                          | 40.50 – 2.30<br>40.50 – 2.30                                                                                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.7 (40.50-2.30)<br>91.4 (40.50-2.30)                                                                                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                                                                                                          | Depositor        |
| $R_{sym}$                                                               | 0.06                                                                                                                                          | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.23 (at 2.31Å)                                                                                                                               | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                                                                                                               | Depositor        |
| R, $R_{free}$                                                           | 0.240 , 0.273<br>0.251 , 0.275                                                                                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 20322 reflections (4.59%)                                                                                                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.8                                                                                                                                          | Xtriage          |
| Anisotropy                                                              | 1.104                                                                                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 20.3                                                                                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$                                                                                   | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -k,h,l<br>0.000 for k,-h,l<br>0.146 for h,-k,-l<br>0.459 for -h,k,-l<br>0.146 for -h,-k,l<br>0.000 for -k,-h,-l<br>0.000 for k,h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                                                                                                          | EDS              |
| Total number of atoms                                                   | 63144                                                                                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                                                                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2482e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ADP, ZN, MG

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     | 0.72         | 0/3874          | 0.98        | 4/5244 (0.1%)   |
| 1   | D     | 0.72         | 0/3874          | 0.97        | 4/5244 (0.1%)   |
| 1   | G     | 0.72         | 2/3874 (0.1%)   | 0.96        | 5/5244 (0.1%)   |
| 1   | J     | 0.75         | 2/3874 (0.1%)   | 0.97        | 4/5244 (0.1%)   |
| 1   | M     | 0.70         | 0/3874          | 0.96        | 1/5244 (0.0%)   |
| 1   | P     | 0.73         | 1/3874 (0.0%)   | 0.97        | 4/5244 (0.1%)   |
| 1   | S     | 0.72         | 1/3874 (0.0%)   | 0.98        | 1/5244 (0.0%)   |
| 1   | V     | 0.74         | 0/3874          | 0.99        | 8/5244 (0.2%)   |
| 2   | B     | 0.64         | 0/3371          | 0.93        | 3/4541 (0.1%)   |
| 2   | E     | 0.71         | 2/3371 (0.1%)   | 0.94        | 6/4541 (0.1%)   |
| 2   | H     | 0.68         | 0/3371          | 0.94        | 3/4541 (0.1%)   |
| 2   | K     | 0.68         | 0/3371          | 0.94        | 3/4541 (0.1%)   |
| 2   | N     | 0.69         | 1/3371 (0.0%)   | 0.94        | 3/4541 (0.1%)   |
| 2   | Q     | 0.69         | 1/3371 (0.0%)   | 0.96        | 5/4541 (0.1%)   |
| 2   | T     | 0.69         | 0/3371          | 0.94        | 3/4541 (0.1%)   |
| 2   | W     | 0.69         | 2/3371 (0.1%)   | 0.92        | 4/4541 (0.1%)   |
| 3   | C     | 0.72         | 2/778 (0.3%)    | 1.00        | 0/1050          |
| 3   | F     | 0.65         | 0/778           | 0.97        | 1/1050 (0.1%)   |
| 3   | I     | 0.73         | 3/778 (0.4%)    | 0.93        | 0/1050          |
| 3   | L     | 0.67         | 0/778           | 1.01        | 5/1050 (0.5%)   |
| 3   | O     | 0.66         | 0/778           | 0.95        | 2/1050 (0.2%)   |
| 3   | R     | 0.68         | 0/778           | 1.02        | 1/1050 (0.1%)   |
| 3   | U     | 0.63         | 0/778           | 0.92        | 0/1050          |
| 3   | X     | 0.66         | 0/778           | 0.98        | 1/1050 (0.1%)   |
| All | All   | 0.70         | 17/64184 (0.0%) | 0.96        | 71/86680 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |
| 3   | I     | 0                   | 1                   |
| 3   | O     | 0                   | 1                   |
| 3   | U     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 299 | ILE  | CA-CB   | 9.16  | 1.59        | 1.54     |
| 1   | J     | 299 | ILE  | CA-CB   | 9.11  | 1.59        | 1.54     |
| 1   | G     | 299 | ILE  | CA-CB   | 7.26  | 1.58        | 1.54     |
| 2   | E     | 110 | ASN  | CG-OD1  | 6.16  | 1.35        | 1.23     |
| 3   | I     | 27  | GLN  | CD-OE1  | 5.73  | 1.34        | 1.23     |
| 1   | S     | 299 | ILE  | CA-CB   | 5.64  | 1.57        | 1.54     |
| 3   | I     | 53  | GLN  | CD-OE1  | 5.57  | 1.34        | 1.23     |
| 2   | W     | 216 | ASN  | CG-OD1  | 5.51  | 1.34        | 1.23     |
| 2   | W     | 345 | ASN  | CG-OD1  | 5.40  | 1.33        | 1.23     |
| 2   | Q     | 135 | HIS  | ND1-CE1 | 5.40  | 1.38        | 1.32     |
| 2   | E     | 323 | HIS  | ND1-CE1 | 5.36  | 1.38        | 1.32     |
| 3   | I     | 53  | GLN  | CD-NE2  | -5.17 | 1.22        | 1.33     |
| 1   | G     | 434 | ILE  | CA-CB   | 5.14  | 1.58        | 1.54     |
| 3   | C     | 53  | GLN  | CD-OE1  | 5.10  | 1.33        | 1.23     |
| 3   | C     | 53  | GLN  | CD-NE2  | -5.05 | 1.22        | 1.33     |
| 1   | J     | 53  | GLN  | CD-OE1  | 5.05  | 1.33        | 1.23     |
| 2   | N     | 323 | HIS  | ND1-CE1 | 5.04  | 1.37        | 1.32     |

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 295 | VAL  | CB-CA-C   | -7.74 | 101.90      | 112.04   |
| 2   | W     | 98  | GLU  | N-CA-C    | -6.98 | 101.31      | 110.53   |
| 2   | B     | 88  | LEU  | CA-C-N    | 6.68  | 126.47      | 119.05   |
| 2   | B     | 88  | LEU  | C-N-CA    | 6.68  | 126.47      | 119.05   |
| 2   | E     | 323 | HIS  | CB-CG-CD2 | -6.68 | 122.52      | 131.20   |
| 2   | N     | 323 | HIS  | CB-CG-CD2 | -6.64 | 122.57      | 131.20   |
| 1   | M     | 434 | ILE  | N-CA-CB   | -6.58 | 105.39      | 112.37   |
| 2   | T     | 98  | GLU  | N-CA-C    | -6.57 | 101.86      | 110.53   |
| 1   | G     | 434 | ILE  | N-CA-CB   | -6.50 | 105.48      | 112.37   |
| 2   | Q     | 135 | HIS  | CB-CG-CD2 | -6.48 | 122.78      | 131.20   |
| 2   | Q     | 98  | GLU  | N-CA-C    | -6.34 | 101.56      | 110.50   |
| 1   | S     | 43  | ILE  | N-CA-C    | -6.31 | 105.58      | 111.45   |
| 1   | V     | 43  | ILE  | N-CA-C    | -6.29 | 105.60      | 111.45   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | K     | 98  | GLU  | N-CA-C    | -6.17 | 101.81      | 110.50   |
| 3   | L     | 46  | GLU  | N-CA-C    | -6.15 | 101.31      | 110.23   |
| 2   | H     | 91  | GLY  | N-CA-C    | -6.13 | 107.21      | 115.36   |
| 3   | O     | 58  | THR  | CA-C-N    | 6.08  | 127.44      | 119.84   |
| 3   | O     | 58  | THR  | C-N-CA    | 6.08  | 127.44      | 119.84   |
| 2   | E     | 88  | LEU  | CA-C-N    | 5.96  | 125.83      | 119.28   |
| 2   | E     | 88  | LEU  | C-N-CA    | 5.96  | 125.83      | 119.28   |
| 3   | F     | 46  | GLU  | N-CA-C    | -5.89 | 101.68      | 110.23   |
| 2   | H     | 98  | GLU  | N-CA-C    | -5.89 | 102.20      | 110.50   |
| 2   | B     | 91  | GLY  | N-CA-C    | -5.85 | 107.25      | 115.32   |
| 2   | E     | 323 | HIS  | CB-CG-ND1 | 5.84  | 131.46      | 122.70   |
| 2   | W     | 91  | GLY  | N-CA-C    | -5.84 | 107.60      | 115.36   |
| 1   | V     | 113 | GLY  | N-CA-C    | 5.83  | 119.08      | 110.63   |
| 2   | N     | 98  | GLU  | N-CA-C    | -5.82 | 102.29      | 110.50   |
| 2   | E     | 98  | GLU  | N-CA-C    | -5.80 | 102.33      | 110.50   |
| 1   | J     | 295 | VAL  | N-CA-CB   | 5.71  | 117.61      | 110.47   |
| 2   | W     | 88  | LEU  | CA-C-N    | 5.70  | 125.55      | 119.28   |
| 2   | W     | 88  | LEU  | C-N-CA    | 5.70  | 125.55      | 119.28   |
| 2   | H     | 360 | ILE  | N-CA-C    | 5.66  | 116.64      | 108.48   |
| 2   | Q     | 135 | HIS  | CB-CG-ND1 | 5.63  | 131.15      | 122.70   |
| 2   | N     | 323 | HIS  | CB-CG-ND1 | 5.58  | 131.07      | 122.70   |
| 1   | D     | 43  | ILE  | N-CA-C    | -5.57 | 106.27      | 111.45   |
| 3   | L     | 58  | THR  | CA-C-N    | 5.56  | 126.43      | 119.98   |
| 3   | L     | 58  | THR  | C-N-CA    | 5.56  | 126.43      | 119.98   |
| 1   | P     | 245 | VAL  | CB-CA-C   | -5.55 | 104.64      | 112.14   |
| 1   | P     | 143 | VAL  | N-CA-CB   | -5.55 | 103.44      | 111.21   |
| 3   | X     | 46  | GLU  | N-CA-C    | -5.52 | 102.22      | 110.23   |
| 2   | E     | 91  | GLY  | N-CA-C    | -5.49 | 108.06      | 115.36   |
| 1   | P     | 295 | VAL  | N-CA-CB   | 5.46  | 117.29      | 110.47   |
| 3   | R     | 46  | GLU  | N-CA-C    | -5.45 | 102.32      | 110.23   |
| 1   | G     | 245 | VAL  | CB-CA-C   | -5.42 | 104.82      | 112.14   |
| 1   | A     | 43  | ILE  | N-CA-C    | -5.39 | 106.44      | 111.45   |
| 1   | J     | 43  | ILE  | N-CA-C    | -5.36 | 106.47      | 111.45   |
| 1   | J     | 185 | LYS  | CA-C-N    | 5.36  | 125.35      | 120.21   |
| 1   | J     | 185 | LYS  | C-N-CA    | 5.36  | 125.35      | 120.21   |
| 2   | K     | 91  | GLY  | N-CA-C    | -5.31 | 108.30      | 115.36   |
| 3   | L     | 46  | GLU  | CA-C-N    | -5.26 | 115.52      | 124.31   |
| 3   | L     | 46  | GLU  | C-N-CA    | -5.26 | 115.52      | 124.31   |
| 1   | V     | 295 | VAL  | N-CA-CB   | 5.19  | 116.95      | 110.47   |
| 1   | V     | 143 | VAL  | N-CA-CB   | -5.18 | 103.96      | 111.21   |
| 1   | A     | 36  | GLU  | N-CA-C    | 5.15  | 116.90      | 111.28   |
| 2   | Q     | 91  | GLY  | N-CA-C    | -5.12 | 108.18      | 115.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 266 | GLN  | CA-C-N  | 5.12  | 125.16      | 119.32   |
| 1   | D     | 266 | GLN  | C-N-CA  | 5.12  | 125.16      | 119.32   |
| 2   | Q     | 344 | VAL  | CB-CA-C | -5.12 | 105.23      | 112.14   |
| 1   | G     | 433 | SER  | CA-C-N  | 5.07  | 127.74      | 123.33   |
| 1   | G     | 433 | SER  | C-N-CA  | 5.07  | 127.74      | 123.33   |
| 1   | V     | 36  | GLU  | N-CA-C  | 5.07  | 116.80      | 111.28   |
| 1   | A     | 39  | VAL  | N-CA-C  | 5.07  | 115.29      | 110.53   |
| 1   | V     | 115 | THR  | N-CA-CB | -5.07 | 102.02      | 110.23   |
| 1   | V     | 245 | VAL  | CB-CA-C | -5.04 | 105.33      | 112.14   |
| 1   | G     | 397 | THR  | CB-CA-C | 5.04  | 116.76      | 109.45   |
| 1   | D     | 115 | THR  | CB-CA-C | 5.04  | 118.02      | 109.50   |
| 2   | K     | 218 | ASN  | N-CA-C  | 5.02  | 119.09      | 112.92   |
| 1   | V     | 295 | VAL  | CB-CA-C | -5.01 | 105.47      | 112.04   |
| 1   | P     | 43  | ILE  | N-CA-C  | -5.00 | 106.80      | 111.45   |
| 2   | T     | 88  | LEU  | CA-C-N  | 5.00  | 124.78      | 119.28   |
| 2   | T     | 88  | LEU  | C-N-CA  | 5.00  | 124.78      | 119.28   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 39  | VAL  | Peptide |
| 2   | B     | 97  | TYR  | Peptide |
| 3   | I     | 45  | THR  | Peptide |
| 3   | O     | 45  | THR  | Peptide |
| 3   | U     | 45  | THR  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3784  | 0        | 3816     | 96      | 0            |
| 1   | D     | 3784  | 0        | 3816     | 80      | 0            |
| 1   | G     | 3784  | 0        | 3816     | 93      | 0            |
| 1   | J     | 3784  | 0        | 3816     | 74      | 0            |
| 1   | M     | 3784  | 0        | 3816     | 73      | 0            |
| 1   | P     | 3784  | 0        | 3816     | 77      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | S     | 3784  | 0        | 3816     | 92      | 0            |
| 1   | V     | 3784  | 0        | 3816     | 101     | 0            |
| 2   | B     | 3308  | 0        | 3354     | 85      | 0            |
| 2   | E     | 3308  | 0        | 3353     | 77      | 0            |
| 2   | H     | 3308  | 0        | 3353     | 77      | 0            |
| 2   | K     | 3308  | 0        | 3353     | 67      | 0            |
| 2   | N     | 3308  | 0        | 3353     | 68      | 0            |
| 2   | Q     | 3308  | 0        | 3353     | 66      | 0            |
| 2   | T     | 3308  | 0        | 3353     | 77      | 0            |
| 2   | W     | 3308  | 0        | 3353     | 77      | 0            |
| 3   | C     | 764   | 0        | 755      | 11      | 0            |
| 3   | F     | 764   | 0        | 755      | 17      | 0            |
| 3   | I     | 764   | 0        | 755      | 18      | 0            |
| 3   | L     | 764   | 0        | 755      | 22      | 0            |
| 3   | O     | 764   | 0        | 755      | 16      | 0            |
| 3   | R     | 764   | 0        | 755      | 15      | 0            |
| 3   | U     | 764   | 0        | 755      | 15      | 0            |
| 3   | X     | 764   | 0        | 755      | 17      | 0            |
| 4   | A     | 8     | 0        | 3        | 1       | 0            |
| 4   | D     | 8     | 0        | 3        | 1       | 0            |
| 4   | G     | 8     | 0        | 3        | 0       | 0            |
| 4   | J     | 8     | 0        | 3        | 0       | 0            |
| 4   | M     | 8     | 0        | 3        | 0       | 0            |
| 4   | P     | 8     | 0        | 3        | 1       | 0            |
| 4   | S     | 8     | 0        | 3        | 1       | 0            |
| 4   | V     | 8     | 0        | 3        | 0       | 0            |
| 5   | B     | 27    | 0        | 12       | 1       | 0            |
| 5   | E     | 27    | 0        | 12       | 0       | 0            |
| 5   | H     | 27    | 0        | 12       | 0       | 0            |
| 5   | K     | 27    | 0        | 12       | 0       | 0            |
| 5   | N     | 27    | 0        | 12       | 0       | 0            |
| 5   | Q     | 27    | 0        | 12       | 0       | 0            |
| 5   | T     | 27    | 0        | 12       | 1       | 0            |
| 5   | W     | 27    | 0        | 12       | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 1     | 0        | 0        | 0       | 0            |
| 6   | K     | 1     | 0        | 0        | 0       | 0            |
| 6   | N     | 1     | 0        | 0        | 0       | 0            |
| 6   | Q     | 1     | 0        | 0        | 0       | 0            |
| 6   | T     | 1     | 0        | 0        | 0       | 0            |
| 6   | W     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | E     | 1     | 0        | 0        | 0       | 0            |
| 7   | H     | 1     | 0        | 0        | 0       | 0            |
| 7   | K     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| 7   | Q     | 1     | 0        | 0        | 0       | 0            |
| 7   | T     | 1     | 0        | 0        | 0       | 0            |
| 7   | W     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 63144 | 0        | 63513    | 1283    | 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 10.

All (1283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:77:VAL:CG2   | 1:V:114:LYS:HZ2  | 1.57                     | 1.16              |
| 1:A:190:ARG:HG3  | 1:A:190:ARG:HH11 | 1.05                     | 1.16              |
| 1:V:77:VAL:HG21  | 1:V:114:LYS:NZ   | 1.61                     | 1.13              |
| 1:V:77:VAL:HG21  | 1:V:114:LYS:HZ2  | 0.94                     | 1.08              |
| 1:A:47:TYR:O     | 1:A:51:LEU:HD13  | 1.54                     | 1.07              |
| 1:V:190:ARG:HG3  | 1:V:190:ARG:HH11 | 1.10                     | 1.06              |
| 1:P:31:ARG:HH11  | 1:P:31:ARG:CG    | 1.69                     | 1.05              |
| 3:L:92:VAL:HG22  | 3:L:92:VAL:O     | 1.58                     | 1.04              |
| 1:D:190:ARG:HD3  | 1:D:241:TRP:HH2  | 1.20                     | 1.03              |
| 1:M:88:ILE:HG23  | 1:M:343:GLY:HA3  | 1.40                     | 1.03              |
| 1:S:376:ARG:HG3  | 1:S:376:ARG:HH11 | 1.24                     | 1.02              |
| 2:N:21:THR:HG21  | 3:O:61:ARG:HH12  | 1.24                     | 1.01              |
| 2:B:21:THR:HB    | 3:C:63:ASP:OD1   | 1.61                     | 1.01              |
| 1:V:336:TYR:O    | 1:V:339:THR:HG22 | 1.61                     | 1.00              |
| 2:B:21:THR:HG21  | 3:C:61:ARG:HH12  | 1.25                     | 1.00              |
| 2:E:21:THR:HG21  | 3:F:61:ARG:HH12  | 1.23                     | 1.00              |
| 1:D:376:ARG:HG3  | 1:D:376:ARG:HH11 | 1.25                     | 0.98              |
| 2:T:21:THR:HG21  | 3:U:61:ARG:HH12  | 1.26                     | 0.97              |
| 2:H:21:THR:HG21  | 3:I:61:ARG:HH12  | 1.26                     | 0.97              |
| 1:P:190:ARG:HD3  | 1:P:241:TRP:HH2  | 1.27                     | 0.97              |
| 1:J:376:ARG:HG3  | 1:J:376:ARG:HH11 | 1.26                     | 0.96              |
| 2:K:360:ILE:HD11 | 2:K:365:SER:HA   | 1.45                     | 0.96              |
| 1:A:47:TYR:CE2   | 1:A:112:VAL:CG1  | 2.48                     | 0.96              |
| 1:D:138:TRP:CE2  | 1:D:438:TRP:HH2  | 1.81                     | 0.96              |
| 1:A:47:TYR:CE2   | 1:A:112:VAL:HG11 | 2.00                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:17:MET:HE3   | 2:E:60:TYR:HB2   | 1.48                     | 0.95              |
| 1:V:77:VAL:CG2   | 1:V:114:LYS:NZ   | 2.23                     | 0.95              |
| 1:P:352:ILE:O    | 1:P:356:THR:HG22 | 1.66                     | 0.94              |
| 2:T:21:THR:HB    | 3:U:63:ASP:OD1   | 1.65                     | 0.94              |
| 2:K:100:PRO:HB3  | 2:K:123:ARG:HH21 | 1.32                     | 0.94              |
| 1:S:155:VAL:HG12 | 1:S:181:VAL:HG21 | 1.48                     | 0.94              |
| 1:J:190:ARG:HD3  | 1:J:241:TRP:HH2  | 1.32                     | 0.93              |
| 1:M:352:ILE:O    | 1:M:356:THR:HG22 | 1.67                     | 0.93              |
| 1:D:138:TRP:CE2  | 1:D:438:TRP:CH2  | 2.56                     | 0.93              |
| 2:W:17:MET:CE    | 2:W:60:TYR:HB2   | 1.99                     | 0.93              |
| 2:E:17:MET:HE1   | 2:E:57:ALA:HA    | 1.52                     | 0.92              |
| 2:Q:360:ILE:HD11 | 2:Q:365:SER:HA   | 1.52                     | 0.91              |
| 1:G:85:ALA:HB2   | 1:G:117:LEU:HD13 | 1.53                     | 0.91              |
| 1:D:72:LYS:HA    | 1:D:115:THR:HG22 | 1.50                     | 0.90              |
| 2:W:252:ASP:HB3  | 2:W:255:THR:HG22 | 1.54                     | 0.90              |
| 2:B:162:THR:HG22 | 2:B:165:GLU:H    | 1.33                     | 0.90              |
| 2:K:156:THR:HG22 | 2:K:157:GLU:O    | 1.70                     | 0.90              |
| 2:H:252:ASP:HB3  | 2:H:255:THR:HG22 | 1.53                     | 0.89              |
| 2:B:100:PRO:HB3  | 2:B:123:ARG:HH21 | 1.35                     | 0.89              |
| 2:W:103:THR:HG22 | 2:W:104:ASN:OD1  | 1.73                     | 0.88              |
| 1:P:31:ARG:HH11  | 1:P:31:ARG:HG2   | 1.36                     | 0.88              |
| 1:S:386:PHE:HB3  | 1:S:451:LYS:HE2  | 1.54                     | 0.88              |
| 2:B:17:MET:HE1   | 2:B:57:ALA:HA    | 1.56                     | 0.88              |
| 1:V:190:ARG:HG3  | 1:V:190:ARG:NH1  | 1.84                     | 0.88              |
| 1:A:68:PRO:HB3   | 1:A:112:VAL:HG21 | 1.55                     | 0.87              |
| 2:T:17:MET:HE1   | 2:T:57:ALA:HA    | 1.58                     | 0.86              |
| 2:E:17:MET:HE3   | 2:E:60:TYR:CB    | 2.06                     | 0.85              |
| 2:H:252:ASP:HB3  | 2:H:255:THR:CG2  | 2.05                     | 0.85              |
| 2:H:17:MET:HE2   | 2:H:60:TYR:HB3   | 1.58                     | 0.85              |
| 2:B:40:CYS:O     | 2:B:44:LEU:HB2   | 1.76                     | 0.85              |
| 2:W:34:GLU:O     | 2:W:37:THR:HG22  | 1.77                     | 0.85              |
| 2:W:39:VAL:HG13  | 2:W:44:LEU:HD11  | 1.57                     | 0.85              |
| 2:E:17:MET:CE    | 2:E:60:TYR:HB2   | 2.06                     | 0.84              |
| 2:E:252:ASP:HB3  | 2:E:255:THR:HG22 | 1.57                     | 0.84              |
| 2:N:21:THR:CG2   | 3:O:61:ARG:HH12  | 1.90                     | 0.84              |
| 1:M:190:ARG:HD3  | 1:M:241:TRP:HH2  | 1.43                     | 0.84              |
| 1:A:47:TYR:CD2   | 1:A:112:VAL:CG1  | 2.61                     | 0.84              |
| 1:M:88:ILE:HD11  | 1:M:120:PHE:CE2  | 2.11                     | 0.83              |
| 2:T:156:THR:HG22 | 2:T:157:GLU:O    | 1.78                     | 0.83              |
| 1:A:190:ARG:HG3  | 1:A:190:ARG:NH1  | 1.84                     | 0.83              |
| 2:B:21:THR:CG2   | 3:C:61:ARG:HH12  | 1.92                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:422:VAL:N    | 1:G:423:PRO:CD   | 2.43                     | 0.82              |
| 2:T:103:THR:HG22 | 2:T:104:ASN:OD1  | 1.78                     | 0.81              |
| 2:W:17:MET:HE3   | 2:W:60:TYR:HB2   | 1.59                     | 0.81              |
| 1:A:279:GLU:HG3  | 1:A:468:LYS:NZ   | 1.94                     | 0.81              |
| 1:D:190:ARG:HD3  | 1:D:241:TRP:CH2  | 2.12                     | 0.81              |
| 2:B:17:MET:HE3   | 2:B:60:TYR:HB2   | 1.61                     | 0.81              |
| 1:A:138:TRP:CE2  | 1:A:438:TRP:HH2  | 1.98                     | 0.81              |
| 2:Q:21:THR:CG2   | 3:R:61:ARG:HH12  | 1.94                     | 0.80              |
| 1:P:370:LYS:HZ2  | 3:R:45:THR:HB    | 1.46                     | 0.80              |
| 1:A:47:TYR:CD2   | 1:A:112:VAL:HG13 | 2.17                     | 0.80              |
| 1:G:85:ALA:CB    | 1:G:117:LEU:HD13 | 2.11                     | 0.80              |
| 1:M:88:ILE:HD11  | 1:M:120:PHE:CZ   | 2.16                     | 0.80              |
| 1:G:190:ARG:HD3  | 1:G:241:TRP:HH2  | 1.44                     | 0.80              |
| 1:S:376:ARG:HG3  | 1:S:376:ARG:NH1  | 1.97                     | 0.80              |
| 2:B:39:VAL:HG13  | 2:B:44:LEU:HD11  | 1.64                     | 0.80              |
| 1:A:138:TRP:CE2  | 1:A:438:TRP:CH2  | 2.70                     | 0.80              |
| 1:A:95:PRO:HG2   | 2:B:46:MET:HE1   | 1.64                     | 0.79              |
| 3:L:92:VAL:O     | 3:L:92:VAL:CG2   | 2.30                     | 0.79              |
| 1:V:71:VAL:HB    | 1:V:114:LYS:HZ1  | 1.46                     | 0.79              |
| 1:P:31:ARG:HH11  | 1:P:31:ARG:HG3   | 1.47                     | 0.79              |
| 2:N:162:THR:HG22 | 2:N:165:GLU:H    | 1.45                     | 0.79              |
| 1:D:77:VAL:HG23  | 1:D:114:LYS:NZ   | 1.98                     | 0.79              |
| 1:S:81:LYS:HE2   | 1:S:91:ASN:HA    | 1.64                     | 0.79              |
| 2:K:21:THR:HG21  | 3:L:61:ARG:HH12  | 1.46                     | 0.78              |
| 2:W:17:MET:HE3   | 2:W:60:TYR:CB    | 2.13                     | 0.78              |
| 2:E:17:MET:CE    | 2:E:57:ALA:HA    | 2.13                     | 0.78              |
| 1:G:352:ILE:O    | 1:G:356:THR:HG23 | 1.84                     | 0.78              |
| 1:J:352:ILE:O    | 1:J:356:THR:HG22 | 1.84                     | 0.78              |
| 1:P:190:ARG:HD3  | 1:P:241:TRP:CH2  | 2.17                     | 0.78              |
| 2:T:17:MET:HE3   | 2:T:60:TYR:HB2   | 1.65                     | 0.78              |
| 2:B:17:MET:CE    | 2:B:57:ALA:HA    | 2.14                     | 0.77              |
| 1:D:194:TYR:CD1  | 1:D:229:LYS:HB3  | 2.19                     | 0.77              |
| 1:V:190:ARG:HH11 | 1:V:190:ARG:CG   | 1.95                     | 0.77              |
| 1:P:31:ARG:HG2   | 1:P:31:ARG:NH1   | 1.97                     | 0.77              |
| 2:W:17:MET:HE1   | 2:W:57:ALA:HA    | 1.67                     | 0.77              |
| 2:N:21:THR:HB    | 3:O:63:ASP:OD1   | 1.85                     | 0.76              |
| 2:T:85:TYR:HD2   | 2:T:87:ASP:OD1   | 1.69                     | 0.76              |
| 2:Q:17:MET:CE    | 2:Q:60:TYR:HB2   | 2.15                     | 0.76              |
| 1:A:190:ARG:HH11 | 1:A:190:ARG:CG   | 1.94                     | 0.76              |
| 2:K:21:THR:CG2   | 3:L:61:ARG:HH12  | 1.97                     | 0.76              |
| 1:M:95:PRO:HG2   | 2:N:46:MET:CE    | 2.16                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:156:THR:HG22 | 2:Q:157:GLU:O    | 1.84                     | 0.76              |
| 1:S:190:ARG:HD3  | 1:S:241:TRP:HH2  | 1.51                     | 0.75              |
| 2:B:17:MET:CE    | 2:B:60:TYR:HB2   | 2.16                     | 0.75              |
| 2:Q:109:LEU:HD11 | 2:Q:169:PHE:HA   | 1.68                     | 0.75              |
| 2:B:21:THR:HG21  | 3:C:61:ARG:NH1   | 2.00                     | 0.75              |
| 1:D:352:ILE:O    | 1:D:356:THR:HG23 | 1.86                     | 0.75              |
| 2:E:21:THR:HB    | 3:F:63:ASP:OD1   | 1.87                     | 0.75              |
| 2:H:17:MET:CE    | 2:H:60:TYR:HB3   | 2.17                     | 0.74              |
| 1:V:279:GLU:HG3  | 1:V:468:LYS:NZ   | 2.03                     | 0.74              |
| 1:J:174:GLN:HG3  | 1:J:175:PRO:HD3  | 1.70                     | 0.74              |
| 2:N:109:LEU:HD11 | 2:N:169:PHE:HA   | 1.70                     | 0.73              |
| 2:W:21:THR:CG2   | 3:X:61:ARG:HH12  | 1.99                     | 0.73              |
| 2:H:21:THR:CG2   | 3:I:61:ARG:HH12  | 1.99                     | 0.73              |
| 2:H:103:THR:CG2  | 2:H:104:ASN:OD1  | 2.36                     | 0.73              |
| 2:W:252:ASP:HB3  | 2:W:255:THR:CG2  | 2.17                     | 0.73              |
| 1:J:352:ILE:O    | 1:J:356:THR:CG2  | 2.35                     | 0.73              |
| 2:K:109:LEU:HD11 | 2:K:169:PHE:HA   | 1.71                     | 0.73              |
| 1:P:306:ALA:HB3  | 1:P:307:PRO:HD3  | 1.70                     | 0.73              |
| 1:M:138:TRP:CE2  | 1:M:438:TRP:CH2  | 2.77                     | 0.73              |
| 1:V:193:ARG:NH1  | 1:V:232:THR:OG1  | 2.22                     | 0.72              |
| 2:W:97:TYR:O     | 2:W:123:ARG:NH2  | 2.22                     | 0.72              |
| 2:W:21:THR:HG21  | 3:X:61:ARG:HH12  | 1.53                     | 0.72              |
| 2:B:213:GLU:OE1  | 2:B:215:LYS:HE3  | 1.89                     | 0.72              |
| 2:B:252:ASP:HB3  | 2:B:255:THR:HG22 | 1.71                     | 0.72              |
| 2:B:156:THR:HG22 | 2:B:157:GLU:O    | 1.90                     | 0.71              |
| 1:M:185:LYS:NZ   | 1:M:429:LEU:O    | 2.24                     | 0.71              |
| 2:B:17:MET:HE1   | 2:B:57:ALA:O     | 1.88                     | 0.71              |
| 2:H:20:LYS:HE2   | 2:H:56:ARG:HH12  | 1.55                     | 0.71              |
| 1:A:110:LEU:O    | 1:A:112:VAL:HG23 | 1.90                     | 0.71              |
| 2:B:39:VAL:CG1   | 2:B:44:LEU:HD11  | 2.21                     | 0.71              |
| 2:T:17:MET:CE    | 2:T:57:ALA:HA    | 2.20                     | 0.71              |
| 1:D:138:TRP:CZ2  | 1:D:438:TRP:CH2  | 2.78                     | 0.71              |
| 1:D:182:ILE:HG12 | 1:D:434:ILE:HD12 | 1.71                     | 0.71              |
| 2:E:17:MET:HE1   | 2:E:57:ALA:O     | 1.91                     | 0.71              |
| 2:N:156:THR:HG22 | 2:N:157:GLU:O    | 1.90                     | 0.71              |
| 2:E:17:MET:HE1   | 2:E:57:ALA:CA    | 2.21                     | 0.71              |
| 1:V:352:ILE:O    | 1:V:356:THR:HG23 | 1.89                     | 0.71              |
| 2:N:21:THR:HG21  | 3:O:61:ARG:NH1   | 2.04                     | 0.70              |
| 1:A:47:TYR:O     | 1:A:51:LEU:CD1   | 2.37                     | 0.70              |
| 2:B:17:MET:HE3   | 2:B:60:TYR:CB    | 2.20                     | 0.70              |
| 2:T:21:THR:CG2   | 3:U:61:ARG:HH12  | 2.00                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:115:THR:HG21 | 1:D:151:SER:OG   | 1.90                     | 0.70              |
| 1:P:31:ARG:CG    | 1:P:31:ARG:NH1   | 2.40                     | 0.70              |
| 2:N:360:ILE:HD11 | 2:N:365:SER:HA   | 1.74                     | 0.70              |
| 1:G:270:LYS:HE3  | 1:G:274:GLU:OE2  | 1.91                     | 0.70              |
| 3:L:46:GLU:O     | 3:L:47:ASN:HB2   | 1.91                     | 0.70              |
| 3:F:23:ILE:O     | 3:F:27:GLN:HG3   | 1.92                     | 0.69              |
| 2:H:17:MET:CE    | 2:H:60:TYR:CB    | 2.70                     | 0.69              |
| 2:W:123:ARG:NH1  | 2:W:125:HIS:ND1  | 2.40                     | 0.69              |
| 1:J:190:ARG:HD3  | 1:J:241:TRP:CH2  | 2.23                     | 0.69              |
| 2:Q:17:MET:CE    | 2:Q:60:TYR:CB    | 2.70                     | 0.69              |
| 2:W:402:THR:HG22 | 2:W:403:PRO:HD2  | 1.74                     | 0.69              |
| 2:E:21:THR:HG21  | 3:F:61:ARG:NH1   | 2.03                     | 0.69              |
| 2:E:156:THR:HG22 | 2:E:157:GLU:O    | 1.91                     | 0.69              |
| 2:H:17:MET:HE2   | 2:H:60:TYR:CB    | 2.22                     | 0.69              |
| 1:S:182:ILE:HG12 | 1:S:434:ILE:HD12 | 1.74                     | 0.69              |
| 2:W:17:MET:CE    | 2:W:57:ALA:HA    | 2.22                     | 0.69              |
| 1:G:13:LEU:HB3   | 1:G:19:VAL:HG12  | 1.75                     | 0.69              |
| 1:G:190:ARG:HD3  | 1:G:241:TRP:CH2  | 2.26                     | 0.69              |
| 2:H:95:SER:HB3   | 2:H:127:GLU:HB3  | 1.73                     | 0.69              |
| 2:T:402:THR:OG1  | 2:T:405:GLN:HB2  | 1.93                     | 0.69              |
| 2:H:109:LEU:HD11 | 2:H:169:PHE:HA   | 1.74                     | 0.69              |
| 1:V:204:ASP:O    | 1:V:205:GLN:HG2  | 1.93                     | 0.69              |
| 2:E:103:THR:HG22 | 2:E:104:ASN:OD1  | 1.93                     | 0.68              |
| 1:M:115:THR:HG21 | 1:M:151:SER:OG   | 1.93                     | 0.68              |
| 2:T:17:MET:CE    | 2:T:60:TYR:HB2   | 2.24                     | 0.68              |
| 2:T:17:MET:HE1   | 2:T:57:ALA:O     | 1.94                     | 0.68              |
| 2:K:85:TYR:OH    | 3:L:91:VAL:HG11  | 1.92                     | 0.68              |
| 1:D:376:ARG:HG3  | 1:D:376:ARG:NH1  | 2.01                     | 0.68              |
| 2:H:97:TYR:O     | 2:H:123:ARG:NH2  | 2.27                     | 0.68              |
| 2:K:95:SER:CB    | 2:K:127:GLU:HB3  | 2.23                     | 0.68              |
| 2:N:17:MET:HE2   | 2:N:60:TYR:HB3   | 1.75                     | 0.68              |
| 2:T:255:THR:HG21 | 2:T:259:TYR:OH   | 1.92                     | 0.68              |
| 1:M:90:GLU:O     | 1:M:91:ASN:HB2   | 1.92                     | 0.68              |
| 1:M:190:ARG:HD3  | 1:M:241:TRP:CH2  | 2.28                     | 0.68              |
| 2:W:17:MET:HE1   | 2:W:57:ALA:O     | 1.93                     | 0.68              |
| 1:G:306:ALA:HB3  | 1:G:307:PRO:HD3  | 1.75                     | 0.68              |
| 2:K:17:MET:HE2   | 2:K:60:TYR:CB    | 2.23                     | 0.68              |
| 1:S:155:VAL:CG1  | 1:S:181:VAL:HG21 | 2.24                     | 0.68              |
| 1:D:77:VAL:HG23  | 1:D:114:LYS:HZ2  | 1.59                     | 0.67              |
| 2:E:310:TYR:CE1  | 2:E:334:VAL:HG11 | 2.28                     | 0.67              |
| 2:K:3:GLU:HA     | 2:K:3:GLU:OE1    | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:336:TYR:O    | 1:V:339:THR:CG2  | 2.41                     | 0.67              |
| 1:V:138:TRP:CE2  | 1:V:438:TRP:CH2  | 2.81                     | 0.67              |
| 2:W:156:THR:HG22 | 2:W:157:GLU:O    | 1.94                     | 0.67              |
| 1:M:69:ILE:HD11  | 1:M:164:LEU:HD13 | 1.76                     | 0.67              |
| 2:Q:21:THR:HG21  | 3:R:61:ARG:HH12  | 1.59                     | 0.67              |
| 2:Q:162:THR:HG22 | 2:Q:165:GLU:H    | 1.59                     | 0.67              |
| 2:B:17:MET:HG2   | 2:B:152:MET:HE3  | 1.76                     | 0.67              |
| 2:K:74:GLU:HG2   | 2:K:283:VAL:O    | 1.95                     | 0.67              |
| 1:V:77:VAL:HG21  | 1:V:114:LYS:CE   | 2.24                     | 0.67              |
| 1:G:422:VAL:HG22 | 1:G:423:PRO:HD3  | 1.75                     | 0.67              |
| 1:S:83:THR:HG22  | 1:S:90:GLU:HA    | 1.77                     | 0.67              |
| 2:T:252:ASP:HB3  | 2:T:255:THR:HG22 | 1.77                     | 0.67              |
| 1:G:85:ALA:HB2   | 1:G:117:LEU:CD1  | 2.23                     | 0.67              |
| 1:A:279:GLU:HG3  | 1:A:468:LYS:HZ3  | 1.55                     | 0.67              |
| 1:G:115:THR:HG21 | 1:G:151:SER:OG   | 1.95                     | 0.67              |
| 1:A:352:ILE:O    | 1:A:356:THR:HG23 | 1.94                     | 0.67              |
| 2:B:17:MET:HE1   | 2:B:57:ALA:CA    | 2.24                     | 0.66              |
| 2:B:156:THR:CG2  | 2:B:157:GLU:O    | 2.42                     | 0.66              |
| 2:B:402:THR:HG22 | 2:B:403:PRO:HD2  | 1.77                     | 0.66              |
| 1:M:163:SER:HB3  | 1:M:209:PHE:HB2  | 1.77                     | 0.66              |
| 1:S:167:ASP:HB2  | 1:S:172:ILE:HD12 | 1.76                     | 0.66              |
| 1:A:438:TRP:CH2  | 1:A:443:PRO:HG3  | 2.31                     | 0.66              |
| 2:B:39:VAL:HG13  | 2:B:44:LEU:CD1   | 2.24                     | 0.66              |
| 2:W:213:GLU:OE2  | 2:W:215:LYS:HE3  | 1.95                     | 0.66              |
| 2:H:375:LEU:HD13 | 2:H:396:MET:HE1  | 1.77                     | 0.66              |
| 2:K:17:MET:CE    | 2:K:60:TYR:CB    | 2.73                     | 0.66              |
| 1:D:174:GLN:HG3  | 1:D:175:PRO:HD3  | 1.77                     | 0.66              |
| 2:E:252:ASP:HB3  | 2:E:255:THR:CG2  | 2.24                     | 0.66              |
| 3:U:46:GLU:O     | 3:U:47:ASN:HB2   | 1.95                     | 0.66              |
| 1:M:155:VAL:CG2  | 1:M:163:SER:HB2  | 2.26                     | 0.66              |
| 1:S:190:ARG:HD3  | 1:S:241:TRP:CH2  | 2.29                     | 0.66              |
| 1:J:376:ARG:HG3  | 1:J:376:ARG:NH1  | 1.94                     | 0.66              |
| 1:M:174:GLN:HG3  | 1:M:175:PRO:HD3  | 1.78                     | 0.66              |
| 2:B:103:THR:CG2  | 2:B:104:ASN:OD1  | 2.44                     | 0.66              |
| 2:E:103:THR:CG2  | 2:E:104:ASN:OD1  | 2.44                     | 0.66              |
| 2:K:95:SER:HB2   | 2:K:127:GLU:HB3  | 1.76                     | 0.66              |
| 1:M:95:PRO:HG2   | 2:N:46:MET:HE1   | 1.78                     | 0.65              |
| 2:T:21:THR:HG21  | 3:U:61:ARG:NH1   | 2.07                     | 0.65              |
| 1:D:292:LEU:O    | 1:D:295:VAL:HG22 | 1.97                     | 0.65              |
| 1:M:138:TRP:CE2  | 1:M:438:TRP:HH2  | 2.13                     | 0.65              |
| 1:D:69:ILE:HD11  | 1:D:164:LEU:HD13 | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:299:ILE:HG13 | 1:P:419:ILE:HG22 | 1.78                     | 0.65              |
| 2:B:73:HIS:NE2   | 2:B:103:THR:HB   | 2.12                     | 0.65              |
| 2:Q:17:MET:HE2   | 2:Q:60:TYR:HB2   | 1.79                     | 0.65              |
| 1:S:143:VAL:HG12 | 1:S:145:GLY:H    | 1.60                     | 0.65              |
| 2:W:103:THR:CG2  | 2:W:104:ASN:OD1  | 2.44                     | 0.65              |
| 1:J:178:PHE:HE1  | 1:J:397:THR:HG21 | 1.62                     | 0.65              |
| 1:G:421:THR:C    | 1:G:423:PRO:HD2  | 2.22                     | 0.65              |
| 2:Q:17:MET:HG2   | 2:Q:152:MET:HE2  | 1.78                     | 0.65              |
| 2:Q:95:SER:HB3   | 2:Q:127:GLU:CB   | 2.26                     | 0.64              |
| 1:S:299:ILE:HG13 | 1:S:419:ILE:HG22 | 1.79                     | 0.64              |
| 2:K:17:MET:HE2   | 2:K:60:TYR:HB3   | 1.79                     | 0.64              |
| 2:B:302:ARG:HD3  | 2:B:321:VAL:HG22 | 1.80                     | 0.64              |
| 1:P:95:PRO:HG2   | 2:Q:46:MET:CE    | 2.27                     | 0.64              |
| 2:N:103:THR:HG23 | 2:N:104:ASN:OD1  | 1.98                     | 0.64              |
| 2:T:103:THR:CG2  | 2:T:104:ASN:OD1  | 2.45                     | 0.64              |
| 3:X:23:ILE:O     | 3:X:27:GLN:HG3   | 1.96                     | 0.64              |
| 1:J:306:ALA:HB3  | 1:J:307:PRO:HD3  | 1.80                     | 0.64              |
| 1:M:86:SER:OG    | 1:M:88:ILE:HG13  | 1.98                     | 0.64              |
| 1:G:300:PRO:HG2  | 3:I:39:GLN:HG3   | 1.80                     | 0.64              |
| 1:G:422:VAL:CG2  | 1:G:423:PRO:HD3  | 2.28                     | 0.64              |
| 2:H:220:PHE:O    | 2:H:223:VAL:HG22 | 1.97                     | 0.64              |
| 1:J:138:TRP:CE2  | 1:J:438:TRP:CH2  | 2.86                     | 0.64              |
| 1:D:2:LEU:HD23   | 1:D:27:SER:HB2   | 1.79                     | 0.63              |
| 1:M:376:ARG:HG3  | 1:M:376:ARG:HH11 | 1.62                     | 0.63              |
| 2:N:100:PRO:HB3  | 2:N:123:ARG:NH2  | 2.13                     | 0.63              |
| 1:S:352:ILE:O    | 1:S:356:THR:HG23 | 1.97                     | 0.63              |
| 1:G:90:GLU:O     | 1:G:91:ASN:HB2   | 1.98                     | 0.63              |
| 1:J:90:GLU:O     | 1:J:91:ASN:HB2   | 1.98                     | 0.63              |
| 2:N:39:VAL:HG13  | 2:N:44:LEU:HD11  | 1.79                     | 0.63              |
| 1:P:174:GLN:HG3  | 1:P:175:PRO:HD3  | 1.79                     | 0.63              |
| 2:Q:213:GLU:OE2  | 2:Q:215:LYS:HE3  | 1.98                     | 0.63              |
| 2:W:17:MET:HG2   | 2:W:152:MET:HE3  | 1.81                     | 0.63              |
| 1:V:115:THR:HG21 | 1:V:151:SER:OG   | 1.99                     | 0.63              |
| 1:P:185:LYS:NZ   | 1:P:429:LEU:O    | 2.30                     | 0.63              |
| 2:E:21:THR:CG2   | 3:F:61:ARG:HH12  | 2.07                     | 0.63              |
| 1:V:292:LEU:HB2  | 1:V:295:VAL:HG22 | 1.79                     | 0.63              |
| 2:K:170:LEU:CD1  | 2:K:223:VAL:HG21 | 2.29                     | 0.63              |
| 2:Q:95:SER:HB3   | 2:Q:127:GLU:HB2  | 1.81                     | 0.63              |
| 1:V:190:ARG:HD2  | 1:V:455:GLU:OE2  | 1.99                     | 0.62              |
| 2:B:330:PHE:CE1  | 2:B:344:VAL:HG13 | 2.34                     | 0.62              |
| 1:G:95:PRO:HG2   | 2:H:46:MET:CE    | 2.30                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:163:SER:HB3  | 1:J:209:PHE:HB2  | 1.81                     | 0.62              |
| 2:H:23:MET:CE    | 2:H:126:ILE:HG21 | 2.29                     | 0.62              |
| 2:E:39:VAL:HG22  | 2:E:44:LEU:HG    | 1.81                     | 0.62              |
| 2:T:17:MET:HE1   | 2:T:57:ALA:CA    | 2.27                     | 0.62              |
| 2:B:40:CYS:O     | 2:B:44:LEU:CB    | 2.47                     | 0.62              |
| 2:B:109:LEU:HD11 | 2:B:169:PHE:HA   | 1.82                     | 0.62              |
| 1:V:118:ASP:OD2  | 1:V:147:SER:HA   | 2.00                     | 0.62              |
| 1:V:350:ARG:NH1  | 3:X:29:GLN:OE1   | 2.33                     | 0.62              |
| 2:E:170:LEU:HD12 | 2:E:223:VAL:HG21 | 1.80                     | 0.62              |
| 1:G:299:ILE:HG13 | 1:G:419:ILE:HG22 | 1.81                     | 0.62              |
| 1:P:138:TRP:CE2  | 1:P:438:TRP:CH2  | 2.87                     | 0.62              |
| 2:B:97:TYR:O     | 2:B:123:ARG:NH2  | 2.33                     | 0.62              |
| 1:S:306:ALA:HB3  | 1:S:307:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:30:ASP:O     | 1:A:34:GLN:HG3   | 2.00                     | 0.61              |
| 2:K:17:MET:CE    | 2:K:60:TYR:HB3   | 2.29                     | 0.61              |
| 2:H:103:THR:HG22 | 2:H:104:ASN:OD1  | 2.00                     | 0.61              |
| 2:N:17:MET:CE    | 2:N:60:TYR:CB    | 2.79                     | 0.61              |
| 1:P:31:ARG:NE    | 1:P:157:VAL:O    | 2.32                     | 0.61              |
| 2:T:17:MET:HE3   | 2:T:60:TYR:CB    | 2.29                     | 0.61              |
| 2:B:146:ARG:HG2  | 2:B:146:ARG:HH11 | 1.66                     | 0.61              |
| 1:G:262:GLU:OE1  | 1:G:262:GLU:HA   | 2.01                     | 0.61              |
| 2:H:162:THR:HG22 | 2:H:165:GLU:H    | 1.65                     | 0.61              |
| 2:K:17:MET:CE    | 2:K:60:TYR:HB2   | 2.31                     | 0.61              |
| 2:N:17:MET:HE2   | 2:N:60:TYR:CB    | 2.29                     | 0.61              |
| 2:T:61:ALA:HA    | 2:T:152:MET:HE2  | 1.81                     | 0.61              |
| 1:A:78:GLU:N     | 1:A:97:ASP:OD1   | 2.24                     | 0.61              |
| 2:H:201:ARG:HD2  | 2:H:207:GLU:O    | 2.00                     | 0.61              |
| 1:M:138:TRP:CD2  | 1:M:438:TRP:HZ3  | 2.18                     | 0.61              |
| 1:M:299:ILE:N    | 1:M:300:PRO:HD2  | 2.15                     | 0.61              |
| 3:C:23:ILE:O     | 3:C:27:GLN:HG3   | 2.01                     | 0.61              |
| 1:P:3:TRP:CE3    | 1:P:31:ARG:HD2   | 2.36                     | 0.61              |
| 2:N:17:MET:CE    | 2:N:60:TYR:HB3   | 2.30                     | 0.61              |
| 1:V:81:LYS:HE2   | 1:V:91:ASN:HA    | 1.83                     | 0.61              |
| 2:B:39:VAL:HG13  | 2:B:40:CYS:N     | 2.15                     | 0.60              |
| 2:E:310:TYR:HE1  | 2:E:334:VAL:HG11 | 1.66                     | 0.60              |
| 2:B:8:VAL:HG12   | 2:B:158:PRO:HB2  | 1.84                     | 0.60              |
| 1:S:376:ARG:HD2  | 3:U:49:GLU:O     | 2.02                     | 0.60              |
| 2:W:109:LEU:HD11 | 2:W:169:PHE:HA   | 1.82                     | 0.60              |
| 1:M:279:GLU:HG3  | 1:M:468:LYS:NZ   | 2.16                     | 0.60              |
| 1:S:13:LEU:HB3   | 1:S:19:VAL:HG12  | 1.83                     | 0.60              |
| 1:D:88:ILE:HG13  | 1:D:343:GLY:HA3  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:220:PHE:O    | 2:K:223:VAL:HG22 | 2.01                     | 0.60              |
| 2:N:220:PHE:O    | 2:N:223:VAL:HG22 | 2.00                     | 0.60              |
| 1:A:2:LEU:HD23   | 1:A:27:SER:HB2   | 1.83                     | 0.60              |
| 2:H:21:THR:HB    | 3:I:63:ASP:OD1   | 2.02                     | 0.60              |
| 2:H:73:HIS:NE2   | 2:H:103:THR:HB   | 2.16                     | 0.60              |
| 2:H:320:LEU:HD22 | 2:H:326:VAL:HG12 | 1.83                     | 0.60              |
| 1:V:270:LYS:O    | 1:V:274:GLU:HG3  | 2.01                     | 0.60              |
| 1:V:71:VAL:CB    | 1:V:114:LYS:HZ1  | 2.12                     | 0.60              |
| 1:M:88:ILE:HD11  | 1:M:120:PHE:HE2  | 1.63                     | 0.60              |
| 1:D:138:TRP:NE1  | 1:D:438:TRP:HH2  | 1.99                     | 0.59              |
| 1:D:352:ILE:O    | 1:D:356:THR:CG2  | 2.49                     | 0.59              |
| 2:N:346:TRP:O    | 2:N:350:ASP:HB2  | 2.02                     | 0.59              |
| 2:T:396:MET:HG3  | 2:T:406:ILE:HD11 | 1.84                     | 0.59              |
| 1:D:68:PRO:HB3   | 1:D:112:VAL:HG11 | 1.84                     | 0.59              |
| 1:G:81:LYS:HE2   | 1:G:91:ASN:HA    | 1.83                     | 0.59              |
| 1:G:422:VAL:N    | 1:G:423:PRO:HD2  | 2.16                     | 0.59              |
| 3:O:46:GLU:O     | 3:O:47:ASN:HB2   | 2.03                     | 0.59              |
| 1:G:69:ILE:HD11  | 1:G:164:LEU:HD13 | 1.84                     | 0.59              |
| 2:Q:156:THR:CG2  | 2:Q:157:GLU:O    | 2.50                     | 0.59              |
| 3:R:46:GLU:O     | 3:R:47:ASN:HB2   | 2.00                     | 0.59              |
| 1:S:297:TYR:O    | 1:S:300:PRO:HD2  | 2.01                     | 0.59              |
| 1:M:138:TRP:CZ2  | 1:M:438:TRP:CH2  | 2.90                     | 0.59              |
| 2:K:201:ARG:HG3  | 2:K:205:SER:OG   | 2.03                     | 0.59              |
| 2:T:340:PRO:O    | 2:T:344:VAL:HG22 | 2.02                     | 0.59              |
| 1:V:172:ILE:C    | 1:V:175:PRO:HD2  | 2.28                     | 0.59              |
| 2:B:103:THR:HG22 | 2:B:104:ASN:OD1  | 2.03                     | 0.59              |
| 2:K:90:LYS:NZ    | 2:K:128:GLU:OE2  | 2.31                     | 0.59              |
| 2:N:375:LEU:HD13 | 2:N:396:MET:HE1  | 1.84                     | 0.59              |
| 1:D:245:VAL:HG12 | 1:D:459:LEU:HB3  | 1.84                     | 0.59              |
| 1:D:356:THR:HG21 | 3:F:14:ALA:HB2   | 1.85                     | 0.59              |
| 2:H:346:TRP:O    | 2:H:350:ASP:HB2  | 2.02                     | 0.59              |
| 2:K:360:ILE:HD11 | 2:K:366:PRO:HD3  | 1.84                     | 0.59              |
| 1:J:299:ILE:HG13 | 1:J:419:ILE:HG22 | 1.85                     | 0.58              |
| 2:K:103:THR:CG2  | 2:K:104:ASN:OD1  | 2.51                     | 0.58              |
| 2:K:140:THR:OG1  | 3:L:90:ARG:HA    | 2.02                     | 0.58              |
| 2:N:80:ARG:HE    | 2:N:275:ASP:CG   | 2.10                     | 0.58              |
| 1:V:95:PRO:HG2   | 2:W:46:MET:HE3   | 1.83                     | 0.58              |
| 2:B:297:GLU:OE2  | 2:B:302:ARG:HA   | 2.02                     | 0.58              |
| 1:V:438:TRP:CZ3  | 1:V:443:PRO:HG3  | 2.38                     | 0.58              |
| 1:A:25:VAL:CG1   | 1:A:51:LEU:HD12  | 2.34                     | 0.58              |
| 1:S:190:ARG:HG3  | 1:S:190:ARG:HH11 | 1.68                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:W:21:THR:HB    | 3:X:63:ASP:OD1   | 2.03                     | 0.58              |
| 2:H:23:MET:HE2   | 2:H:126:ILE:HG21 | 1.84                     | 0.58              |
| 1:V:172:ILE:O    | 1:V:175:PRO:HD2  | 2.03                     | 0.58              |
| 1:A:306:ALA:HB3  | 1:A:307:PRO:HD3  | 1.84                     | 0.58              |
| 2:E:100:PRO:HB3  | 2:E:123:ARG:NH2  | 2.18                     | 0.58              |
| 2:W:170:LEU:HD12 | 2:W:223:VAL:HG21 | 1.86                     | 0.58              |
| 2:K:170:LEU:HD12 | 2:K:223:VAL:HG21 | 1.85                     | 0.58              |
| 1:D:143:VAL:CG1  | 1:D:145:GLY:H    | 2.17                     | 0.58              |
| 2:B:375:LEU:HD22 | 2:B:396:MET:HE1  | 1.85                     | 0.57              |
| 1:S:194:TYR:CD1  | 1:S:229:LYS:HB3  | 2.39                     | 0.57              |
| 1:G:72:LYS:HA    | 1:G:115:THR:HG22 | 1.86                     | 0.57              |
| 1:G:397:THR:HG23 | 1:G:399:THR:O    | 2.03                     | 0.57              |
| 2:H:95:SER:HB3   | 2:H:127:GLU:CB   | 2.33                     | 0.57              |
| 2:H:95:SER:CB    | 2:H:127:GLU:HB3  | 2.34                     | 0.57              |
| 1:M:306:ALA:HB3  | 1:M:307:PRO:HD3  | 1.86                     | 0.57              |
| 2:N:14:HIS:CD2   | 2:N:127:GLU:OE2  | 2.57                     | 0.57              |
| 1:S:163:SER:HB3  | 1:S:209:PHE:HB2  | 1.84                     | 0.57              |
| 2:T:355:LEU:HD21 | 2:T:365:SER:HB2  | 1.86                     | 0.57              |
| 2:K:360:ILE:CD1  | 2:K:366:PRO:HD3  | 2.34                     | 0.57              |
| 1:D:201:SER:HB2  | 2:E:276:PRO:HG2  | 1.87                     | 0.57              |
| 2:W:17:MET:HE1   | 2:W:60:TYR:HB2   | 1.85                     | 0.57              |
| 1:D:83:THR:HG22  | 1:D:90:GLU:HA    | 1.87                     | 0.57              |
| 1:G:138:TRP:CE2  | 1:G:438:TRP:CZ3  | 2.92                     | 0.57              |
| 1:M:395:PRO:O    | 1:M:420:LEU:HD13 | 2.04                     | 0.57              |
| 1:J:138:TRP:CE2  | 1:J:438:TRP:CZ3  | 2.92                     | 0.57              |
| 1:P:438:TRP:CH2  | 1:P:443:PRO:HG3  | 2.39                     | 0.57              |
| 1:S:138:TRP:CE2  | 1:S:438:TRP:CH2  | 2.93                     | 0.57              |
| 1:S:193:ARG:NH1  | 1:S:232:THR:OG1  | 2.38                     | 0.57              |
| 2:T:170:LEU:CD1  | 2:T:223:VAL:HG21 | 2.34                     | 0.57              |
| 3:F:46:GLU:O     | 3:F:47:ASN:HB2   | 2.05                     | 0.57              |
| 2:W:130:ALA:O    | 2:W:146:ARG:HG2  | 2.05                     | 0.57              |
| 2:E:118:LYS:NZ   | 1:G:291:SER:HB3  | 2.19                     | 0.57              |
| 2:K:374:GLU:O    | 2:K:377:LYS:HB3  | 2.05                     | 0.57              |
| 2:W:252:ASP:CB   | 2:W:255:THR:HG22 | 2.30                     | 0.57              |
| 1:A:292:LEU:O    | 1:A:295:VAL:HG22 | 2.04                     | 0.57              |
| 1:G:329:TYR:CE2  | 3:I:89:PRO:HG3   | 2.40                     | 0.57              |
| 1:J:72:LYS:HA    | 1:J:115:THR:HG22 | 1.87                     | 0.57              |
| 1:A:95:PRO:CG    | 2:B:46:MET:HE1   | 2.35                     | 0.56              |
| 1:J:292:LEU:HB2  | 1:J:295:VAL:HG22 | 1.86                     | 0.56              |
| 2:N:394:LYS:HE2  | 1:P:141:GLU:OE2  | 2.05                     | 0.56              |
| 2:Q:137:GLY:O    | 3:R:90:ARG:NH1   | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:98:GLU:O     | 2:B:98:GLU:HG3   | 2.05                     | 0.56              |
| 1:D:204:ASP:O    | 1:D:205:GLN:HG2  | 2.06                     | 0.56              |
| 1:V:138:TRP:CZ2  | 1:V:438:TRP:CH2  | 2.93                     | 0.56              |
| 2:W:156:THR:CG2  | 2:W:157:GLU:O    | 2.53                     | 0.56              |
| 1:A:376:ARG:HG3  | 1:A:376:ARG:HH11 | 1.69                     | 0.56              |
| 2:B:201:ARG:HD2  | 2:B:207:GLU:O    | 2.05                     | 0.56              |
| 2:E:41:PRO:HB3   | 2:E:46:MET:HE2   | 1.88                     | 0.56              |
| 1:J:397:THR:HG22 | 1:J:399:THR:H    | 1.70                     | 0.56              |
| 1:S:138:TRP:CZ2  | 1:S:438:TRP:CH2  | 2.94                     | 0.56              |
| 1:S:143:VAL:CG1  | 1:S:145:GLY:H    | 2.19                     | 0.56              |
| 1:G:376:ARG:HH11 | 1:G:376:ARG:HG3  | 1.71                     | 0.56              |
| 2:H:80:ARG:HE    | 2:H:275:ASP:CG   | 2.13                     | 0.56              |
| 1:M:299:ILE:HG13 | 1:M:419:ILE:HG22 | 1.88                     | 0.56              |
| 2:Q:252:ASP:HB3  | 2:Q:255:THR:HG23 | 1.87                     | 0.56              |
| 1:V:190:ARG:HD3  | 1:V:241:TRP:HH2  | 1.69                     | 0.56              |
| 2:W:17:MET:HE1   | 2:W:57:ALA:CA    | 2.35                     | 0.56              |
| 2:K:128:GLU:HB2  | 2:K:148:GLY:HA2  | 1.88                     | 0.56              |
| 1:M:245:VAL:HG12 | 1:M:459:LEU:HB3  | 1.87                     | 0.56              |
| 1:P:163:SER:HB3  | 1:P:209:PHE:HB2  | 1.87                     | 0.56              |
| 1:P:172:ILE:HD13 | 1:P:207:GLY:HA3  | 1.88                     | 0.56              |
| 2:Q:95:SER:CB    | 2:Q:127:GLU:HB3  | 2.35                     | 0.56              |
| 2:Q:340:PRO:O    | 2:Q:344:VAL:HG22 | 2.04                     | 0.56              |
| 2:T:128:GLU:HB2  | 2:T:148:GLY:HA2  | 1.86                     | 0.56              |
| 1:P:438:TRP:CZ3  | 1:P:443:PRO:HG3  | 2.40                     | 0.56              |
| 1:V:138:TRP:CE2  | 1:V:438:TRP:CZ3  | 2.93                     | 0.56              |
| 1:D:104:LEU:HD11 | 1:D:164:LEU:HD21 | 1.86                     | 0.56              |
| 1:G:138:TRP:CD2  | 1:G:438:TRP:HZ3  | 2.23                     | 0.56              |
| 1:M:245:VAL:CG1  | 1:M:459:LEU:HB3  | 2.36                     | 0.56              |
| 1:V:162:VAL:HG21 | 1:V:219:VAL:HG21 | 1.88                     | 0.56              |
| 1:V:299:ILE:HG13 | 1:V:419:ILE:HG22 | 1.87                     | 0.56              |
| 1:D:77:VAL:CG2   | 1:D:114:LYS:NZ   | 2.67                     | 0.56              |
| 1:P:178:PHE:HE1  | 1:P:397:THR:HG21 | 1.70                     | 0.56              |
| 1:S:351:ARG:NH1  | 4:S:907:ASN:O    | 2.26                     | 0.56              |
| 1:V:138:TRP:CD2  | 1:V:438:TRP:HZ3  | 2.24                     | 0.56              |
| 1:M:182:ILE:HG12 | 1:M:434:ILE:HD12 | 1.87                     | 0.56              |
| 2:Q:17:MET:HE2   | 2:Q:60:TYR:CB    | 2.35                     | 0.56              |
| 2:E:109:LEU:HD11 | 2:E:169:PHE:HA   | 1.88                     | 0.55              |
| 2:H:17:MET:HE1   | 2:H:60:TYR:CB    | 2.35                     | 0.55              |
| 1:S:292:LEU:O    | 1:S:295:VAL:HG22 | 2.06                     | 0.55              |
| 2:T:156:THR:CG2  | 2:T:157:GLU:O    | 2.51                     | 0.55              |
| 1:D:376:ARG:HD2  | 3:F:49:GLU:O     | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:220:PHE:O    | 2:E:223:VAL:HG22 | 2.07                     | 0.55              |
| 2:T:109:LEU:HD11 | 2:T:169:PHE:HA   | 1.88                     | 0.55              |
| 2:Q:17:MET:HE1   | 2:Q:60:TYR:HB2   | 1.87                     | 0.55              |
| 2:Q:21:THR:HB    | 3:R:63:ASP:OD1   | 2.07                     | 0.55              |
| 1:V:26:GLU:HG3   | 1:V:51:LEU:HD11  | 1.89                     | 0.55              |
| 3:U:23:ILE:O     | 3:U:27:GLN:HG3   | 2.07                     | 0.55              |
| 1:V:138:TRP:CE2  | 1:V:438:TRP:HH2  | 2.25                     | 0.55              |
| 2:N:201:ARG:HD2  | 2:N:207:GLU:O    | 2.07                     | 0.55              |
| 2:W:73:HIS:NE2   | 2:W:103:THR:HB   | 2.21                     | 0.55              |
| 2:T:140:THR:OG1  | 3:U:90:ARG:HA    | 2.05                     | 0.55              |
| 1:P:138:TRP:CE2  | 1:P:438:TRP:CZ3  | 2.95                     | 0.55              |
| 2:Q:21:THR:HG21  | 3:R:61:ARG:NH1   | 2.21                     | 0.55              |
| 1:A:299:ILE:HG13 | 1:A:419:ILE:HG22 | 1.89                     | 0.55              |
| 2:H:156:THR:HG22 | 2:H:157:GLU:N    | 2.21                     | 0.55              |
| 2:K:21:THR:HG21  | 3:L:61:ARG:NH1   | 2.17                     | 0.55              |
| 2:E:21:THR:HG22  | 2:E:22:LYS:O     | 2.07                     | 0.55              |
| 2:E:375:LEU:HD22 | 2:E:396:MET:HE1  | 1.88                     | 0.55              |
| 1:P:143:VAL:HG13 | 1:P:145:GLY:H    | 1.70                     | 0.55              |
| 1:P:352:ILE:O    | 1:P:356:THR:CG2  | 2.50                     | 0.55              |
| 1:D:57:LEU:HD22  | 1:D:65:PHE:CE1   | 2.42                     | 0.55              |
| 1:D:81:LYS:HE2   | 1:D:91:ASN:HA    | 1.89                     | 0.55              |
| 1:G:138:TRP:CZ2  | 1:G:438:TRP:CH2  | 2.95                     | 0.55              |
| 1:S:1:MET:O      | 1:S:1:MET:HG2    | 2.06                     | 0.55              |
| 3:X:33:ILE:O     | 3:X:37:ILE:HG12  | 2.07                     | 0.55              |
| 1:G:138:TRP:CE2  | 1:G:438:TRP:CH2  | 2.95                     | 0.54              |
| 2:K:255:THR:HG21 | 2:K:259:TYR:OH   | 2.07                     | 0.54              |
| 2:Q:230:GLU:OE2  | 2:Q:233:ARG:NH1  | 2.40                     | 0.54              |
| 2:W:252:ASP:OD2  | 2:W:255:THR:HG22 | 2.07                     | 0.54              |
| 2:W:162:THR:HG22 | 2:W:164:GLU:H    | 1.72                     | 0.54              |
| 1:A:174:GLN:CB   | 1:A:175:PRO:HD3  | 2.37                     | 0.54              |
| 2:E:40:CYS:O     | 2:E:44:LEU:HB2   | 2.07                     | 0.54              |
| 2:E:162:THR:HG22 | 2:E:164:GLU:H    | 1.72                     | 0.54              |
| 1:G:356:THR:HG21 | 3:I:14:ALA:HB2   | 1.88                     | 0.54              |
| 1:M:138:TRP:CE2  | 1:M:438:TRP:CZ3  | 2.96                     | 0.54              |
| 1:V:143:VAL:HG13 | 1:V:145:GLY:H    | 1.72                     | 0.54              |
| 2:H:255:THR:HG21 | 2:H:259:TYR:OH   | 2.07                     | 0.54              |
| 2:T:162:THR:HG22 | 2:T:164:GLU:H    | 1.73                     | 0.54              |
| 2:W:8:VAL:HG12   | 2:W:158:PRO:HB2  | 1.89                     | 0.54              |
| 1:A:115:THR:HG21 | 1:A:151:SER:OG   | 2.06                     | 0.54              |
| 2:B:310:TYR:CE1  | 2:B:334:VAL:HG11 | 2.43                     | 0.54              |
| 3:C:39:GLN:O     | 3:C:42:GLU:HG3   | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:139:LYS:HG2  | 3:F:87:VAL:CG1   | 2.38                     | 0.54              |
| 1:G:126:THR:O    | 1:G:126:THR:HG22 | 2.07                     | 0.54              |
| 1:J:138:TRP:CD2  | 1:J:438:TRP:HZ3  | 2.25                     | 0.54              |
| 1:V:185:LYS:NZ   | 1:V:186:PRO:O    | 2.39                     | 0.54              |
| 1:A:25:VAL:HG11  | 1:A:51:LEU:HD12  | 1.89                     | 0.54              |
| 1:P:3:TRP:CZ3    | 1:P:31:ARG:HD2   | 2.43                     | 0.54              |
| 1:P:370:LYS:NZ   | 3:R:45:THR:HB    | 2.22                     | 0.54              |
| 1:D:1:MET:HE2    | 1:D:3:TRP:HE1    | 1.73                     | 0.54              |
| 2:E:96:GLN:HB2   | 2:E:125:HIS:HB2  | 1.90                     | 0.54              |
| 2:K:39:VAL:HG13  | 2:K:44:LEU:HD11  | 1.88                     | 0.54              |
| 1:D:104:LEU:HD11 | 1:D:164:LEU:CD2  | 2.38                     | 0.54              |
| 2:E:128:GLU:HB2  | 2:E:148:GLY:HA2  | 1.90                     | 0.54              |
| 2:Q:220:PHE:O    | 2:Q:223:VAL:HG22 | 2.07                     | 0.54              |
| 1:A:142:ARG:NH2  | 1:A:403:LYS:HE3  | 2.23                     | 0.54              |
| 1:G:100:VAL:HG12 | 1:G:223:ILE:HB   | 1.90                     | 0.54              |
| 2:H:17:MET:CE    | 2:H:60:TYR:HB2   | 2.38                     | 0.54              |
| 2:Q:374:GLU:OE1  | 2:Q:402:THR:HG22 | 2.08                     | 0.54              |
| 1:S:322:TYR:CZ   | 2:T:47:PRO:HD3   | 2.43                     | 0.54              |
| 1:V:60:ARG:HA    | 1:V:65:PHE:CD1   | 2.43                     | 0.54              |
| 1:A:185:LYS:NZ   | 1:A:429:LEU:O    | 2.42                     | 0.53              |
| 2:Q:85:TYR:HD2   | 2:Q:87:ASP:OD1   | 1.91                     | 0.53              |
| 2:W:128:GLU:HB2  | 2:W:148:GLY:HA2  | 1.91                     | 0.53              |
| 2:E:113:ASN:ND2  | 2:E:115:GLU:HG2  | 2.23                     | 0.53              |
| 1:P:81:LYS:HE2   | 1:P:91:ASN:HA    | 1.89                     | 0.53              |
| 2:B:40:CYS:SG    | 2:B:41:PRO:HD2   | 2.48                     | 0.53              |
| 1:D:245:VAL:CG1  | 1:D:459:LEU:HB3  | 2.39                     | 0.53              |
| 2:K:17:MET:HE2   | 2:K:60:TYR:HB2   | 1.90                     | 0.53              |
| 1:P:174:GLN:HG3  | 1:P:175:PRO:CD   | 2.38                     | 0.53              |
| 2:T:95:SER:HB3   | 2:T:127:GLU:OE1  | 2.09                     | 0.53              |
| 2:B:360:ILE:HD11 | 2:B:365:SER:HA   | 1.90                     | 0.53              |
| 1:P:16:ARG:HB2   | 1:P:18:GLU:OE2   | 2.08                     | 0.53              |
| 2:Q:21:THR:HG23  | 3:R:61:ARG:HH12  | 1.72                     | 0.53              |
| 2:T:146:ARG:HH11 | 2:T:146:ARG:HG2  | 1.73                     | 0.53              |
| 1:V:163:SER:HB3  | 1:V:209:PHE:HB2  | 1.91                     | 0.53              |
| 1:A:138:TRP:NE1  | 1:A:438:TRP:HH2  | 2.06                     | 0.53              |
| 1:P:90:GLU:O     | 1:P:91:ASN:HB2   | 2.08                     | 0.53              |
| 1:S:8:SER:HA     | 1:S:11:ARG:HH21  | 1.73                     | 0.53              |
| 1:S:69:ILE:HD11  | 1:S:164:LEU:HD13 | 1.90                     | 0.53              |
| 1:S:69:ILE:HD12  | 1:S:162:VAL:HG13 | 1.91                     | 0.53              |
| 2:T:8:VAL:HG12   | 2:T:158:PRO:HB2  | 1.90                     | 0.53              |
| 1:A:60:ARG:HA    | 1:A:65:PHE:CD1   | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:252:ASP:HB3  | 2:K:255:THR:CG2  | 2.38                     | 0.53              |
| 1:S:64:LEU:HD21  | 1:S:218:LEU:HG   | 1.90                     | 0.53              |
| 2:W:337:PHE:CE2  | 2:W:377:LYS:HA   | 2.44                     | 0.53              |
| 2:W:348:ILE:HA   | 2:W:352:LEU:HD22 | 1.90                     | 0.53              |
| 1:M:90:GLU:O     | 1:M:91:ASN:CB    | 2.57                     | 0.53              |
| 1:A:118:ASP:OD1  | 1:A:126:THR:HA   | 2.09                     | 0.53              |
| 1:G:418:ASP:O    | 1:G:422:VAL:HG13 | 2.09                     | 0.53              |
| 1:G:418:ASP:HB3  | 1:G:422:VAL:HG13 | 1.91                     | 0.53              |
| 2:K:85:TYR:OH    | 3:L:91:VAL:CG1   | 2.57                     | 0.53              |
| 1:P:178:PHE:CE1  | 1:P:397:THR:HG21 | 2.43                     | 0.53              |
| 1:S:201:SER:HB2  | 2:T:276:PRO:HG2  | 1.90                     | 0.53              |
| 2:W:162:THR:HG22 | 2:W:164:GLU:N    | 2.24                     | 0.53              |
| 2:B:184:LYS:HB2  | 2:B:191:GLN:OE1  | 2.09                     | 0.52              |
| 1:D:322:TYR:CZ   | 2:E:47:PRO:HD3   | 2.43                     | 0.52              |
| 2:E:77:VAL:HG23  | 2:E:99:LYS:HD2   | 1.91                     | 0.52              |
| 2:N:90:LYS:NZ    | 2:N:128:GLU:OE2  | 2.42                     | 0.52              |
| 2:Q:128:GLU:HB2  | 2:Q:148:GLY:HA2  | 1.90                     | 0.52              |
| 2:T:370:GLU:CD   | 2:T:370:GLU:H    | 2.17                     | 0.52              |
| 2:W:17:MET:HE3   | 2:W:60:TYR:HB3   | 1.88                     | 0.52              |
| 2:E:252:ASP:CB   | 2:E:255:THR:HG22 | 2.35                     | 0.52              |
| 1:M:338:ARG:HG3  | 3:O:17:GLU:OE1   | 2.09                     | 0.52              |
| 2:T:96:GLN:HB2   | 2:T:125:HIS:HB2  | 1.90                     | 0.52              |
| 2:W:220:PHE:O    | 2:W:223:VAL:HG22 | 2.09                     | 0.52              |
| 2:B:170:LEU:HD12 | 2:B:223:VAL:HG21 | 1.91                     | 0.52              |
| 2:H:85:TYR:HD2   | 2:H:87:ASP:OD1   | 1.92                     | 0.52              |
| 2:N:74:GLU:HG2   | 2:N:283:VAL:O    | 2.08                     | 0.52              |
| 2:N:167:ARG:HG3  | 2:N:220:PHE:HB3  | 1.92                     | 0.52              |
| 2:W:396:MET:HG3  | 2:W:406:ILE:HD11 | 1.92                     | 0.52              |
| 1:S:138:TRP:CE2  | 1:S:438:TRP:CZ3  | 2.97                     | 0.52              |
| 1:V:339:THR:HG23 | 1:V:340:ARG:N    | 2.24                     | 0.52              |
| 3:X:21:GLU:O     | 3:X:25:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:46:LEU:HG    | 1:A:113:GLY:HA2  | 1.90                     | 0.52              |
| 1:D:90:GLU:O     | 1:D:91:ASN:HB2   | 2.10                     | 0.52              |
| 2:E:85:TYR:HD2   | 2:E:87:ASP:OD1   | 1.93                     | 0.52              |
| 2:K:73:HIS:NE2   | 2:K:103:THR:HB   | 2.25                     | 0.52              |
| 2:Q:170:LEU:CD1  | 2:Q:223:VAL:HG21 | 2.38                     | 0.52              |
| 2:E:17:MET:HE1   | 2:E:57:ALA:C     | 2.34                     | 0.52              |
| 2:H:146:ARG:HH11 | 2:H:146:ARG:HG2  | 1.75                     | 0.52              |
| 2:K:372:LEU:O    | 2:K:376:VAL:HG23 | 2.10                     | 0.52              |
| 3:L:28:LYS:NZ    | 3:L:32:ASP:OD2   | 2.43                     | 0.52              |
| 1:S:463:TYR:O    | 1:S:467:GLN:HG2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:W:96:GLN:HB2   | 2:W:125:HIS:HB2  | 1.92                     | 0.52              |
| 2:B:17:MET:HE1   | 2:B:57:ALA:C     | 2.33                     | 0.52              |
| 2:B:252:ASP:OD2  | 2:B:255:THR:HG22 | 2.09                     | 0.52              |
| 2:B:310:TYR:HE1  | 2:B:334:VAL:HG11 | 1.74                     | 0.52              |
| 2:B:396:MET:HG3  | 2:B:406:ILE:HD11 | 1.90                     | 0.52              |
| 1:D:199:PHE:CD1  | 1:D:199:PHE:C    | 2.87                     | 0.52              |
| 2:E:222:PHE:CZ   | 2:E:253:PRO:HB3  | 2.45                     | 0.52              |
| 2:H:23:MET:HE2   | 2:H:126:ILE:CG2  | 2.40                     | 0.52              |
| 2:H:123:ARG:NH1  | 2:H:125:HIS:CE1  | 2.77                     | 0.52              |
| 2:Q:140:THR:OG1  | 3:R:90:ARG:HA    | 2.10                     | 0.52              |
| 1:A:167:ASP:HB2  | 1:A:172:ILE:HD12 | 1.92                     | 0.52              |
| 2:H:17:MET:HE1   | 2:H:61:ALA:N     | 2.25                     | 0.52              |
| 1:J:292:LEU:CB   | 1:J:295:VAL:HG22 | 2.40                     | 0.52              |
| 1:V:181:VAL:HG13 | 1:V:210:GLY:O    | 2.09                     | 0.52              |
| 1:A:98:ALA:HA    | 1:A:195:GLY:HA3  | 1.92                     | 0.52              |
| 2:B:211:ARG:HD3  | 5:B:701:ADP:C5   | 2.45                     | 0.52              |
| 2:H:14:HIS:CD2   | 2:H:127:GLU:OE2  | 2.63                     | 0.52              |
| 1:J:178:PHE:CE1  | 1:J:397:THR:HG21 | 2.45                     | 0.52              |
| 2:Q:95:SER:HB3   | 2:Q:127:GLU:HB3  | 1.91                     | 0.52              |
| 1:V:292:LEU:HB2  | 1:V:295:VAL:CG2  | 2.40                     | 0.52              |
| 1:D:299:ILE:HG13 | 1:D:419:ILE:HG22 | 1.90                     | 0.52              |
| 2:E:95:SER:CB    | 2:E:127:GLU:HB3  | 2.39                     | 0.52              |
| 1:M:422:VAL:N    | 1:M:423:PRO:CD   | 2.73                     | 0.52              |
| 2:T:252:ASP:OD2  | 2:T:255:THR:HG22 | 2.10                     | 0.52              |
| 1:V:292:LEU:O    | 1:V:295:VAL:HG22 | 2.10                     | 0.52              |
| 1:D:77:VAL:HG23  | 1:D:114:LYS:HZ1  | 1.71                     | 0.51              |
| 2:E:146:ARG:HH11 | 2:E:146:ARG:HG2  | 1.74                     | 0.51              |
| 1:J:438:TRP:CZ3  | 1:J:443:PRO:HG3  | 2.46                     | 0.51              |
| 2:K:85:TYR:HD2   | 2:K:87:ASP:OD1   | 1.93                     | 0.51              |
| 2:K:252:ASP:HB3  | 2:K:255:THR:HG22 | 1.91                     | 0.51              |
| 2:Q:17:MET:CE    | 2:Q:60:TYR:HB3   | 2.38                     | 0.51              |
| 2:T:170:LEU:HD12 | 2:T:223:VAL:HG21 | 1.90                     | 0.51              |
| 1:V:203:LEU:HD23 | 1:V:375:ARG:NH2  | 2.25                     | 0.51              |
| 2:E:396:MET:HG3  | 2:E:406:ILE:HD11 | 1.92                     | 0.51              |
| 1:J:90:GLU:O     | 1:J:91:ASN:CB    | 2.58                     | 0.51              |
| 2:T:360:ILE:HD11 | 2:T:365:SER:HA   | 1.91                     | 0.51              |
| 2:B:128:GLU:HB2  | 2:B:148:GLY:HA2  | 1.92                     | 0.51              |
| 1:D:422:VAL:N    | 1:D:423:PRO:CD   | 2.74                     | 0.51              |
| 2:Q:74:GLU:HG2   | 2:Q:283:VAL:O    | 2.09                     | 0.51              |
| 2:Q:201:ARG:HG3  | 2:Q:205:SER:OG   | 2.10                     | 0.51              |
| 1:A:95:PRO:HG2   | 2:B:46:MET:CE    | 2.38                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:71:VAL:HG11  | 1:D:101:ILE:HD11 | 1.93                     | 0.51              |
| 2:H:39:VAL:HG13  | 2:H:44:LEU:HD11  | 1.93                     | 0.51              |
| 2:N:128:GLU:HB2  | 2:N:148:GLY:HA2  | 1.93                     | 0.51              |
| 2:B:98:GLU:O     | 2:B:99:LYS:HB2   | 2.11                     | 0.51              |
| 1:V:190:ARG:HD3  | 1:V:241:TRP:CH2  | 2.46                     | 0.51              |
| 1:A:155:VAL:HG21 | 1:A:163:SER:HB3  | 1.93                     | 0.51              |
| 2:B:252:ASP:HB3  | 2:B:255:THR:CG2  | 2.38                     | 0.51              |
| 1:D:306:ALA:HB3  | 1:D:307:PRO:HD3  | 1.93                     | 0.51              |
| 1:J:47:TYR:CD2   | 1:J:112:VAL:HG22 | 2.45                     | 0.51              |
| 2:N:282:LYS:HD3  | 3:O:55:PHE:CZ    | 2.46                     | 0.51              |
| 1:S:100:VAL:HG12 | 1:S:223:ILE:HB   | 1.93                     | 0.51              |
| 1:J:374:VAL:O    | 1:J:378:ILE:HG13 | 2.11                     | 0.51              |
| 2:N:302:ARG:HD3  | 2:N:321:VAL:HG22 | 1.93                     | 0.51              |
| 1:A:199:PHE:CD1  | 1:A:199:PHE:C    | 2.89                     | 0.51              |
| 2:K:17:MET:HG2   | 2:K:152:MET:HE2  | 1.92                     | 0.51              |
| 1:V:292:LEU:CB   | 1:V:295:VAL:HG22 | 2.41                     | 0.51              |
| 2:B:142:VAL:HB   | 3:C:86:PHE:HB2   | 1.92                     | 0.51              |
| 2:E:170:LEU:CD1  | 2:E:223:VAL:HG21 | 2.40                     | 0.51              |
| 3:F:7:VAL:HG21   | 3:F:27:GLN:HG2   | 1.93                     | 0.51              |
| 1:G:199:PHE:C    | 1:G:199:PHE:CD1  | 2.88                     | 0.51              |
| 2:W:263:THR:HB   | 2:W:265:GLU:HG3  | 1.92                     | 0.51              |
| 1:D:138:TRP:CD2  | 1:D:438:TRP:CZ3  | 2.99                     | 0.50              |
| 2:E:21:THR:CG2   | 2:E:22:LYS:N     | 2.74                     | 0.50              |
| 2:E:340:PRO:O    | 2:E:344:VAL:HG22 | 2.11                     | 0.50              |
| 1:V:279:GLU:HG3  | 1:V:468:LYS:HZ3  | 1.75                     | 0.50              |
| 2:H:17:MET:HG2   | 2:H:152:MET:HE2  | 1.92                     | 0.50              |
| 2:K:162:THR:HG22 | 2:K:165:GLU:H    | 1.77                     | 0.50              |
| 2:T:100:PRO:HB3  | 2:T:123:ARG:NH1  | 2.26                     | 0.50              |
| 2:T:106:TRP:CD1  | 2:T:118:LYS:HE2  | 2.46                     | 0.50              |
| 2:E:156:THR:HG22 | 2:E:157:GLU:N    | 2.26                     | 0.50              |
| 2:T:22:LYS:HD2   | 2:T:27:CYS:HB2   | 1.92                     | 0.50              |
| 1:D:265:LEU:HD11 | 1:D:395:PRO:HG2  | 1.93                     | 0.50              |
| 1:G:72:LYS:HD3   | 1:G:74:ASN:OD1   | 2.12                     | 0.50              |
| 2:N:17:MET:CE    | 2:N:60:TYR:HB2   | 2.41                     | 0.50              |
| 1:S:104:LEU:HD11 | 1:S:164:LEU:HD21 | 1.93                     | 0.50              |
| 1:G:422:VAL:N    | 1:G:423:PRO:HD3  | 2.25                     | 0.50              |
| 1:A:151:SER:HB3  | 1:A:163:SER:OG   | 2.11                     | 0.50              |
| 1:A:403:LYS:O    | 1:A:406:GLU:HB2  | 2.12                     | 0.50              |
| 1:D:123:GLY:N    | 4:D:902:ASN:OXT  | 2.45                     | 0.50              |
| 1:M:86:SER:HB2   | 1:M:119:GLU:HG3  | 1.93                     | 0.50              |
| 1:M:138:TRP:CD2  | 1:M:438:TRP:CZ3  | 2.98                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:90:GLU:O     | 1:S:91:ASN:HB2   | 2.12                     | 0.50              |
| 1:V:360:SER:HA   | 2:W:269:ASP:OD2  | 2.12                     | 0.50              |
| 1:V:384:LYS:O    | 1:V:387:GLU:HB2  | 2.12                     | 0.50              |
| 1:G:178:PHE:HE1  | 1:G:397:THR:HG21 | 1.76                     | 0.50              |
| 1:J:438:TRP:CH2  | 1:J:443:PRO:HG3  | 2.46                     | 0.50              |
| 2:K:40:CYS:HB2   | 2:K:41:PRO:HD2   | 1.93                     | 0.50              |
| 2:K:375:LEU:HD13 | 2:K:396:MET:HE1  | 1.92                     | 0.50              |
| 1:M:329:TYR:CE2  | 3:O:89:PRO:HG3   | 2.46                     | 0.50              |
| 1:P:167:ASP:HA   | 1:P:171:SER:HB2  | 1.94                     | 0.50              |
| 1:S:298:SER:HB3  | 1:S:422:VAL:HG23 | 1.94                     | 0.50              |
| 2:T:77:VAL:HG23  | 2:T:99:LYS:HD2   | 1.94                     | 0.50              |
| 2:E:119:VAL:HG12 | 2:E:156:THR:HG23 | 1.93                     | 0.50              |
| 2:K:17:MET:HE1   | 2:K:60:TYR:HB2   | 1.94                     | 0.50              |
| 1:M:279:GLU:HG3  | 1:M:468:LYS:HZ1  | 1.75                     | 0.50              |
| 1:S:190:ARG:HG3  | 1:S:190:ARG:NH1  | 2.27                     | 0.50              |
| 2:T:167:ARG:HG3  | 2:T:220:PHE:HB3  | 1.92                     | 0.50              |
| 1:V:279:GLU:HG3  | 1:V:468:LYS:HZ1  | 1.76                     | 0.50              |
| 2:B:59:GLU:OE2   | 2:B:63:ARG:NH2   | 2.44                     | 0.49              |
| 1:J:162:VAL:HG11 | 1:J:219:VAL:HG21 | 1.94                     | 0.49              |
| 2:N:96:GLN:HB2   | 2:N:125:HIS:HB2  | 1.94                     | 0.49              |
| 1:A:118:ASP:OD1  | 1:A:126:THR:CA   | 2.60                     | 0.49              |
| 1:J:167:ASP:HA   | 1:J:171:SER:HB2  | 1.94                     | 0.49              |
| 2:Q:73:HIS:NE2   | 2:Q:103:THR:HB   | 2.27                     | 0.49              |
| 1:S:245:VAL:CG1  | 1:S:459:LEU:HB3  | 2.42                     | 0.49              |
| 2:T:23:MET:HE2   | 2:T:126:ILE:HG21 | 1.94                     | 0.49              |
| 2:T:39:VAL:HG13  | 2:T:44:LEU:HD11  | 1.93                     | 0.49              |
| 2:T:77:VAL:CG2   | 2:T:99:LYS:HD2   | 2.42                     | 0.49              |
| 1:D:291:SER:HB3  | 2:H:118:LYS:NZ   | 2.27                     | 0.49              |
| 2:N:197:ASN:HB3  | 2:N:211:ARG:HD2  | 1.95                     | 0.49              |
| 1:D:279:GLU:HG3  | 1:D:468:LYS:NZ   | 2.27                     | 0.49              |
| 1:D:463:TYR:O    | 1:D:467:GLN:HG2  | 2.12                     | 0.49              |
| 2:E:280:PRO:HD2  | 3:F:55:PHE:CZ    | 2.47                     | 0.49              |
| 2:H:128:GLU:HB2  | 2:H:148:GLY:HA2  | 1.93                     | 0.49              |
| 2:K:340:PRO:O    | 2:K:344:VAL:HG22 | 2.12                     | 0.49              |
| 1:G:373:LYS:HE2  | 3:I:50:PRO:HD3   | 1.93                     | 0.49              |
| 1:G:376:ARG:HG3  | 1:G:376:ARG:NH1  | 2.26                     | 0.49              |
| 2:Q:375:LEU:HD22 | 2:Q:396:MET:HE1  | 1.93                     | 0.49              |
| 2:E:21:THR:HG22  | 2:E:22:LYS:N     | 2.27                     | 0.49              |
| 2:E:22:LYS:HD2   | 2:E:27:CYS:HB2   | 1.95                     | 0.49              |
| 1:J:172:ILE:HD13 | 1:J:207:GLY:HA3  | 1.95                     | 0.49              |
| 2:K:85:TYR:CZ    | 3:L:91:VAL:HG11  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:81:LYS:HE2   | 1:S:91:ASN:CA    | 2.38                     | 0.49              |
| 1:V:116:ASN:ND2  | 1:V:132:PHE:O    | 2.45                     | 0.49              |
| 3:X:46:GLU:O     | 3:X:47:ASN:HB2   | 2.13                     | 0.49              |
| 1:A:7:LEU:HD22   | 1:A:67:ILE:HD12  | 1.95                     | 0.49              |
| 1:A:138:TRP:CZ2  | 1:A:438:TRP:CH2  | 3.01                     | 0.49              |
| 2:H:197:ASN:HB3  | 2:H:211:ARG:HD2  | 1.95                     | 0.49              |
| 1:S:464:LEU:HD12 | 1:S:464:LEU:O    | 2.13                     | 0.49              |
| 2:T:95:SER:CB    | 2:T:127:GLU:HB3  | 2.42                     | 0.49              |
| 1:V:318:ASP:HB2  | 1:V:336:TYR:HE1  | 1.78                     | 0.49              |
| 1:A:190:ARG:HD2  | 1:A:455:GLU:OE2  | 2.13                     | 0.49              |
| 2:B:280:PRO:HD2  | 3:C:55:PHE:CZ    | 2.48                     | 0.49              |
| 2:Q:360:ILE:CD1  | 2:Q:366:PRO:HD3  | 2.43                     | 0.49              |
| 2:E:140:THR:OG1  | 3:F:90:ARG:HA    | 2.13                     | 0.49              |
| 1:J:329:TYR:CE2  | 3:L:89:PRO:HG3   | 2.47                     | 0.49              |
| 1:M:201:SER:HB2  | 2:N:276:PRO:HG2  | 1.95                     | 0.49              |
| 1:M:298:SER:HB3  | 1:M:422:VAL:HG23 | 1.94                     | 0.49              |
| 2:N:156:THR:HG22 | 2:N:157:GLU:N    | 2.27                     | 0.49              |
| 1:P:384:LYS:O    | 1:P:387:GLU:HB2  | 2.13                     | 0.49              |
| 1:S:395:PRO:O    | 1:S:420:LEU:HD13 | 2.12                     | 0.49              |
| 1:V:432:ILE:HG12 | 1:V:434:ILE:HD13 | 1.93                     | 0.49              |
| 2:H:340:PRO:O    | 2:H:344:VAL:HG22 | 2.12                     | 0.49              |
| 1:J:156:ALA:O    | 1:J:211:ARG:NH1  | 2.46                     | 0.49              |
| 1:M:88:ILE:HD11  | 1:M:120:PHE:HZ   | 1.75                     | 0.49              |
| 1:S:297:TYR:C    | 1:S:300:PRO:HD2  | 2.38                     | 0.49              |
| 2:W:56:ARG:HD2   | 3:X:63:ASP:OD2   | 2.13                     | 0.49              |
| 2:B:220:PHE:O    | 2:B:223:VAL:HG22 | 2.13                     | 0.48              |
| 2:H:17:MET:HE1   | 2:H:60:TYR:HB2   | 1.94                     | 0.48              |
| 2:K:21:THR:HB    | 3:L:63:ASP:OD1   | 2.12                     | 0.48              |
| 1:A:397:THR:HG22 | 1:A:398:PRO:HD2  | 1.95                     | 0.48              |
| 1:D:143:VAL:HG13 | 1:D:145:GLY:H    | 1.79                     | 0.48              |
| 2:E:402:THR:HG22 | 2:E:403:PRO:HD2  | 1.95                     | 0.48              |
| 1:P:138:TRP:CD2  | 1:P:438:TRP:HZ3  | 2.31                     | 0.48              |
| 2:E:17:MET:HG2   | 2:E:152:MET:HE2  | 1.93                     | 0.48              |
| 1:J:330:LYS:HG2  | 1:J:334:GLU:CD   | 2.38                     | 0.48              |
| 2:N:22:LYS:HD2   | 2:N:27:CYS:HB2   | 1.94                     | 0.48              |
| 2:Q:170:LEU:HD12 | 2:Q:223:VAL:HG21 | 1.94                     | 0.48              |
| 1:V:162:VAL:HG22 | 1:V:163:SER:H    | 1.77                     | 0.48              |
| 2:W:375:LEU:HD22 | 2:W:396:MET:HE1  | 1.94                     | 0.48              |
| 1:A:172:ILE:HD13 | 1:A:207:GLY:HA3  | 1.95                     | 0.48              |
| 2:H:170:LEU:HD12 | 2:H:223:VAL:HG21 | 1.95                     | 0.48              |
| 2:N:83:TYR:CZ    | 2:N:88:LEU:HD22  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:167:ASP:HB3  | 1:P:185:LYS:HG3  | 1.94                     | 0.48              |
| 2:T:8:VAL:HG13   | 2:T:161:ARG:HH12 | 1.79                     | 0.48              |
| 2:T:348:ILE:HA   | 2:T:352:LEU:HD22 | 1.96                     | 0.48              |
| 1:D:403:LYS:O    | 1:D:406:GLU:HB2  | 2.14                     | 0.48              |
| 2:H:167:ARG:HG3  | 2:H:220:PHE:HB3  | 1.93                     | 0.48              |
| 2:N:17:MET:HG2   | 2:N:152:MET:HE2  | 1.94                     | 0.48              |
| 2:N:282:LYS:HD3  | 3:O:55:PHE:CE2   | 2.49                     | 0.48              |
| 2:Q:39:VAL:HG13  | 2:Q:44:LEU:HD11  | 1.94                     | 0.48              |
| 1:S:172:ILE:HD13 | 1:S:207:GLY:HA3  | 1.95                     | 0.48              |
| 1:V:77:VAL:CG2   | 1:V:114:LYS:HZ3  | 2.24                     | 0.48              |
| 1:A:5:LYS:HB2    | 1:A:10:LEU:HD13  | 1.94                     | 0.48              |
| 1:A:321:ARG:HD2  | 2:B:44:LEU:O     | 2.14                     | 0.48              |
| 1:D:157:VAL:HG23 | 1:D:159:SER:H    | 1.77                     | 0.48              |
| 2:E:118:LYS:HZ1  | 1:G:291:SER:CB   | 2.27                     | 0.48              |
| 2:H:96:GLN:HB2   | 2:H:125:HIS:HB2  | 1.94                     | 0.48              |
| 1:P:138:TRP:CE2  | 1:P:438:TRP:HH2  | 2.32                     | 0.48              |
| 2:Q:17:MET:HE1   | 2:Q:57:ALA:O     | 2.13                     | 0.48              |
| 2:Q:372:LEU:O    | 2:Q:376:VAL:HG23 | 2.13                     | 0.48              |
| 1:V:88:ILE:HA    | 1:V:324:TYR:HB3  | 1.95                     | 0.48              |
| 2:W:142:VAL:HB   | 3:X:86:PHE:HB2   | 1.95                     | 0.48              |
| 2:K:167:ARG:HG3  | 2:K:220:PHE:HB3  | 1.96                     | 0.48              |
| 1:M:376:ARG:HG3  | 1:M:376:ARG:NH1  | 2.24                     | 0.48              |
| 1:S:2:LEU:HB3    | 1:S:27:SER:OG    | 2.13                     | 0.48              |
| 1:S:199:PHE:C    | 1:S:199:PHE:CD1  | 2.92                     | 0.48              |
| 1:V:98:ALA:HA    | 1:V:195:GLY:HA3  | 1.95                     | 0.48              |
| 1:D:163:SER:HB3  | 1:D:209:PHE:HB2  | 1.95                     | 0.48              |
| 2:E:17:MET:HE3   | 2:E:60:TYR:HB3   | 1.91                     | 0.48              |
| 2:N:8:VAL:HG12   | 2:N:158:PRO:HB2  | 1.94                     | 0.48              |
| 1:P:28:PHE:CD2   | 1:P:68:PRO:HG2   | 2.49                     | 0.48              |
| 2:Q:360:ILE:HD11 | 2:Q:366:PRO:HD3  | 1.95                     | 0.48              |
| 2:B:39:VAL:HG13  | 2:B:40:CYS:H     | 1.76                     | 0.47              |
| 2:B:100:PRO:CB   | 2:B:123:ARG:HH21 | 2.18                     | 0.47              |
| 2:H:230:GLU:OE2  | 2:H:233:ARG:NH1  | 2.47                     | 0.47              |
| 1:M:297:TYR:CE2  | 3:O:43:LEU:HD21  | 2.48                     | 0.47              |
| 1:S:245:VAL:HG12 | 1:S:459:LEU:HB3  | 1.95                     | 0.47              |
| 2:K:252:ASP:CG   | 2:K:255:THR:HG22 | 2.39                     | 0.47              |
| 1:S:190:ARG:HD2  | 1:S:455:GLU:OE2  | 2.13                     | 0.47              |
| 2:H:8:VAL:CG1    | 2:H:158:PRO:HB2  | 2.44                     | 0.47              |
| 2:N:85:TYR:HD2   | 2:N:87:ASP:OD1   | 1.97                     | 0.47              |
| 3:O:36:PHE:O     | 3:O:39:GLN:NE2   | 2.43                     | 0.47              |
| 2:Q:355:LEU:HD21 | 2:Q:365:SER:HB2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:17:MET:HG2   | 2:T:152:MET:HE3  | 1.96                     | 0.47              |
| 2:W:233:ARG:HD2  | 2:W:249:ARG:NH2  | 2.29                     | 0.47              |
| 1:D:398:PRO:HG3  | 1:D:419:ILE:HD11 | 1.97                     | 0.47              |
| 1:G:163:SER:HB3  | 1:G:209:PHE:HB2  | 1.96                     | 0.47              |
| 2:N:170:LEU:HB3  | 2:N:220:PHE:CE1  | 2.48                     | 0.47              |
| 2:Q:374:GLU:O    | 2:Q:377:LYS:HB3  | 2.14                     | 0.47              |
| 2:T:17:MET:HE1   | 2:T:57:ALA:C     | 2.39                     | 0.47              |
| 2:T:220:PHE:O    | 2:T:223:VAL:HG22 | 2.15                     | 0.47              |
| 2:K:40:CYS:HB2   | 2:K:41:PRO:CD    | 2.44                     | 0.47              |
| 2:W:331:GLU:O    | 2:W:334:VAL:HG12 | 2.13                     | 0.47              |
| 1:A:76:LEU:HD22  | 1:A:96:TYR:CE1   | 2.49                     | 0.47              |
| 2:B:8:VAL:HG11   | 2:B:208:PHE:HE1  | 1.80                     | 0.47              |
| 2:E:80:ARG:HE    | 2:E:275:ASP:CG   | 2.23                     | 0.47              |
| 1:G:167:ASP:HB2  | 1:G:172:ILE:HD12 | 1.95                     | 0.47              |
| 1:G:418:ASP:HB3  | 1:G:422:VAL:CG1  | 2.44                     | 0.47              |
| 1:P:138:TRP:NE1  | 1:P:438:TRP:HH2  | 2.12                     | 0.47              |
| 1:S:138:TRP:CD2  | 1:S:438:TRP:HZ3  | 2.32                     | 0.47              |
| 2:T:331:GLU:HA   | 2:T:334:VAL:HG12 | 1.96                     | 0.47              |
| 1:V:138:TRP:CD2  | 1:V:438:TRP:CZ3  | 3.02                     | 0.47              |
| 2:W:201:ARG:HD2  | 2:W:207:GLU:O    | 2.15                     | 0.47              |
| 1:A:88:ILE:HA    | 1:A:324:TYR:HB3  | 1.96                     | 0.47              |
| 1:G:344:PHE:O    | 1:G:349:LYS:HE2  | 2.15                     | 0.47              |
| 1:P:199:PHE:CD1  | 1:P:199:PHE:C    | 2.92                     | 0.47              |
| 1:A:162:VAL:HG21 | 1:A:219:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:201:SER:HB2  | 2:B:276:PRO:HG2  | 1.96                     | 0.47              |
| 2:H:119:VAL:CG1  | 2:H:156:THR:HG21 | 2.45                     | 0.47              |
| 1:A:157:VAL:HG23 | 1:A:159:SER:H    | 1.80                     | 0.47              |
| 1:G:438:TRP:CD1  | 1:G:438:TRP:N    | 2.83                     | 0.47              |
| 1:J:245:VAL:HG12 | 1:J:459:LEU:HB3  | 1.97                     | 0.47              |
| 2:W:330:PHE:CE1  | 2:W:344:VAL:HG13 | 2.50                     | 0.47              |
| 2:N:36:ASN:ND2   | 3:O:84:GLY:O     | 2.37                     | 0.46              |
| 2:N:355:LEU:HD22 | 2:N:360:ILE:HG12 | 1.97                     | 0.46              |
| 1:D:100:VAL:HG12 | 1:D:223:ILE:HB   | 1.96                     | 0.46              |
| 1:D:464:LEU:HD12 | 1:D:464:LEU:O    | 2.14                     | 0.46              |
| 2:H:282:LYS:HD3  | 3:I:55:PHE:CE2   | 2.50                     | 0.46              |
| 1:J:138:TRP:CE2  | 1:J:438:TRP:HH2  | 2.31                     | 0.46              |
| 2:K:310:TYR:CE1  | 2:K:334:VAL:HG11 | 2.50                     | 0.46              |
| 2:N:348:ILE:HA   | 2:N:352:LEU:HD22 | 1.97                     | 0.46              |
| 1:V:42:TYR:CE2   | 1:V:113:GLY:HA3  | 2.51                     | 0.46              |
| 1:A:77:VAL:HG21  | 1:A:114:LYS:HD3  | 1.97                     | 0.46              |
| 1:A:189:GLY:H    | 1:A:205:GLN:NE2  | 2.13                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:437:ALA:C    | 1:G:438:TRP:CD1  | 2.93                     | 0.46              |
| 1:M:155:VAL:HG21 | 1:M:163:SER:HB2  | 1.96                     | 0.46              |
| 2:N:41:PRO:HB3   | 2:N:46:MET:HE2   | 1.97                     | 0.46              |
| 1:V:316:ARG:O    | 1:V:321:ARG:NH2  | 2.48                     | 0.46              |
| 1:V:438:TRP:CH2  | 1:V:443:PRO:HG3  | 2.50                     | 0.46              |
| 1:A:174:GLN:HB3  | 1:A:175:PRO:HD3  | 1.97                     | 0.46              |
| 2:K:331:GLU:HA   | 2:K:334:VAL:HG12 | 1.98                     | 0.46              |
| 1:P:83:THR:HG22  | 1:P:90:GLU:HA    | 1.97                     | 0.46              |
| 3:I:46:GLU:O     | 3:I:47:ASN:HB2   | 2.15                     | 0.46              |
| 2:K:392:VAL:C    | 2:K:396:MET:HE3  | 2.41                     | 0.46              |
| 1:P:1:MET:HE2    | 1:P:3:TRP:HE1    | 1.80                     | 0.46              |
| 1:S:174:GLN:HB3  | 1:S:175:PRO:HD3  | 1.97                     | 0.46              |
| 1:J:292:LEU:O    | 1:J:295:VAL:HG22 | 2.16                     | 0.46              |
| 2:Q:54:ASN:HB2   | 3:R:61:ARG:NH2   | 2.31                     | 0.46              |
| 1:S:6:SER:HB3    | 1:S:212:ARG:CZ   | 2.45                     | 0.46              |
| 1:S:27:SER:O     | 1:S:30:ASP:HB2   | 2.16                     | 0.46              |
| 1:S:218:LEU:O    | 1:S:222:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:68:PRO:HB3   | 1:G:112:VAL:HG11 | 1.98                     | 0.46              |
| 1:G:86:SER:HB2   | 1:G:119:GLU:HG3  | 1.98                     | 0.46              |
| 1:S:438:TRP:CZ3  | 1:S:443:PRO:HG3  | 2.51                     | 0.46              |
| 1:A:47:TYR:CE2   | 1:A:112:VAL:HG12 | 2.47                     | 0.46              |
| 1:D:44:THR:HB    | 1:D:114:LYS:HB2  | 1.98                     | 0.46              |
| 1:D:182:ILE:HG12 | 1:D:434:ILE:CD1  | 2.42                     | 0.46              |
| 2:E:8:VAL:HG12   | 2:E:158:PRO:HB2  | 1.98                     | 0.46              |
| 1:G:83:THR:HG22  | 1:G:90:GLU:HA    | 1.98                     | 0.46              |
| 1:J:376:ARG:HH11 | 1:J:376:ARG:CG   | 2.13                     | 0.46              |
| 2:N:217:VAL:HG11 | 2:N:223:VAL:HA   | 1.98                     | 0.46              |
| 1:P:318:ASP:HB2  | 1:P:336:TYR:CE1  | 2.50                     | 0.46              |
| 1:S:81:LYS:CE    | 1:S:91:ASN:HA    | 2.40                     | 0.46              |
| 2:W:21:THR:HG21  | 3:X:61:ARG:NH1   | 2.24                     | 0.46              |
| 1:A:155:VAL:CG2  | 1:A:163:SER:HB3  | 2.46                     | 0.46              |
| 2:B:100:PRO:HB3  | 2:B:123:ARG:NH2  | 2.15                     | 0.46              |
| 2:E:73:HIS:NE2   | 2:E:103:THR:HB   | 2.31                     | 0.46              |
| 1:G:172:ILE:HD13 | 1:G:207:GLY:HA3  | 1.97                     | 0.46              |
| 1:J:316:ARG:O    | 1:J:321:ARG:NH2  | 2.46                     | 0.46              |
| 1:V:265:LEU:HD23 | 1:V:398:PRO:HA   | 1.98                     | 0.46              |
| 2:B:331:GLU:O    | 2:B:334:VAL:HG12 | 2.16                     | 0.46              |
| 1:G:297:TYR:CE2  | 3:I:43:LEU:HD21  | 2.51                     | 0.46              |
| 2:H:21:THR:HG21  | 3:I:61:ARG:NH1   | 2.10                     | 0.46              |
| 1:J:338:ARG:CG   | 3:L:17:GLU:OE1   | 2.63                     | 0.46              |
| 2:N:117:LYS:HG2  | 2:N:118:LYS:N    | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:398:GLU:OE1  | 2:N:398:GLU:HA   | 2.15                     | 0.46              |
| 2:Q:129:ASP:CG   | 2:Q:146:ARG:HH11 | 2.24                     | 0.46              |
| 1:S:318:ASP:HB2  | 1:S:336:TYR:CE1  | 2.50                     | 0.46              |
| 2:T:80:ARG:HE    | 2:T:275:ASP:CG   | 2.24                     | 0.46              |
| 2:T:132:LYS:HE2  | 2:T:146:ARG:HH21 | 1.81                     | 0.46              |
| 2:E:118:LYS:HZ1  | 1:G:291:SER:HB3  | 1.81                     | 0.45              |
| 2:H:21:THR:HG22  | 2:H:54:ASN:ND2   | 2.31                     | 0.45              |
| 1:J:138:TRP:CZ2  | 1:J:438:TRP:CH2  | 3.04                     | 0.45              |
| 1:P:306:ALA:HB3  | 1:P:307:PRO:CD   | 2.42                     | 0.45              |
| 2:W:141:LEU:HD12 | 3:X:87:VAL:HG22  | 1.98                     | 0.45              |
| 1:D:143:VAL:HG12 | 1:D:145:GLY:H    | 1.80                     | 0.45              |
| 2:E:106:TRP:CE3  | 1:G:293:PRO:HG3  | 2.51                     | 0.45              |
| 1:M:72:LYS:HA    | 1:M:115:THR:HG22 | 1.99                     | 0.45              |
| 1:G:377:LEU:HD23 | 1:G:377:LEU:HA   | 1.81                     | 0.45              |
| 2:K:379:ILE:HD13 | 2:K:384:ILE:HG13 | 1.99                     | 0.45              |
| 2:W:310:TYR:CE1  | 2:W:334:VAL:HG11 | 2.51                     | 0.45              |
| 2:H:119:VAL:CG1  | 2:H:156:THR:CG2  | 2.95                     | 0.45              |
| 1:P:25:VAL:HG12  | 1:P:51:LEU:HD12  | 1.97                     | 0.45              |
| 1:S:57:LEU:HD22  | 1:S:65:PHE:CE1   | 2.51                     | 0.45              |
| 1:V:9:GLU:O      | 1:V:13:LEU:HD13  | 2.16                     | 0.45              |
| 1:G:259:GLU:CD   | 1:G:292:LEU:H    | 2.25                     | 0.45              |
| 1:V:318:ASP:HB2  | 1:V:336:TYR:CE1  | 2.52                     | 0.45              |
| 1:V:422:VAL:N    | 1:V:423:PRO:CD   | 2.80                     | 0.45              |
| 2:H:8:VAL:HG12   | 2:H:158:PRO:HB2  | 1.98                     | 0.45              |
| 1:J:422:VAL:N    | 1:J:423:PRO:CD   | 2.80                     | 0.45              |
| 2:K:162:THR:HG22 | 2:K:164:GLU:N    | 2.31                     | 0.45              |
| 2:B:96:GLN:HB2   | 2:B:125:HIS:HB2  | 1.99                     | 0.45              |
| 2:H:103:THR:HG23 | 2:H:104:ASN:OD1  | 2.13                     | 0.45              |
| 2:H:170:LEU:HB3  | 2:H:220:PHE:CE1  | 2.52                     | 0.45              |
| 2:N:8:VAL:CG1    | 2:N:158:PRO:HB2  | 2.47                     | 0.45              |
| 1:P:90:GLU:O     | 1:P:91:ASN:CB    | 2.65                     | 0.45              |
| 1:V:171:SER:O    | 1:V:175:PRO:HG2  | 2.17                     | 0.45              |
| 1:V:241:TRP:O    | 1:V:245:VAL:HG22 | 2.17                     | 0.45              |
| 2:W:340:PRO:O    | 2:W:344:VAL:HG22 | 2.17                     | 0.45              |
| 1:A:94:ALA:HA    | 1:A:95:PRO:HD3   | 1.80                     | 0.45              |
| 2:B:141:LEU:HD23 | 3:C:85:PHE:CD2   | 2.50                     | 0.45              |
| 2:B:340:PRO:O    | 2:B:344:VAL:HG22 | 2.16                     | 0.45              |
| 2:B:393:ILE:HA   | 2:B:396:MET:HE3  | 1.98                     | 0.45              |
| 2:N:95:SER:HB3   | 2:N:127:GLU:CB   | 2.47                     | 0.45              |
| 1:S:104:LEU:HD11 | 1:S:164:LEU:CD2  | 2.47                     | 0.45              |
| 1:S:318:ASP:HB2  | 1:S:336:TYR:CD1  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:W:85:TYR:HD2   | 2:W:87:ASP:OD1   | 1.99                     | 0.45              |
| 1:A:234:ALA:HB1  | 1:A:236:VAL:HG23 | 1.98                     | 0.45              |
| 1:D:172:ILE:CD1  | 1:D:207:GLY:HA3  | 2.47                     | 0.45              |
| 1:D:337:ALA:HA   | 3:F:15:ARG:O     | 2.17                     | 0.45              |
| 1:J:155:VAL:HG23 | 1:J:163:SER:HB2  | 1.98                     | 0.45              |
| 1:M:126:THR:HG22 | 1:M:126:THR:O    | 2.16                     | 0.45              |
| 1:P:16:ARG:CB    | 1:P:18:GLU:OE2   | 2.65                     | 0.45              |
| 1:S:157:VAL:HG23 | 1:S:159:SER:H    | 1.81                     | 0.45              |
| 2:T:211:ARG:HD3  | 5:T:707:ADP:C5   | 2.52                     | 0.45              |
| 1:A:69:ILE:HD11  | 1:A:164:LEU:HD13 | 1.99                     | 0.45              |
| 2:B:336:HIS:CE1  | 2:B:370:GLU:HG3  | 2.52                     | 0.45              |
| 1:D:39:VAL:HG21  | 1:D:157:VAL:HG11 | 1.98                     | 0.45              |
| 2:H:184:LYS:HB2  | 2:H:191:GLN:OE1  | 2.17                     | 0.45              |
| 1:S:162:VAL:HG21 | 1:S:219:VAL:HG21 | 1.98                     | 0.45              |
| 2:W:17:MET:HE1   | 2:W:57:ALA:C     | 2.42                     | 0.45              |
| 1:G:94:ALA:HA    | 1:G:95:PRO:HD3   | 1.81                     | 0.44              |
| 1:G:138:TRP:CE2  | 1:G:438:TRP:HZ3  | 2.34                     | 0.44              |
| 1:J:384:LYS:O    | 1:J:387:GLU:HB2  | 2.17                     | 0.44              |
| 2:K:132:LYS:HB2  | 2:K:146:ARG:HH21 | 1.82                     | 0.44              |
| 2:N:17:MET:HE1   | 2:N:60:TYR:CB    | 2.47                     | 0.44              |
| 2:N:95:SER:HB3   | 2:N:127:GLU:HB3  | 1.99                     | 0.44              |
| 1:P:174:GLN:HE21 | 1:P:174:GLN:HB2  | 1.56                     | 0.44              |
| 2:W:137:GLY:O    | 3:X:90:ARG:HD2   | 2.17                     | 0.44              |
| 1:A:270:LYS:HE3  | 1:A:274:GLU:OE2  | 2.17                     | 0.44              |
| 1:G:134:THR:HG22 | 1:G:144:PRO:HG3  | 1.98                     | 0.44              |
| 1:G:397:THR:CG2  | 1:G:399:THR:O    | 2.64                     | 0.44              |
| 1:M:234:ALA:HB1  | 1:M:236:VAL:HG23 | 1.99                     | 0.44              |
| 2:N:170:LEU:HD12 | 2:N:223:VAL:HG21 | 1.99                     | 0.44              |
| 1:P:1:MET:O      | 1:P:1:MET:HG2    | 2.17                     | 0.44              |
| 2:Q:123:ARG:NH1  | 2:Q:125:HIS:ND1  | 2.64                     | 0.44              |
| 1:S:178:PHE:CE2  | 1:S:402:PHE:CE2  | 3.05                     | 0.44              |
| 2:W:355:LEU:HD21 | 2:W:365:SER:HB2  | 2.00                     | 0.44              |
| 1:A:99:THR:O     | 1:A:103:ARG:HG3  | 2.18                     | 0.44              |
| 1:M:353:MET:O    | 1:M:356:THR:HG23 | 2.17                     | 0.44              |
| 1:V:174:GLN:N    | 1:V:175:PRO:CD   | 2.81                     | 0.44              |
| 1:A:422:VAL:N    | 1:A:423:PRO:CD   | 2.80                     | 0.44              |
| 1:J:199:PHE:CD1  | 1:J:199:PHE:C    | 2.96                     | 0.44              |
| 1:J:403:LYS:O    | 1:J:406:GLU:HB2  | 2.17                     | 0.44              |
| 1:S:98:ALA:HA    | 1:S:195:GLY:HA3  | 2.00                     | 0.44              |
| 1:V:356:THR:HG21 | 3:X:14:ALA:HB2   | 2.00                     | 0.44              |
| 2:H:275:ASP:OD1  | 2:H:276:PRO:HD2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:184:LYS:HB2  | 2:N:191:GLN:OE1  | 2.17                     | 0.44              |
| 1:P:376:ARG:O    | 1:P:376:ARG:HG3  | 2.17                     | 0.44              |
| 1:P:422:VAL:N    | 1:P:423:PRO:CD   | 2.81                     | 0.44              |
| 2:H:394:LYS:HB2  | 2:H:394:LYS:HE3  | 1.82                     | 0.44              |
| 2:Q:346:TRP:O    | 2:Q:350:ASP:HB2  | 2.16                     | 0.44              |
| 1:S:120:PHE:HE1  | 1:S:197:VAL:HG11 | 1.82                     | 0.44              |
| 1:S:126:THR:O    | 1:S:126:THR:HG22 | 2.18                     | 0.44              |
| 2:T:21:THR:HG22  | 2:T:54:ASN:HD22  | 1.82                     | 0.44              |
| 2:T:193:ARG:HH11 | 2:T:193:ARG:HG3  | 1.83                     | 0.44              |
| 1:V:29:TYR:O     | 1:V:29:TYR:HD1   | 2.00                     | 0.44              |
| 1:V:203:LEU:CD2  | 1:V:375:ARG:NH2  | 2.80                     | 0.44              |
| 1:D:438:TRP:CH2  | 1:D:443:PRO:HG3  | 2.52                     | 0.44              |
| 1:J:1:MET:HE2    | 1:J:3:TRP:HE1    | 1.82                     | 0.44              |
| 1:M:68:PRO:HB3   | 1:M:112:VAL:HG21 | 1.99                     | 0.44              |
| 1:M:134:THR:HG22 | 1:M:144:PRO:HG3  | 2.00                     | 0.44              |
| 1:M:190:ARG:HD2  | 1:M:455:GLU:OE2  | 2.18                     | 0.44              |
| 1:S:356:THR:HG21 | 3:U:14:ALA:HB2   | 2.00                     | 0.44              |
| 2:E:374:GLU:OE1  | 2:E:402:THR:HG22 | 2.17                     | 0.44              |
| 2:E:374:GLU:OE2  | 2:E:404:SER:HB3  | 2.17                     | 0.44              |
| 1:G:201:SER:HB2  | 2:H:276:PRO:HG2  | 1.98                     | 0.44              |
| 1:G:258:LYS:HE2  | 1:G:289:GLU:HB3  | 1.99                     | 0.44              |
| 1:G:395:PRO:O    | 1:G:420:LEU:HD13 | 2.18                     | 0.44              |
| 1:J:292:LEU:HB2  | 1:J:295:VAL:CG2  | 2.47                     | 0.44              |
| 1:J:352:ILE:O    | 1:J:356:THR:HG23 | 2.16                     | 0.44              |
| 3:L:89:PRO:O     | 3:L:90:ARG:C     | 2.60                     | 0.44              |
| 2:N:402:THR:HG22 | 2:N:403:PRO:HD2  | 2.00                     | 0.44              |
| 1:P:115:THR:HG21 | 1:P:151:SER:OG   | 2.18                     | 0.44              |
| 2:Q:310:TYR:CE1  | 2:Q:334:VAL:HG11 | 2.53                     | 0.44              |
| 1:S:46:LEU:HD11  | 1:S:80:GLU:HG3   | 2.00                     | 0.44              |
| 1:S:168:THR:HG21 | 1:S:199:PHE:CE2  | 2.53                     | 0.44              |
| 3:U:58:THR:HA    | 3:U:59:PRO:HD2   | 1.88                     | 0.44              |
| 1:V:69:ILE:HD11  | 1:V:164:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:151:SER:HB3  | 1:A:163:SER:HG   | 1.83                     | 0.44              |
| 1:A:245:VAL:HG12 | 1:A:459:LEU:HB3  | 1.99                     | 0.44              |
| 1:G:297:TYR:OH   | 3:I:42:GLU:OE1   | 2.33                     | 0.44              |
| 1:G:376:ARG:HG2  | 1:G:380:ASN:ND2  | 2.33                     | 0.44              |
| 2:H:85:TYR:CG    | 2:H:86:PRO:HD2   | 2.53                     | 0.44              |
| 1:J:155:VAL:O    | 1:J:211:ARG:HD2  | 2.18                     | 0.44              |
| 1:S:14:LEU:HD11  | 1:S:24:VAL:HG21  | 1.99                     | 0.44              |
| 2:T:41:PRO:HB3   | 2:T:46:MET:HE2   | 2.00                     | 0.44              |
| 2:B:179:TYR:CE1  | 2:B:324:LYS:HB2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:138:TRP:CD2  | 1:J:438:TRP:CZ3  | 3.06                     | 0.43              |
| 2:K:330:PHE:CE1  | 2:K:344:VAL:HG13 | 2.52                     | 0.43              |
| 1:P:234:ALA:HB1  | 1:P:236:VAL:HG23 | 1.99                     | 0.43              |
| 1:P:351:ARG:NH1  | 4:P:906:ASN:O    | 2.31                     | 0.43              |
| 1:S:354:LEU:HD11 | 3:U:34:LEU:HD13  | 1.99                     | 0.43              |
| 2:T:8:VAL:HG13   | 2:T:161:ARG:NH1  | 2.33                     | 0.43              |
| 2:T:95:SER:HB3   | 2:T:127:GLU:CB   | 2.48                     | 0.43              |
| 2:W:320:LEU:CD2  | 2:W:326:VAL:HG12 | 2.48                     | 0.43              |
| 1:A:32:TYR:CE1   | 1:A:36:GLU:HG2   | 2.53                     | 0.43              |
| 1:D:21:PRO:O     | 1:D:25:VAL:HG23  | 2.18                     | 0.43              |
| 2:E:106:TRP:CZ3  | 1:G:293:PRO:HG3  | 2.54                     | 0.43              |
| 1:G:298:SER:HB3  | 1:G:422:VAL:HG23 | 2.00                     | 0.43              |
| 2:H:75:GLU:HG3   | 2:H:282:LYS:HG3  | 2.00                     | 0.43              |
| 1:J:294:HIS:HB2  | 1:J:381:ASP:OD2  | 2.18                     | 0.43              |
| 1:P:214:GLU:OE2  | 1:P:463:TYR:CE1  | 2.71                     | 0.43              |
| 2:T:375:LEU:HD22 | 2:T:396:MET:HE1  | 1.99                     | 0.43              |
| 1:V:157:VAL:HG23 | 1:V:159:SER:H    | 1.83                     | 0.43              |
| 2:W:35:PRO:HG3   | 3:X:85:PHE:CE2   | 2.54                     | 0.43              |
| 1:A:95:PRO:CD    | 2:B:46:MET:HE1   | 2.49                     | 0.43              |
| 1:V:337:ALA:HA   | 3:X:15:ARG:O     | 2.18                     | 0.43              |
| 2:W:8:VAL:HG13   | 2:W:161:ARG:NH1  | 2.34                     | 0.43              |
| 1:A:42:TYR:CE2   | 1:A:113:GLY:HA3  | 2.54                     | 0.43              |
| 2:B:399:THR:OG1  | 2:B:400:GLY:N    | 2.51                     | 0.43              |
| 1:G:300:PRO:HG2  | 3:I:39:GLN:CG    | 2.48                     | 0.43              |
| 2:K:103:THR:HG23 | 2:K:104:ASN:OD1  | 2.18                     | 0.43              |
| 2:N:141:LEU:HD12 | 3:O:87:VAL:HG22  | 1.99                     | 0.43              |
| 2:Q:41:PRO:HB3   | 2:Q:46:MET:HE2   | 2.00                     | 0.43              |
| 1:S:403:LYS:O    | 1:S:406:GLU:HB2  | 2.19                     | 0.43              |
| 1:V:212:ARG:NH2  | 1:V:472:TYR:CE1  | 2.86                     | 0.43              |
| 1:G:337:ALA:HA   | 3:I:15:ARG:O     | 2.19                     | 0.43              |
| 1:J:185:LYS:NZ   | 1:J:429:LEU:O    | 2.49                     | 0.43              |
| 1:J:374:VAL:HG11 | 3:L:40:LEU:HD22  | 2.01                     | 0.43              |
| 2:N:340:PRO:O    | 2:N:344:VAL:HG22 | 2.17                     | 0.43              |
| 2:N:368:LYS:HB3  | 2:N:370:GLU:OE2  | 2.18                     | 0.43              |
| 1:S:178:PHE:HE2  | 1:S:402:PHE:CE2  | 2.36                     | 0.43              |
| 2:T:320:LEU:HD22 | 2:T:326:VAL:HG12 | 2.01                     | 0.43              |
| 1:V:259:GLU:CD   | 1:V:292:LEU:H    | 2.27                     | 0.43              |
| 1:A:171:SER:N    | 4:A:901:ASN:OD1  | 2.52                     | 0.43              |
| 1:A:317:TYR:O    | 1:A:340:ARG:NH1  | 2.49                     | 0.43              |
| 1:G:57:LEU:HD22  | 1:G:65:PHE:CE1   | 2.54                     | 0.43              |
| 1:J:138:TRP:NE1  | 1:J:438:TRP:HH2  | 2.16                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:57:LEU:HD22  | 1:M:65:PHE:CE1   | 2.54                     | 0.43              |
| 3:O:51:TYR:C     | 3:O:51:TYR:CD2   | 2.97                     | 0.43              |
| 2:Q:402:THR:HG22 | 2:Q:403:PRO:HD2  | 1.99                     | 0.43              |
| 1:S:422:VAL:N    | 1:S:423:PRO:CD   | 2.81                     | 0.43              |
| 1:A:353:MET:HE3  | 1:A:353:MET:HB3  | 1.89                     | 0.43              |
| 3:C:58:THR:HA    | 3:C:59:PRO:HD2   | 1.81                     | 0.43              |
| 2:E:201:ARG:HG3  | 2:E:205:SER:HB3  | 2.01                     | 0.43              |
| 1:P:117:LEU:O    | 1:P:129:SER:HB2  | 2.19                     | 0.43              |
| 1:P:138:TRP:CZ2  | 1:P:438:TRP:CH2  | 3.06                     | 0.43              |
| 1:P:190:ARG:HH11 | 1:P:190:ARG:HG3  | 1.83                     | 0.43              |
| 1:P:245:VAL:HG12 | 1:P:459:LEU:HB3  | 2.01                     | 0.43              |
| 2:Q:348:ILE:HA   | 2:Q:352:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:404:PHE:HB3  | 2:E:390:LYS:HE3  | 2.00                     | 0.43              |
| 2:B:46:MET:HB3   | 2:B:46:MET:HE2   | 1.51                     | 0.43              |
| 2:E:255:THR:HG23 | 2:E:257:LYS:H    | 1.83                     | 0.43              |
| 2:E:262:ARG:H    | 2:E:262:ARG:HG2  | 1.50                     | 0.43              |
| 2:K:41:PRO:HB3   | 2:K:46:MET:HE2   | 2.00                     | 0.43              |
| 1:M:354:LEU:HD21 | 3:O:33:ILE:HG21  | 2.00                     | 0.43              |
| 1:P:62:LEU:HA    | 1:P:63:PRO:HD3   | 1.85                     | 0.43              |
| 2:Q:83:TYR:CZ    | 2:Q:88:LEU:HD22  | 2.54                     | 0.43              |
| 3:U:33:ILE:O     | 3:U:37:ILE:HG12  | 2.19                     | 0.43              |
| 2:W:3:GLU:OE2    | 2:W:235:ILE:HD13 | 2.19                     | 0.43              |
| 1:A:337:ALA:HA   | 3:C:15:ARG:O     | 2.18                     | 0.43              |
| 2:B:302:ARG:NH2  | 2:B:328:ASP:OD1  | 2.52                     | 0.43              |
| 3:F:21:GLU:H     | 3:F:21:GLU:CD    | 2.27                     | 0.43              |
| 1:G:279:GLU:HG3  | 1:G:468:LYS:NZ   | 2.34                     | 0.43              |
| 1:M:199:PHE:CD1  | 1:M:199:PHE:C    | 2.97                     | 0.43              |
| 3:R:51:TYR:CD2   | 3:R:51:TYR:C     | 2.97                     | 0.43              |
| 1:S:337:ALA:HA   | 3:U:15:ARG:O     | 2.17                     | 0.43              |
| 1:V:49:LYS:NZ    | 1:V:80:GLU:HG2   | 2.34                     | 0.43              |
| 1:V:169:GLY:HA2  | 1:V:425:ASN:OD1  | 2.18                     | 0.43              |
| 2:B:146:ARG:HG2  | 2:B:146:ARG:NH1  | 2.32                     | 0.43              |
| 2:E:162:THR:HG22 | 2:E:164:GLU:N    | 2.32                     | 0.43              |
| 2:E:306:LEU:HB3  | 2:E:312:LEU:HD12 | 2.01                     | 0.43              |
| 2:H:156:THR:HG22 | 2:H:157:GLU:O    | 2.19                     | 0.43              |
| 2:H:396:MET:HG3  | 2:H:406:ILE:HD11 | 2.00                     | 0.43              |
| 1:P:292:LEU:HB2  | 1:P:295:VAL:HG22 | 2.01                     | 0.43              |
| 1:P:292:LEU:O    | 1:P:295:VAL:HG22 | 2.19                     | 0.43              |
| 2:T:360:ILE:CD1  | 2:T:366:PRO:HD3  | 2.49                     | 0.43              |
| 1:V:126:THR:OG1  | 1:V:149:GLY:HA3  | 2.19                     | 0.43              |
| 1:M:88:ILE:HG23  | 1:M:343:GLY:CA   | 2.30                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:21:THR:HG22  | 2:Q:54:ASN:ND2   | 2.34                     | 0.42              |
| 2:Q:392:VAL:C    | 2:Q:396:MET:HE3  | 2.44                     | 0.42              |
| 1:V:434:ILE:HD12 | 1:V:434:ILE:HA   | 1.82                     | 0.42              |
| 2:W:297:GLU:OE2  | 2:W:302:ARG:HA   | 2.18                     | 0.42              |
| 1:A:265:LEU:HD22 | 1:A:398:PRO:HA   | 2.00                     | 0.42              |
| 1:A:279:GLU:HG3  | 1:A:468:LYS:HZ1  | 1.78                     | 0.42              |
| 1:D:30:ASP:O     | 1:D:34:GLN:HG3   | 2.19                     | 0.42              |
| 3:F:58:THR:HA    | 3:F:59:PRO:HD2   | 1.83                     | 0.42              |
| 1:G:90:GLU:O     | 1:G:91:ASN:CB    | 2.62                     | 0.42              |
| 2:N:146:ARG:HG2  | 2:N:146:ARG:HH11 | 1.84                     | 0.42              |
| 1:P:172:ILE:O    | 1:P:175:PRO:HD2  | 2.19                     | 0.42              |
| 1:A:72:LYS:HE2   | 1:A:117:LEU:HD13 | 2.01                     | 0.42              |
| 2:H:282:LYS:HD3  | 3:I:55:PHE:CZ    | 2.54                     | 0.42              |
| 1:P:95:PRO:HG2   | 2:Q:46:MET:HE3   | 1.99                     | 0.42              |
| 2:Q:355:LEU:CD2  | 2:Q:365:SER:HB2  | 2.50                     | 0.42              |
| 1:S:94:ALA:HA    | 1:S:95:PRO:HD3   | 1.82                     | 0.42              |
| 1:S:172:ILE:HG22 | 1:S:173:ARG:N    | 2.33                     | 0.42              |
| 2:T:11:LEU:H     | 2:T:156:THR:HB   | 1.85                     | 0.42              |
| 1:A:32:TYR:CE1   | 1:A:36:GLU:CG    | 3.02                     | 0.42              |
| 1:A:325:ARG:HA   | 1:A:339:THR:HG23 | 2.00                     | 0.42              |
| 2:B:360:ILE:HD11 | 2:B:364:GLU:O    | 2.20                     | 0.42              |
| 1:M:277:ILE:HD13 | 1:M:280:LEU:HD12 | 2.00                     | 0.42              |
| 1:P:94:ALA:HA    | 1:P:95:PRO:HD3   | 1.86                     | 0.42              |
| 2:Q:85:TYR:HA    | 2:Q:86:PRO:HD3   | 1.93                     | 0.42              |
| 2:Q:192:LEU:C    | 2:Q:192:LEU:HD23 | 2.45                     | 0.42              |
| 1:V:71:VAL:HB    | 1:V:114:LYS:NZ   | 2.25                     | 0.42              |
| 2:W:101:LEU:HD22 | 2:W:126:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:340:ARG:NH2  | 3:F:14:ALA:O     | 2.49                     | 0.42              |
| 2:E:255:THR:HG21 | 2:E:259:TYR:OH   | 2.18                     | 0.42              |
| 2:H:89:PRO:HG3   | 2:H:144:LEU:HD22 | 2.01                     | 0.42              |
| 1:M:299:ILE:N    | 1:M:300:PRO:CD   | 2.81                     | 0.42              |
| 1:S:138:TRP:CE2  | 1:S:438:TRP:HH2  | 2.37                     | 0.42              |
| 2:T:95:SER:HB3   | 2:T:127:GLU:HB3  | 2.01                     | 0.42              |
| 2:W:95:SER:HB2   | 2:W:96:GLN:H     | 1.69                     | 0.42              |
| 2:W:170:LEU:HB3  | 2:W:220:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:168:THR:HG22 | 1:A:302:TYR:OH   | 2.20                     | 0.42              |
| 1:G:226:TRP:CE2  | 1:G:235:LYS:HE2  | 2.54                     | 0.42              |
| 1:S:265:LEU:HD23 | 1:S:398:PRO:HA   | 2.02                     | 0.42              |
| 1:V:178:PHE:CE1  | 1:V:397:THR:HG21 | 2.54                     | 0.42              |
| 1:A:178:PHE:CE1  | 1:A:397:THR:HG21 | 2.55                     | 0.42              |
| 1:G:137:PRO:HB3  | 1:G:157:VAL:HG13 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:168:THR:C    | 1:G:425:ASN:ND2  | 2.78                     | 0.42              |
| 1:M:83:THR:HG22  | 1:M:90:GLU:HA    | 2.02                     | 0.42              |
| 1:P:337:ALA:HA   | 3:R:15:ARG:O     | 2.20                     | 0.42              |
| 2:Q:64:ALA:O     | 2:Q:68:LEU:HG    | 2.19                     | 0.42              |
| 2:T:355:LEU:CD2  | 2:T:365:SER:HB2  | 2.50                     | 0.42              |
| 1:V:438:TRP:CD1  | 1:V:438:TRP:N    | 2.86                     | 0.42              |
| 1:A:90:GLU:O     | 1:A:91:ASN:HB2   | 2.19                     | 0.42              |
| 1:D:76:LEU:HD22  | 1:D:96:TYR:CE1   | 2.55                     | 0.42              |
| 1:D:101:ILE:HA   | 1:D:104:LEU:HD12 | 2.01                     | 0.42              |
| 1:G:297:TYR:O    | 1:G:300:PRO:HD2  | 2.19                     | 0.42              |
| 2:K:17:MET:HE1   | 2:K:60:TYR:CB    | 2.48                     | 0.42              |
| 1:M:318:ASP:HB2  | 1:M:336:TYR:CE1  | 2.54                     | 0.42              |
| 2:N:360:ILE:HD11 | 2:N:364:GLU:O    | 2.20                     | 0.42              |
| 2:Q:162:THR:HG22 | 2:Q:164:GLU:N    | 2.35                     | 0.42              |
| 1:S:173:ARG:HH11 | 1:S:447:GLN:NE2  | 2.17                     | 0.42              |
| 1:V:94:ALA:HA    | 1:V:95:PRO:HD3   | 1.76                     | 0.42              |
| 1:A:265:LEU:HD11 | 1:A:395:PRO:HG2  | 2.01                     | 0.42              |
| 1:D:94:ALA:HA    | 1:D:95:PRO:HD3   | 1.77                     | 0.42              |
| 1:J:348:VAL:O    | 1:J:352:ILE:HG13 | 2.19                     | 0.42              |
| 2:K:355:LEU:HD21 | 2:K:365:SER:HB2  | 2.02                     | 0.42              |
| 1:M:136:ASN:HA   | 1:M:137:PRO:HD2  | 1.96                     | 0.42              |
| 1:M:312:SER:OG   | 2:N:82:HIS:NE2   | 2.35                     | 0.42              |
| 1:M:320:VAL:HG13 | 3:O:88:VAL:CG1   | 2.50                     | 0.42              |
| 1:P:213:THR:HG21 | 1:P:459:LEU:O    | 2.20                     | 0.42              |
| 1:S:341:ASP:OD1  | 3:U:22:GLU:OE1   | 2.38                     | 0.42              |
| 2:T:80:ARG:HD2   | 2:T:273:PHE:CE2  | 2.55                     | 0.42              |
| 2:W:392:VAL:C    | 2:W:396:MET:HE3  | 2.44                     | 0.42              |
| 1:D:6:SER:HB3    | 1:D:212:ARG:CZ   | 2.49                     | 0.42              |
| 1:G:25:VAL:CG1   | 1:G:51:LEU:HD13  | 2.50                     | 0.42              |
| 1:J:337:ALA:HA   | 3:L:15:ARG:O     | 2.20                     | 0.42              |
| 1:J:438:TRP:CD1  | 1:J:438:TRP:N    | 2.87                     | 0.42              |
| 2:K:8:VAL:HG12   | 2:K:158:PRO:HB2  | 2.02                     | 0.42              |
| 1:M:162:VAL:HG21 | 1:M:219:VAL:HG21 | 2.01                     | 0.42              |
| 2:T:23:MET:CE    | 2:T:126:ILE:HG21 | 2.50                     | 0.42              |
| 2:T:402:THR:OG1  | 2:T:405:GLN:CB   | 2.66                     | 0.42              |
| 1:A:139:ASP:CG   | 1:A:142:ARG:HG3  | 2.45                     | 0.41              |
| 1:D:190:ARG:HD2  | 1:D:455:GLU:OE2  | 2.20                     | 0.41              |
| 2:E:252:ASP:OD2  | 2:E:255:THR:HG22 | 2.20                     | 0.41              |
| 2:H:36:ASN:ND2   | 3:I:84:GLY:O     | 2.35                     | 0.41              |
| 1:J:318:ASP:HB2  | 1:J:336:TYR:CE1  | 2.54                     | 0.41              |
| 2:K:142:VAL:HB   | 3:L:86:PHE:HB2   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:20:LYS:HE2   | 2:N:56:ARG:HH12  | 1.84                     | 0.41              |
| 1:S:5:LYS:HB2    | 1:S:10:LEU:HD13  | 2.01                     | 0.41              |
| 1:S:325:ARG:HD2  | 1:S:335:MET:SD   | 2.59                     | 0.41              |
| 1:V:57:LEU:HD12  | 1:V:110:LEU:HD21 | 2.02                     | 0.41              |
| 2:W:70:CYS:HB3   | 2:W:102:ALA:HB1  | 2.00                     | 0.41              |
| 2:W:255:THR:HG23 | 2:W:257:LYS:H    | 1.85                     | 0.41              |
| 2:W:374:GLU:OE2  | 2:W:404:SER:HB3  | 2.20                     | 0.41              |
| 2:B:156:THR:HG23 | 2:B:157:GLU:O    | 2.20                     | 0.41              |
| 1:D:98:ALA:HA    | 1:D:195:GLY:HA3  | 2.02                     | 0.41              |
| 1:G:13:LEU:HB3   | 1:G:19:VAL:CG1   | 2.46                     | 0.41              |
| 1:J:145:GLY:CA   | 1:J:174:GLN:OE1  | 2.68                     | 0.41              |
| 1:P:11:ARG:HG2   | 1:P:15:LYS:HE3   | 2.02                     | 0.41              |
| 1:P:172:ILE:CD1  | 1:P:207:GLY:HA3  | 2.50                     | 0.41              |
| 2:T:90:LYS:HD2   | 2:T:92:TYR:CE2   | 2.55                     | 0.41              |
| 2:T:179:TYR:CE1  | 2:T:324:LYS:HB2  | 2.55                     | 0.41              |
| 1:J:25:VAL:CG1   | 1:J:51:LEU:HD12  | 2.51                     | 0.41              |
| 1:J:266:GLN:HA   | 1:J:267:PRO:HD3  | 1.91                     | 0.41              |
| 1:J:329:TYR:HE2  | 3:L:89:PRO:HG3   | 1.85                     | 0.41              |
| 1:M:137:PRO:HB3  | 1:M:157:VAL:HG13 | 2.02                     | 0.41              |
| 2:N:202:PRO:O    | 2:N:205:SER:HB3  | 2.20                     | 0.41              |
| 1:P:29:TYR:O     | 1:P:32:TYR:HB3   | 2.21                     | 0.41              |
| 2:Q:365:SER:HA   | 2:Q:366:PRO:HD3  | 1.94                     | 0.41              |
| 1:V:162:VAL:HG22 | 1:V:163:SER:N    | 2.35                     | 0.41              |
| 1:V:344:PHE:O    | 1:V:349:LYS:HE2  | 2.20                     | 0.41              |
| 2:W:40:CYS:HB2   | 2:W:41:PRO:HD2   | 2.01                     | 0.41              |
| 1:A:21:PRO:O     | 1:A:25:VAL:HG23  | 2.20                     | 0.41              |
| 1:D:333:PHE:C    | 1:D:333:PHE:CD2  | 2.99                     | 0.41              |
| 1:G:155:VAL:HG21 | 1:G:163:SER:HB3  | 2.02                     | 0.41              |
| 2:H:132:LYS:HG3  | 2:H:133:ASN:N    | 2.35                     | 0.41              |
| 2:Q:214:ILE:HD11 | 2:Q:230:GLU:HG2  | 2.02                     | 0.41              |
| 1:S:78:GLU:HB2   | 1:S:97:ASP:OD1   | 2.21                     | 0.41              |
| 2:W:261:MET:HE3  | 2:W:261:MET:HB2  | 1.98                     | 0.41              |
| 1:A:136:ASN:HA   | 1:A:137:PRO:HD2  | 1.84                     | 0.41              |
| 3:I:58:THR:HA    | 3:I:59:PRO:HD2   | 1.87                     | 0.41              |
| 1:J:241:TRP:CD1  | 1:J:456:THR:HG1  | 2.38                     | 0.41              |
| 2:K:192:LEU:HD23 | 2:K:192:LEU:C    | 2.45                     | 0.41              |
| 1:M:98:ALA:HA    | 1:M:195:GLY:HA3  | 2.02                     | 0.41              |
| 2:N:17:MET:HE1   | 2:N:60:TYR:HB2   | 2.01                     | 0.41              |
| 2:W:365:SER:HA   | 2:W:366:PRO:HD3  | 1.94                     | 0.41              |
| 1:A:69:ILE:HD12  | 1:A:162:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:77:VAL:HG23  | 1:A:114:LYS:NZ   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:95:SER:CB    | 2:B:127:GLU:HB3  | 2.51                     | 0.41              |
| 2:B:346:TRP:O    | 2:B:350:ASP:HB2  | 2.19                     | 0.41              |
| 1:G:319:GLY:O    | 3:I:79:PRO:HG2   | 2.20                     | 0.41              |
| 2:H:20:LYS:HE2   | 2:H:56:ARG:NH1   | 2.28                     | 0.41              |
| 2:H:365:SER:HA   | 2:H:366:PRO:HD3  | 1.94                     | 0.41              |
| 3:R:46:GLU:O     | 3:R:47:ASN:CB    | 2.65                     | 0.41              |
| 1:D:279:GLU:OE2  | 1:D:282:LYS:HD2  | 2.21                     | 0.41              |
| 2:E:88:LEU:HA    | 2:E:89:PRO:HD2   | 1.85                     | 0.41              |
| 1:G:49:LYS:HE2   | 1:G:53:GLN:NE2   | 2.35                     | 0.41              |
| 1:J:111:ILE:HD12 | 1:J:111:ILE:N    | 2.35                     | 0.41              |
| 2:K:95:SER:CB    | 2:K:127:GLU:CB   | 2.97                     | 0.41              |
| 3:L:58:THR:HA    | 3:L:59:PRO:HD3   | 1.93                     | 0.41              |
| 1:M:65:PHE:O     | 1:M:108:GLY:O    | 2.38                     | 0.41              |
| 1:S:279:GLU:HG3  | 1:S:468:LYS:NZ   | 2.35                     | 0.41              |
| 1:V:21:PRO:HG3   | 1:V:65:PHE:CE2   | 2.55                     | 0.41              |
| 1:V:99:THR:O     | 1:V:103:ARG:HG3  | 2.19                     | 0.41              |
| 2:W:83:TYR:CZ    | 2:W:88:LEU:HD22  | 2.56                     | 0.41              |
| 2:B:213:GLU:OE1  | 2:B:215:LYS:CE   | 2.63                     | 0.41              |
| 1:D:118:ASP:HB2  | 1:D:147:SER:HB3  | 2.03                     | 0.41              |
| 2:H:402:THR:HG22 | 2:H:403:PRO:HD2  | 2.03                     | 0.41              |
| 1:J:94:ALA:HA    | 1:J:95:PRO:HD3   | 1.86                     | 0.41              |
| 1:J:303:TYR:CE2  | 1:J:415:TYR:HB3  | 2.56                     | 0.41              |
| 2:K:156:THR:HG22 | 2:K:157:GLU:N    | 2.35                     | 0.41              |
| 1:M:94:ALA:HA    | 1:M:95:PRO:HD3   | 1.85                     | 0.41              |
| 1:M:437:ALA:C    | 1:M:438:TRP:CD1  | 2.99                     | 0.41              |
| 1:M:463:TYR:O    | 1:M:467:GLN:HG2  | 2.21                     | 0.41              |
| 1:P:25:VAL:CG1   | 1:P:51:LEU:HD12  | 2.51                     | 0.41              |
| 2:T:141:LEU:HD23 | 3:U:85:PHE:CD2   | 2.56                     | 0.41              |
| 1:V:178:PHE:HE1  | 1:V:397:THR:HG21 | 1.86                     | 0.41              |
| 1:A:111:ILE:N    | 1:A:111:ILE:HD12 | 2.35                     | 0.41              |
| 1:A:174:GLN:CG   | 1:A:175:PRO:HD3  | 2.51                     | 0.41              |
| 2:B:252:ASP:CB   | 2:B:255:THR:HG22 | 2.46                     | 0.41              |
| 2:B:348:ILE:HA   | 2:B:352:LEU:HD22 | 2.03                     | 0.41              |
| 1:D:138:TRP:CD2  | 1:D:438:TRP:HZ3  | 2.39                     | 0.41              |
| 2:E:393:ILE:HA   | 2:E:396:MET:HE3  | 2.02                     | 0.41              |
| 1:G:226:TRP:CD1  | 1:G:235:LYS:HG3  | 2.56                     | 0.41              |
| 1:G:403:LYS:O    | 1:G:406:GLU:HB2  | 2.20                     | 0.41              |
| 2:H:252:ASP:CB   | 2:H:255:THR:HG22 | 2.38                     | 0.41              |
| 1:J:126:THR:O    | 1:J:126:THR:HG22 | 2.20                     | 0.41              |
| 1:J:182:ILE:HG12 | 1:J:434:ILE:HG12 | 2.03                     | 0.41              |
| 1:J:434:ILE:HA   | 1:J:435:PRO:HD3  | 1.91                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:138:TRP:NE1  | 1:M:438:TRP:HH2  | 2.19                     | 0.41              |
| 1:P:353:MET:HE3  | 1:P:353:MET:HB3  | 1.97                     | 0.41              |
| 1:S:412:ILE:HA   | 1:S:415:TYR:CD2  | 2.55                     | 0.41              |
| 1:V:336:TYR:C    | 1:V:339:THR:HG22 | 2.40                     | 0.41              |
| 2:W:40:CYS:HB2   | 2:W:41:PRO:CD    | 2.51                     | 0.41              |
| 1:A:47:TYR:CZ    | 1:A:112:VAL:HG12 | 2.56                     | 0.41              |
| 1:A:434:ILE:HD12 | 1:A:465:TRP:CD1  | 2.55                     | 0.41              |
| 2:B:107:VAL:HG23 | 2:B:121:ILE:HD11 | 2.03                     | 0.41              |
| 1:D:67:ILE:HD13  | 1:D:67:ILE:N     | 2.36                     | 0.41              |
| 1:M:76:LEU:HD22  | 1:M:96:TYR:CE1   | 2.56                     | 0.41              |
| 2:N:95:SER:HB2   | 2:N:96:GLN:H     | 1.71                     | 0.41              |
| 2:N:387:LYS:HD3  | 2:N:387:LYS:C    | 2.45                     | 0.41              |
| 1:P:3:TRP:CZ2    | 1:P:31:ARG:HG3   | 2.56                     | 0.41              |
| 1:S:88:ILE:HG13  | 1:S:343:GLY:HA3  | 2.03                     | 0.41              |
| 1:V:339:THR:CG2  | 1:V:340:ARG:N    | 2.83                     | 0.41              |
| 1:V:347:GLU:CD   | 1:V:350:ARG:HE   | 2.28                     | 0.41              |
| 2:W:170:LEU:CD1  | 2:W:223:VAL:HG21 | 2.50                     | 0.41              |
| 3:F:33:ILE:O     | 3:F:37:ILE:HG12  | 2.20                     | 0.40              |
| 1:G:212:ARG:O    | 1:G:215:ASP:HB2  | 2.21                     | 0.40              |
| 1:J:373:LYS:HE2  | 3:L:50:PRO:HD3   | 2.03                     | 0.40              |
| 1:J:422:VAL:CG2  | 1:J:423:PRO:HD3  | 2.51                     | 0.40              |
| 2:K:140:THR:OG1  | 3:L:91:VAL:N     | 2.46                     | 0.40              |
| 1:M:138:TRP:CZ2  | 1:M:438:TRP:HH2  | 2.36                     | 0.40              |
| 2:N:396:MET:HG3  | 2:N:406:ILE:HD11 | 2.02                     | 0.40              |
| 1:P:203:LEU:HD21 | 1:P:426:LEU:HD23 | 2.03                     | 0.40              |
| 3:R:21:GLU:CD    | 3:R:21:GLU:H     | 2.29                     | 0.40              |
| 2:T:88:LEU:HA    | 2:T:89:PRO:HD2   | 1.98                     | 0.40              |
| 1:D:1:MET:HG2    | 1:D:1:MET:O      | 2.21                     | 0.40              |
| 1:D:155:VAL:HG23 | 1:D:163:SER:HB2  | 2.03                     | 0.40              |
| 2:E:225:LYS:HD3  | 2:E:225:LYS:HA   | 1.95                     | 0.40              |
| 1:G:98:ALA:HA    | 1:G:195:GLY:HA3  | 2.04                     | 0.40              |
| 1:G:314:LEU:HD23 | 1:G:352:ILE:HD11 | 2.02                     | 0.40              |
| 2:H:107:VAL:HG23 | 2:H:121:ILE:HD11 | 2.03                     | 0.40              |
| 2:H:119:VAL:HG12 | 2:H:156:THR:HG23 | 2.01                     | 0.40              |
| 1:J:62:LEU:HA    | 1:J:63:PRO:HD3   | 1.90                     | 0.40              |
| 1:J:155:VAL:CG2  | 1:J:163:SER:HB2  | 2.51                     | 0.40              |
| 1:J:185:LYS:NZ   | 1:J:186:PRO:O    | 2.54                     | 0.40              |
| 1:J:270:LYS:HE3  | 1:J:274:GLU:OE2  | 2.22                     | 0.40              |
| 1:J:418:ASP:HB3  | 1:J:422:VAL:HG13 | 2.02                     | 0.40              |
| 1:P:426:LEU:HD23 | 1:P:426:LEU:HA   | 1.81                     | 0.40              |
| 1:V:234:ALA:HB1  | 1:V:236:VAL:HG23 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:SER:O    | 1:A:175:PRO:HG2  | 2.21                     | 0.40              |
| 2:E:119:VAL:CG1  | 2:E:156:THR:CG2  | 2.98                     | 0.40              |
| 2:E:361:SER:HB2  | 2:E:363:GLU:OE1  | 2.21                     | 0.40              |
| 1:G:167:ASP:HA   | 1:G:171:SER:HB2  | 2.03                     | 0.40              |
| 1:M:172:ILE:HD13 | 1:M:207:GLY:HA3  | 2.02                     | 0.40              |
| 2:Q:305:ARG:HG2  | 2:Q:305:ARG:HH11 | 1.87                     | 0.40              |
| 1:S:143:VAL:HG12 | 1:S:145:GLY:N    | 2.30                     | 0.40              |
| 2:T:193:ARG:HG3  | 2:T:193:ARG:NH1  | 2.36                     | 0.40              |
| 1:V:13:LEU:HB3   | 1:V:19:VAL:HG12  | 2.02                     | 0.40              |
| 1:V:64:LEU:O     | 1:V:65:PHE:C     | 2.64                     | 0.40              |
| 1:V:67:ILE:HA    | 1:V:68:PRO:HD3   | 1.97                     | 0.40              |
| 1:V:297:TYR:CE2  | 3:X:43:LEU:HD21  | 2.57                     | 0.40              |
| 1:G:245:VAL:HG12 | 1:G:459:LEU:HB3  | 2.02                     | 0.40              |
| 2:K:355:LEU:CD2  | 2:K:365:SER:HB2  | 2.51                     | 0.40              |
| 1:P:77:VAL:HG22  | 1:P:101:ILE:HG13 | 2.02                     | 0.40              |
| 1:S:64:LEU:O     | 1:S:65:PHE:C     | 2.64                     | 0.40              |
| 2:T:162:THR:HG22 | 2:T:164:GLU:N    | 2.35                     | 0.40              |
| 1:V:62:LEU:HA    | 1:V:63:PRO:HD3   | 1.94                     | 0.40              |
| 2:W:85:TYR:HA    | 2:W:86:PRO:HD3   | 1.93                     | 0.40              |
| 2:B:99:LYS:N     | 2:B:100:PRO:CD   | 2.83                     | 0.40              |
| 1:G:57:LEU:HD12  | 1:G:110:LEU:HD11 | 2.04                     | 0.40              |
| 1:G:95:PRO:HG2   | 2:H:46:MET:HE3   | 2.03                     | 0.40              |
| 1:G:172:ILE:C    | 1:G:175:PRO:HD2  | 2.46                     | 0.40              |
| 2:K:375:LEU:HD22 | 2:K:396:MET:HE1  | 2.04                     | 0.40              |
| 2:Q:25:CYS:SG    | 2:Q:43:CYS:HB3   | 2.62                     | 0.40              |
| 1:S:68:PRO:HB3   | 1:S:112:VAL:HG11 | 2.04                     | 0.40              |
| 2:T:252:ASP:CB   | 2:T:255:THR:HG22 | 2.49                     | 0.40              |
| 1:V:71:VAL:CG1   | 1:V:114:LYS:HZ1  | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 476/478 (100%)  | 455 (96%)  | 19 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | D     | 476/478 (100%)  | 456 (96%)  | 18 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | G     | 476/478 (100%)  | 453 (95%)  | 21 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | J     | 476/478 (100%)  | 457 (96%)  | 17 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | M     | 476/478 (100%)  | 456 (96%)  | 18 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | P     | 476/478 (100%)  | 454 (95%)  | 20 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | S     | 476/478 (100%)  | 454 (95%)  | 20 (4%)  | 2 (0%)   | 30          | 38  |
| 1   | V     | 476/478 (100%)  | 454 (95%)  | 20 (4%)  | 2 (0%)   | 30          | 38  |
| 2   | B     | 408/478 (85%)   | 393 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 2   | E     | 408/478 (85%)   | 394 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 2   | H     | 408/478 (85%)   | 394 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 2   | K     | 408/478 (85%)   | 393 (96%)  | 14 (3%)  | 1 (0%)   | 43          | 55  |
| 2   | N     | 408/478 (85%)   | 394 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 2   | Q     | 408/478 (85%)   | 395 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 2   | T     | 408/478 (85%)   | 396 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 2   | W     | 408/478 (85%)   | 395 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 3   | C     | 89/94 (95%)     | 88 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 3   | F     | 89/94 (95%)     | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | I     | 89/94 (95%)     | 86 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 3   | L     | 89/94 (95%)     | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | O     | 89/94 (95%)     | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | R     | 89/94 (95%)     | 89 (100%)  | 0        | 0        | 100         | 100 |
| 3   | U     | 89/94 (95%)     | 86 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 3   | X     | 89/94 (95%)     | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 7784/8400 (93%) | 7490 (96%) | 277 (4%) | 17 (0%)  | 43          | 55  |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 2   | LEU  |
| 1   | S     | 2   | LEU  |
| 1   | S     | 409 | GLU  |
| 1   | G     | 2   | LEU  |
| 1   | G     | 65  | PHE  |
| 1   | J     | 2   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 2   | LEU  |
| 1   | M     | 65  | PHE  |
| 1   | V     | 2   | LEU  |
| 1   | A     | 2   | LEU  |
| 1   | A     | 65  | PHE  |
| 1   | J     | 65  | PHE  |
| 1   | P     | 2   | LEU  |
| 1   | D     | 65  | PHE  |
| 2   | K     | 113 | ASN  |
| 1   | P     | 65  | PHE  |
| 1   | V     | 65  | PHE  |

### 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     | 406/406 (100%) | 385 (95%) | 21 (5%)  | 21          | 31 |
| 1   | D     | 406/406 (100%) | 377 (93%) | 29 (7%)  | 13          | 19 |
| 1   | G     | 406/406 (100%) | 386 (95%) | 20 (5%)  | 22          | 34 |
| 1   | J     | 406/406 (100%) | 379 (93%) | 27 (7%)  | 15          | 21 |
| 1   | M     | 406/406 (100%) | 384 (95%) | 22 (5%)  | 20          | 29 |
| 1   | P     | 406/406 (100%) | 376 (93%) | 30 (7%)  | 13          | 17 |
| 1   | S     | 406/406 (100%) | 380 (94%) | 26 (6%)  | 16          | 23 |
| 1   | V     | 406/406 (100%) | 387 (95%) | 19 (5%)  | 23          | 35 |
| 2   | B     | 364/427 (85%)  | 341 (94%) | 23 (6%)  | 16          | 23 |
| 2   | E     | 364/427 (85%)  | 340 (93%) | 24 (7%)  | 15          | 21 |
| 2   | H     | 364/427 (85%)  | 338 (93%) | 26 (7%)  | 13          | 19 |
| 2   | K     | 364/427 (85%)  | 342 (94%) | 22 (6%)  | 17          | 25 |
| 2   | N     | 364/427 (85%)  | 337 (93%) | 27 (7%)  | 13          | 17 |
| 2   | Q     | 364/427 (85%)  | 341 (94%) | 23 (6%)  | 16          | 23 |
| 2   | T     | 364/427 (85%)  | 338 (93%) | 26 (7%)  | 13          | 19 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | W     | 364/427 (85%)   | 337 (93%)  | 27 (7%)  | 13          | 17 |
| 3   | C     | 86/89 (97%)     | 80 (93%)   | 6 (7%)   | 14          | 19 |
| 3   | F     | 86/89 (97%)     | 82 (95%)   | 4 (5%)   | 23          | 35 |
| 3   | I     | 86/89 (97%)     | 80 (93%)   | 6 (7%)   | 14          | 19 |
| 3   | L     | 86/89 (97%)     | 82 (95%)   | 4 (5%)   | 23          | 35 |
| 3   | O     | 86/89 (97%)     | 81 (94%)   | 5 (6%)   | 18          | 26 |
| 3   | R     | 86/89 (97%)     | 82 (95%)   | 4 (5%)   | 23          | 35 |
| 3   | U     | 86/89 (97%)     | 81 (94%)   | 5 (6%)   | 18          | 26 |
| 3   | X     | 86/89 (97%)     | 81 (94%)   | 5 (6%)   | 18          | 26 |
| All | All   | 6848/7376 (93%) | 6417 (94%) | 431 (6%) | 16          | 23 |

All (431) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | LEU  |
| 1   | A     | 57  | LEU  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 69  | ILE  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 89  | LEU  |
| 1   | A     | 115 | THR  |
| 1   | A     | 159 | SER  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 190 | ARG  |
| 1   | A     | 199 | PHE  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 245 | VAL  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 295 | VAL  |
| 1   | A     | 356 | THR  |
| 1   | A     | 389 | VAL  |
| 1   | A     | 417 | SER  |
| 1   | A     | 458 | LEU  |
| 1   | A     | 478 | THR  |
| 2   | B     | 20  | LYS  |
| 2   | B     | 21  | THR  |
| 2   | B     | 39  | VAL  |
| 2   | B     | 74  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 103 | THR  |
| 2   | B     | 134 | ILE  |
| 2   | B     | 156 | THR  |
| 2   | B     | 162 | THR  |
| 2   | B     | 188 | GLU  |
| 2   | B     | 189 | LYS  |
| 2   | B     | 203 | LYS  |
| 2   | B     | 213 | GLU  |
| 2   | B     | 217 | VAL  |
| 2   | B     | 244 | VAL  |
| 2   | B     | 250 | THR  |
| 2   | B     | 344 | VAL  |
| 2   | B     | 352 | LEU  |
| 2   | B     | 360 | ILE  |
| 2   | B     | 387 | LYS  |
| 2   | B     | 402 | THR  |
| 2   | B     | 406 | ILE  |
| 2   | B     | 407 | VAL  |
| 2   | B     | 412 | LEU  |
| 3   | C     | 34  | LEU  |
| 3   | C     | 38  | ASP  |
| 3   | C     | 46  | GLU  |
| 3   | C     | 52  | ILE  |
| 3   | C     | 70  | ASP  |
| 3   | C     | 92  | VAL  |
| 1   | D     | 10  | LEU  |
| 1   | D     | 11  | ARG  |
| 1   | D     | 51  | LEU  |
| 1   | D     | 57  | LEU  |
| 1   | D     | 61  | GLU  |
| 1   | D     | 62  | LEU  |
| 1   | D     | 67  | ILE  |
| 1   | D     | 88  | ILE  |
| 1   | D     | 89  | LEU  |
| 1   | D     | 115 | THR  |
| 1   | D     | 143 | VAL  |
| 1   | D     | 164 | LEU  |
| 1   | D     | 174 | GLN  |
| 1   | D     | 181 | VAL  |
| 1   | D     | 185 | LYS  |
| 1   | D     | 199 | PHE  |
| 1   | D     | 245 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 270 | LYS  |
| 1   | D     | 295 | VAL  |
| 1   | D     | 356 | THR  |
| 1   | D     | 376 | ARG  |
| 1   | D     | 384 | LYS  |
| 1   | D     | 388 | GLU  |
| 1   | D     | 389 | VAL  |
| 1   | D     | 392 | ILE  |
| 1   | D     | 397 | THR  |
| 1   | D     | 409 | GLU  |
| 1   | D     | 434 | ILE  |
| 1   | D     | 464 | LEU  |
| 2   | E     | 39  | VAL  |
| 2   | E     | 74  | GLU  |
| 2   | E     | 77  | VAL  |
| 2   | E     | 98  | GLU  |
| 2   | E     | 103 | THR  |
| 2   | E     | 109 | LEU  |
| 2   | E     | 113 | ASN  |
| 2   | E     | 134 | ILE  |
| 2   | E     | 139 | LYS  |
| 2   | E     | 232 | GLU  |
| 2   | E     | 244 | VAL  |
| 2   | E     | 262 | ARG  |
| 2   | E     | 278 | LEU  |
| 2   | E     | 283 | VAL  |
| 2   | E     | 341 | LYS  |
| 2   | E     | 344 | VAL  |
| 2   | E     | 352 | LEU  |
| 2   | E     | 364 | GLU  |
| 2   | E     | 387 | LYS  |
| 2   | E     | 397 | VAL  |
| 2   | E     | 402 | THR  |
| 2   | E     | 406 | ILE  |
| 2   | E     | 407 | VAL  |
| 2   | E     | 412 | LEU  |
| 3   | F     | 34  | LEU  |
| 3   | F     | 39  | GLN  |
| 3   | F     | 46  | GLU  |
| 3   | F     | 52  | ILE  |
| 1   | G     | 10  | LEU  |
| 1   | G     | 26  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 51  | LEU  |
| 1   | G     | 57  | LEU  |
| 1   | G     | 59  | GLU  |
| 1   | G     | 62  | LEU  |
| 1   | G     | 78  | GLU  |
| 1   | G     | 89  | LEU  |
| 1   | G     | 115 | THR  |
| 1   | G     | 117 | LEU  |
| 1   | G     | 164 | LEU  |
| 1   | G     | 199 | PHE  |
| 1   | G     | 245 | VAL  |
| 1   | G     | 327 | LYS  |
| 1   | G     | 356 | THR  |
| 1   | G     | 392 | ILE  |
| 1   | G     | 397 | THR  |
| 1   | G     | 401 | PRO  |
| 1   | G     | 434 | ILE  |
| 1   | G     | 458 | LEU  |
| 2   | H     | 21  | THR  |
| 2   | H     | 39  | VAL  |
| 2   | H     | 74  | GLU  |
| 2   | H     | 98  | GLU  |
| 2   | H     | 103 | THR  |
| 2   | H     | 109 | LEU  |
| 2   | H     | 113 | ASN  |
| 2   | H     | 121 | ILE  |
| 2   | H     | 132 | LYS  |
| 2   | H     | 162 | THR  |
| 2   | H     | 168 | LEU  |
| 2   | H     | 203 | LYS  |
| 2   | H     | 225 | LYS  |
| 2   | H     | 244 | VAL  |
| 2   | H     | 245 | VAL  |
| 2   | H     | 266 | GLU  |
| 2   | H     | 309 | GLU  |
| 2   | H     | 335 | ARG  |
| 2   | H     | 344 | VAL  |
| 2   | H     | 352 | LEU  |
| 2   | H     | 391 | GLU  |
| 2   | H     | 395 | GLU  |
| 2   | H     | 402 | THR  |
| 2   | H     | 406 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 407 | VAL  |
| 2   | H     | 412 | LEU  |
| 3   | I     | 21  | GLU  |
| 3   | I     | 39  | GLN  |
| 3   | I     | 52  | ILE  |
| 3   | I     | 70  | ASP  |
| 3   | I     | 81  | ARG  |
| 3   | I     | 92  | VAL  |
| 1   | J     | 10  | LEU  |
| 1   | J     | 51  | LEU  |
| 1   | J     | 56  | SER  |
| 1   | J     | 57  | LEU  |
| 1   | J     | 59  | GLU  |
| 1   | J     | 62  | LEU  |
| 1   | J     | 78  | GLU  |
| 1   | J     | 88  | ILE  |
| 1   | J     | 89  | LEU  |
| 1   | J     | 112 | VAL  |
| 1   | J     | 115 | THR  |
| 1   | J     | 162 | VAL  |
| 1   | J     | 164 | LEU  |
| 1   | J     | 174 | GLN  |
| 1   | J     | 181 | VAL  |
| 1   | J     | 185 | LYS  |
| 1   | J     | 199 | PHE  |
| 1   | J     | 201 | SER  |
| 1   | J     | 240 | GLU  |
| 1   | J     | 245 | VAL  |
| 1   | J     | 279 | GLU  |
| 1   | J     | 295 | VAL  |
| 1   | J     | 356 | THR  |
| 1   | J     | 376 | ARG  |
| 1   | J     | 434 | ILE  |
| 1   | J     | 458 | LEU  |
| 1   | J     | 478 | THR  |
| 2   | K     | 21  | THR  |
| 2   | K     | 30  | GLU  |
| 2   | K     | 39  | VAL  |
| 2   | K     | 74  | GLU  |
| 2   | K     | 103 | THR  |
| 2   | K     | 109 | LEU  |
| 2   | K     | 113 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 115 | GLU  |
| 2   | K     | 132 | LYS  |
| 2   | K     | 134 | ILE  |
| 2   | K     | 162 | THR  |
| 2   | K     | 244 | VAL  |
| 2   | K     | 245 | VAL  |
| 2   | K     | 266 | GLU  |
| 2   | K     | 338 | LYS  |
| 2   | K     | 341 | LYS  |
| 2   | K     | 344 | VAL  |
| 2   | K     | 352 | LEU  |
| 2   | K     | 360 | ILE  |
| 2   | K     | 363 | GLU  |
| 2   | K     | 405 | GLN  |
| 2   | K     | 412 | LEU  |
| 3   | L     | 34  | LEU  |
| 3   | L     | 52  | ILE  |
| 3   | L     | 91  | VAL  |
| 3   | L     | 92  | VAL  |
| 1   | M     | 10  | LEU  |
| 1   | M     | 40  | LYS  |
| 1   | M     | 51  | LEU  |
| 1   | M     | 57  | LEU  |
| 1   | M     | 62  | LEU  |
| 1   | M     | 78  | GLU  |
| 1   | M     | 88  | ILE  |
| 1   | M     | 89  | LEU  |
| 1   | M     | 112 | VAL  |
| 1   | M     | 115 | THR  |
| 1   | M     | 174 | GLN  |
| 1   | M     | 199 | PHE  |
| 1   | M     | 205 | GLN  |
| 1   | M     | 211 | ARG  |
| 1   | M     | 245 | VAL  |
| 1   | M     | 250 | LYS  |
| 1   | M     | 299 | ILE  |
| 1   | M     | 354 | LEU  |
| 1   | M     | 356 | THR  |
| 1   | M     | 409 | GLU  |
| 1   | M     | 434 | ILE  |
| 1   | M     | 478 | THR  |
| 2   | N     | 21  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 39  | VAL  |
| 2   | N     | 74  | GLU  |
| 2   | N     | 95  | SER  |
| 2   | N     | 98  | GLU  |
| 2   | N     | 103 | THR  |
| 2   | N     | 134 | ILE  |
| 2   | N     | 141 | LEU  |
| 2   | N     | 162 | THR  |
| 2   | N     | 189 | LYS  |
| 2   | N     | 203 | LYS  |
| 2   | N     | 223 | VAL  |
| 2   | N     | 244 | VAL  |
| 2   | N     | 245 | VAL  |
| 2   | N     | 250 | THR  |
| 2   | N     | 266 | GLU  |
| 2   | N     | 320 | LEU  |
| 2   | N     | 344 | VAL  |
| 2   | N     | 360 | ILE  |
| 2   | N     | 382 | LYS  |
| 2   | N     | 387 | LYS  |
| 2   | N     | 390 | LYS  |
| 2   | N     | 391 | GLU  |
| 2   | N     | 395 | GLU  |
| 2   | N     | 402 | THR  |
| 2   | N     | 407 | VAL  |
| 2   | N     | 412 | LEU  |
| 3   | O     | 34  | LEU  |
| 3   | O     | 38  | ASP  |
| 3   | O     | 52  | ILE  |
| 3   | O     | 73  | LYS  |
| 3   | O     | 92  | VAL  |
| 1   | P     | 10  | LEU  |
| 1   | P     | 31  | ARG  |
| 1   | P     | 40  | LYS  |
| 1   | P     | 51  | LEU  |
| 1   | P     | 57  | LEU  |
| 1   | P     | 59  | GLU  |
| 1   | P     | 62  | LEU  |
| 1   | P     | 78  | GLU  |
| 1   | P     | 88  | ILE  |
| 1   | P     | 89  | LEU  |
| 1   | P     | 111 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 115 | THR  |
| 1   | P     | 143 | VAL  |
| 1   | P     | 162 | VAL  |
| 1   | P     | 164 | LEU  |
| 1   | P     | 174 | GLN  |
| 1   | P     | 181 | VAL  |
| 1   | P     | 185 | LYS  |
| 1   | P     | 199 | PHE  |
| 1   | P     | 240 | GLU  |
| 1   | P     | 245 | VAL  |
| 1   | P     | 279 | GLU  |
| 1   | P     | 291 | SER  |
| 1   | P     | 295 | VAL  |
| 1   | P     | 325 | ARG  |
| 1   | P     | 356 | THR  |
| 1   | P     | 434 | ILE  |
| 1   | P     | 458 | LEU  |
| 1   | P     | 464 | LEU  |
| 1   | P     | 478 | THR  |
| 2   | Q     | 21  | THR  |
| 2   | Q     | 39  | VAL  |
| 2   | Q     | 74  | GLU  |
| 2   | Q     | 103 | THR  |
| 2   | Q     | 109 | LEU  |
| 2   | Q     | 132 | LYS  |
| 2   | Q     | 156 | THR  |
| 2   | Q     | 162 | THR  |
| 2   | Q     | 210 | THR  |
| 2   | Q     | 217 | VAL  |
| 2   | Q     | 244 | VAL  |
| 2   | Q     | 245 | VAL  |
| 2   | Q     | 255 | THR  |
| 2   | Q     | 302 | ARG  |
| 2   | Q     | 335 | ARG  |
| 2   | Q     | 344 | VAL  |
| 2   | Q     | 352 | LEU  |
| 2   | Q     | 360 | ILE  |
| 2   | Q     | 365 | SER  |
| 2   | Q     | 387 | LYS  |
| 2   | Q     | 402 | THR  |
| 2   | Q     | 405 | GLN  |
| 2   | Q     | 412 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | R     | 34  | LEU  |
| 3   | R     | 45  | THR  |
| 3   | R     | 52  | ILE  |
| 3   | R     | 56  | GLU  |
| 1   | S     | 10  | LEU  |
| 1   | S     | 11  | ARG  |
| 1   | S     | 51  | LEU  |
| 1   | S     | 57  | LEU  |
| 1   | S     | 59  | GLU  |
| 1   | S     | 62  | LEU  |
| 1   | S     | 69  | ILE  |
| 1   | S     | 88  | ILE  |
| 1   | S     | 89  | LEU  |
| 1   | S     | 140 | LEU  |
| 1   | S     | 155 | VAL  |
| 1   | S     | 164 | LEU  |
| 1   | S     | 172 | ILE  |
| 1   | S     | 181 | VAL  |
| 1   | S     | 192 | SER  |
| 1   | S     | 199 | PHE  |
| 1   | S     | 242 | SER  |
| 1   | S     | 245 | VAL  |
| 1   | S     | 295 | VAL  |
| 1   | S     | 356 | THR  |
| 1   | S     | 376 | ARG  |
| 1   | S     | 384 | LYS  |
| 1   | S     | 389 | VAL  |
| 1   | S     | 392 | ILE  |
| 1   | S     | 458 | LEU  |
| 1   | S     | 464 | LEU  |
| 2   | T     | 21  | THR  |
| 2   | T     | 39  | VAL  |
| 2   | T     | 74  | GLU  |
| 2   | T     | 90  | LYS  |
| 2   | T     | 98  | GLU  |
| 2   | T     | 103 | THR  |
| 2   | T     | 109 | LEU  |
| 2   | T     | 123 | ARG  |
| 2   | T     | 139 | LYS  |
| 2   | T     | 156 | THR  |
| 2   | T     | 164 | GLU  |
| 2   | T     | 189 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | T     | 214 | ILE  |
| 2   | T     | 232 | GLU  |
| 2   | T     | 244 | VAL  |
| 2   | T     | 245 | VAL  |
| 2   | T     | 250 | THR  |
| 2   | T     | 262 | ARG  |
| 2   | T     | 335 | ARG  |
| 2   | T     | 341 | LYS  |
| 2   | T     | 344 | VAL  |
| 2   | T     | 360 | ILE  |
| 2   | T     | 394 | LYS  |
| 2   | T     | 406 | ILE  |
| 2   | T     | 407 | VAL  |
| 2   | T     | 412 | LEU  |
| 3   | U     | 34  | LEU  |
| 3   | U     | 45  | THR  |
| 3   | U     | 52  | ILE  |
| 3   | U     | 54  | GLU  |
| 3   | U     | 70  | ASP  |
| 1   | V     | 10  | LEU  |
| 1   | V     | 53  | GLN  |
| 1   | V     | 57  | LEU  |
| 1   | V     | 62  | LEU  |
| 1   | V     | 88  | ILE  |
| 1   | V     | 89  | LEU  |
| 1   | V     | 115 | THR  |
| 1   | V     | 124 | SER  |
| 1   | V     | 143 | VAL  |
| 1   | V     | 181 | VAL  |
| 1   | V     | 190 | ARG  |
| 1   | V     | 199 | PHE  |
| 1   | V     | 245 | VAL  |
| 1   | V     | 279 | GLU  |
| 1   | V     | 295 | VAL  |
| 1   | V     | 356 | THR  |
| 1   | V     | 392 | ILE  |
| 1   | V     | 434 | ILE  |
| 1   | V     | 478 | THR  |
| 2   | W     | 8   | VAL  |
| 2   | W     | 21  | THR  |
| 2   | W     | 39  | VAL  |
| 2   | W     | 46  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | W     | 74  | GLU  |
| 2   | W     | 95  | SER  |
| 2   | W     | 103 | THR  |
| 2   | W     | 109 | LEU  |
| 2   | W     | 116 | LYS  |
| 2   | W     | 134 | ILE  |
| 2   | W     | 156 | THR  |
| 2   | W     | 162 | THR  |
| 2   | W     | 203 | LYS  |
| 2   | W     | 210 | THR  |
| 2   | W     | 217 | VAL  |
| 2   | W     | 244 | VAL  |
| 2   | W     | 250 | THR  |
| 2   | W     | 302 | ARG  |
| 2   | W     | 344 | VAL  |
| 2   | W     | 352 | LEU  |
| 2   | W     | 358 | LYS  |
| 2   | W     | 364 | GLU  |
| 2   | W     | 387 | LYS  |
| 2   | W     | 402 | THR  |
| 2   | W     | 406 | ILE  |
| 2   | W     | 407 | VAL  |
| 2   | W     | 412 | LEU  |
| 3   | X     | 34  | LEU  |
| 3   | X     | 38  | ASP  |
| 3   | X     | 39  | GLN  |
| 3   | X     | 46  | GLU  |
| 3   | X     | 52  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | ASN  |
| 1   | A     | 205 | GLN  |
| 2   | B     | 218 | ASN  |
| 1   | D     | 34  | GLN  |
| 2   | E     | 218 | ASN  |
| 3   | F     | 39  | GLN  |
| 1   | G     | 53  | GLN  |
| 1   | G     | 380 | ASN  |
| 1   | G     | 471 | HIS  |
| 2   | H     | 371 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 27  | GLN  |
| 2   | K     | 135 | HIS  |
| 2   | K     | 216 | ASN  |
| 2   | K     | 246 | GLN  |
| 2   | K     | 294 | ASN  |
| 2   | K     | 405 | GLN  |
| 1   | M     | 275 | ASN  |
| 2   | N     | 218 | ASN  |
| 2   | N     | 405 | GLN  |
| 1   | P     | 91  | ASN  |
| 2   | Q     | 218 | ASN  |
| 3   | R     | 27  | GLN  |
| 1   | S     | 447 | GLN  |
| 2   | T     | 218 | ASN  |
| 1   | V     | 53  | GLN  |
| 1   | V     | 460 | GLN  |
| 2   | W     | 218 | ASN  |
| 2   | W     | 301 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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 | $\# Z  > 2$ |
| 4   | ASN  | P     | 906 | 1    | 6,7,8        | 1.10 | 0           | 3,8,10      | 1.49 | 0           |
| 5   | ADP  | W     | 708 | -    | 28,29,29     | 1.47 | 5 (17%)     | 43,45,45    | 1.80 | 8 (18%)     |
| 4   | ASN  | G     | 903 | 1    | 6,7,8        | 1.20 | 1 (16%)     | 3,8,10      | 2.38 | 1 (33%)     |
| 4   | ASN  | D     | 902 | 1    | 6,7,8        | 1.12 | 1 (16%)     | 3,8,10      | 1.51 | 1 (33%)     |
| 4   | ASN  | S     | 907 | 1    | 6,7,8        | 1.52 | 2 (33%)     | 3,8,10      | 2.23 | 1 (33%)     |
| 5   | ADP  | N     | 705 | -    | 28,29,29     | 1.61 | 6 (21%)     | 43,45,45    | 1.68 | 8 (18%)     |
| 4   | ASN  | M     | 905 | 1    | 6,7,8        | 1.24 | 1 (16%)     | 3,8,10      | 1.82 | 1 (33%)     |
| 4   | ASN  | A     | 901 | 1    | 6,7,8        | 1.18 | 1 (16%)     | 3,8,10      | 1.25 | 0           |
| 5   | ADP  | K     | 704 | -    | 28,29,29     | 1.50 | 5 (17%)     | 43,45,45    | 1.78 | 6 (13%)     |
| 5   | ADP  | Q     | 706 | -    | 28,29,29     | 1.51 | 4 (14%)     | 43,45,45    | 1.79 | 9 (20%)     |
| 4   | ASN  | V     | 908 | 1    | 6,7,8        | 1.39 | 1 (16%)     | 3,8,10      | 1.58 | 1 (33%)     |
| 5   | ADP  | E     | 702 | -    | 28,29,29     | 1.43 | 6 (21%)     | 43,45,45    | 1.75 | 11 (25%)    |
| 5   | ADP  | H     | 703 | -    | 28,29,29     | 1.66 | 6 (21%)     | 43,45,45    | 1.64 | 6 (13%)     |
| 5   | ADP  | T     | 707 | -    | 28,29,29     | 1.44 | 6 (21%)     | 43,45,45    | 1.75 | 10 (23%)    |
| 4   | ASN  | J     | 904 | 1    | 6,7,8        | 1.24 | 1 (16%)     | 3,8,10      | 1.76 | 1 (33%)     |
| 5   | ADP  | B     | 701 | -    | 28,29,29     | 1.59 | 4 (14%)     | 43,45,45    | 1.78 | 9 (20%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | ASN  | P     | 906 | 1    | -       | 1/7/7/8    | -       |
| 5   | ADP  | W     | 708 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 4   | ASN  | G     | 903 | 1    | -       | 2/7/7/8    | -       |
| 4   | ASN  | D     | 902 | 1    | -       | 2/7/7/8    | -       |
| 4   | ASN  | S     | 907 | 1    | -       | 2/7/7/8    | -       |
| 5   | ADP  | N     | 705 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 4   | ASN  | M     | 905 | 1    | -       | 2/7/7/8    | -       |
| 4   | ASN  | A     | 901 | 1    | -       | 1/7/7/8    | -       |
| 5   | ADP  | K     | 704 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | ADP  | Q     | 706 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 4   | ASN  | V     | 908 | 1    | -       | 0/7/7/8    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | ADP  | E     | 702 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 5   | ADP  | H     | 703 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 5   | ADP  | T     | 707 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 4   | ASN  | J     | 904 | 1    | -       | 2/7/7/8    | -       |
| 5   | ADP  | B     | 701 | -    | -       | 4/16/32/32 | 0/3/3/3 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | B     | 701 | ADP  | C5-C4  | 5.23  | 1.48        | 1.39     |
| 5   | N     | 705 | ADP  | C5-C4  | 4.99  | 1.48        | 1.39     |
| 5   | H     | 703 | ADP  | C5-C4  | 4.90  | 1.47        | 1.39     |
| 5   | W     | 708 | ADP  | C5-C4  | 4.88  | 1.47        | 1.39     |
| 5   | Q     | 706 | ADP  | C5-C4  | 4.84  | 1.47        | 1.39     |
| 5   | K     | 704 | ADP  | C5-C4  | 4.79  | 1.47        | 1.39     |
| 5   | T     | 707 | ADP  | C5-C4  | 4.71  | 1.47        | 1.39     |
| 5   | E     | 702 | ADP  | C5-C4  | 4.67  | 1.47        | 1.39     |
| 5   | H     | 703 | ADP  | PA-O3A | 4.56  | 1.64        | 1.59     |
| 5   | N     | 705 | ADP  | PA-O3A | 3.95  | 1.63        | 1.59     |
| 5   | K     | 704 | ADP  | PA-O3A | 3.36  | 1.63        | 1.59     |
| 5   | B     | 701 | ADP  | PA-O3A | 3.28  | 1.63        | 1.59     |
| 5   | Q     | 706 | ADP  | PA-O3A | 3.05  | 1.62        | 1.59     |
| 5   | B     | 701 | ADP  | C5-C6  | 3.05  | 1.49        | 1.41     |
| 5   | Q     | 706 | ADP  | C8-N7  | 2.95  | 1.37        | 1.31     |
| 5   | W     | 708 | ADP  | C5-C6  | 2.93  | 1.49        | 1.41     |
| 5   | Q     | 706 | ADP  | C5-C6  | 2.84  | 1.48        | 1.41     |
| 5   | B     | 701 | ADP  | C8-N7  | 2.83  | 1.37        | 1.31     |
| 5   | T     | 707 | ADP  | C5-C6  | 2.67  | 1.48        | 1.41     |
| 5   | E     | 702 | ADP  | C5-C6  | 2.62  | 1.48        | 1.41     |
| 5   | H     | 703 | ADP  | C5-C6  | 2.59  | 1.48        | 1.41     |
| 4   | M     | 905 | ASN  | OXT-C  | -2.57 | 1.22        | 1.30     |
| 5   | K     | 704 | ADP  | C5-C6  | 2.56  | 1.48        | 1.41     |
| 5   | E     | 702 | ADP  | PA-O3A | 2.56  | 1.62        | 1.59     |
| 5   | N     | 705 | ADP  | C5-C6  | 2.55  | 1.48        | 1.41     |
| 5   | N     | 705 | ADP  | C5-N7  | -2.53 | 1.34        | 1.39     |
| 5   | H     | 703 | ADP  | C5-N7  | -2.47 | 1.34        | 1.39     |
| 4   | S     | 907 | ASN  | CB-CG  | 2.46  | 1.56        | 1.50     |
| 5   | N     | 705 | ADP  | C4-N9  | -2.43 | 1.32        | 1.37     |
| 5   | W     | 708 | ADP  | PA-O3A | 2.41  | 1.62        | 1.59     |
| 5   | H     | 703 | ADP  | C8-N7  | 2.41  | 1.36        | 1.31     |
| 5   | W     | 708 | ADP  | C8-N7  | 2.39  | 1.36        | 1.31     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | S     | 907 | ASN  | OXT-C  | -2.37 | 1.23        | 1.30     |
| 4   | D     | 902 | ASN  | OXT-C  | -2.36 | 1.23        | 1.30     |
| 4   | G     | 903 | ASN  | OXT-C  | -2.27 | 1.23        | 1.30     |
| 5   | E     | 702 | ADP  | C8-N7  | 2.24  | 1.36        | 1.31     |
| 5   | W     | 708 | ADP  | C5-N7  | -2.23 | 1.35        | 1.39     |
| 5   | E     | 702 | ADP  | C5-N7  | -2.22 | 1.35        | 1.39     |
| 5   | N     | 705 | ADP  | C8-N7  | 2.21  | 1.35        | 1.31     |
| 5   | T     | 707 | ADP  | C8-N7  | 2.19  | 1.35        | 1.31     |
| 5   | T     | 707 | ADP  | C4-N9  | -2.17 | 1.33        | 1.37     |
| 5   | H     | 703 | ADP  | C4-N9  | -2.17 | 1.33        | 1.37     |
| 5   | T     | 707 | ADP  | C5-N7  | -2.17 | 1.35        | 1.39     |
| 5   | E     | 702 | ADP  | C4-N9  | -2.15 | 1.33        | 1.37     |
| 5   | K     | 704 | ADP  | C5-N7  | -2.14 | 1.35        | 1.39     |
| 5   | T     | 707 | ADP  | PA-O3A | 2.13  | 1.61        | 1.59     |
| 5   | K     | 704 | ADP  | C8-N7  | 2.11  | 1.35        | 1.31     |
| 4   | J     | 904 | ASN  | OXT-C  | -2.10 | 1.23        | 1.30     |
| 4   | A     | 901 | ASN  | OXT-C  | -2.01 | 1.24        | 1.30     |
| 4   | V     | 908 | ASN  | CB-CG  | 2.01  | 1.55        | 1.50     |

All (73) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | W     | 708 | ADP  | C5-C4-N3 | -6.03 | 118.42      | 126.72   |
| 5   | Q     | 706 | ADP  | C5-C4-N3 | -5.99 | 118.47      | 126.72   |
| 5   | B     | 701 | ADP  | C5-C4-N3 | -5.89 | 118.60      | 126.72   |
| 5   | T     | 707 | ADP  | C5-C4-N3 | -5.66 | 118.92      | 126.72   |
| 5   | K     | 704 | ADP  | C5-C4-N3 | -5.47 | 119.18      | 126.72   |
| 5   | H     | 703 | ADP  | C5-C4-N3 | -5.31 | 119.41      | 126.72   |
| 5   | E     | 702 | ADP  | C5-C4-N3 | -5.20 | 119.55      | 126.72   |
| 5   | N     | 705 | ADP  | C5-C4-N3 | -5.11 | 119.68      | 126.72   |
| 5   | K     | 704 | ADP  | N3-C4-N9 | 4.84  | 135.41      | 127.17   |
| 5   | T     | 707 | ADP  | N3-C4-N9 | 4.61  | 135.02      | 127.17   |
| 5   | W     | 708 | ADP  | N3-C4-N9 | 4.56  | 134.92      | 127.17   |
| 5   | Q     | 706 | ADP  | N3-C4-N9 | 4.48  | 134.79      | 127.17   |
| 5   | E     | 702 | ADP  | N3-C4-N9 | 4.39  | 134.63      | 127.17   |
| 5   | H     | 703 | ADP  | N3-C4-N9 | 4.33  | 134.52      | 127.17   |
| 5   | B     | 701 | ADP  | N3-C4-N9 | 4.32  | 134.52      | 127.17   |
| 5   | N     | 705 | ADP  | N3-C4-N9 | 4.32  | 134.51      | 127.17   |
| 5   | Q     | 706 | ADP  | C2-N3-C4 | 3.77  | 121.05      | 111.83   |
| 5   | B     | 701 | ADP  | C2-N3-C4 | 3.77  | 121.03      | 111.83   |
| 5   | B     | 701 | ADP  | C4-C5-N7 | -3.73 | 106.32      | 110.58   |
| 5   | W     | 708 | ADP  | C4-C5-N7 | -3.71 | 106.34      | 110.58   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | W     | 708 | ADP  | C2-N3-C4   | 3.71  | 120.88      | 111.83   |
| 5   | K     | 704 | ADP  | C2-N3-C4   | 3.64  | 120.71      | 111.83   |
| 4   | G     | 903 | ASN  | OXT-C-O    | -3.62 | 115.86      | 124.08   |
| 5   | Q     | 706 | ADP  | C4-C5-N7   | -3.61 | 106.45      | 110.58   |
| 5   | K     | 704 | ADP  | N3-C2-N1   | -3.57 | 123.19      | 128.58   |
| 5   | T     | 707 | ADP  | C2-N3-C4   | 3.56  | 120.52      | 111.83   |
| 5   | H     | 703 | ADP  | C2-N3-C4   | 3.48  | 120.34      | 111.83   |
| 4   | S     | 907 | ASN  | OXT-C-O    | -3.46 | 116.23      | 124.08   |
| 5   | E     | 702 | ADP  | C2-N3-C4   | 3.45  | 120.25      | 111.83   |
| 5   | E     | 702 | ADP  | N3-C2-N1   | -3.39 | 123.45      | 128.58   |
| 5   | E     | 702 | ADP  | C4-N9-C8   | 3.35  | 109.25      | 105.74   |
| 5   | T     | 707 | ADP  | C4-C5-N7   | -3.35 | 106.76      | 110.58   |
| 5   | H     | 703 | ADP  | N3-C2-N1   | -3.26 | 123.64      | 128.58   |
| 5   | E     | 702 | ADP  | C4-C5-N7   | -3.23 | 106.89      | 110.58   |
| 5   | N     | 705 | ADP  | C2-N3-C4   | 3.23  | 119.72      | 111.83   |
| 5   | N     | 705 | ADP  | N3-C2-N1   | -3.11 | 123.88      | 128.58   |
| 5   | B     | 701 | ADP  | N3-C2-N1   | -3.09 | 123.90      | 128.58   |
| 5   | T     | 707 | ADP  | N3-C2-N1   | -3.06 | 123.95      | 128.58   |
| 5   | Q     | 706 | ADP  | N3-C2-N1   | -3.03 | 124.00      | 128.58   |
| 5   | T     | 707 | ADP  | C4-N9-C8   | 3.02  | 108.90      | 105.74   |
| 5   | K     | 704 | ADP  | C4-N9-C8   | 2.98  | 108.87      | 105.74   |
| 5   | N     | 705 | ADP  | C4-N9-C8   | 2.94  | 108.82      | 105.74   |
| 5   | N     | 705 | ADP  | C4-C5-N7   | -2.89 | 107.28      | 110.58   |
| 5   | W     | 708 | ADP  | N3-C2-N1   | -2.80 | 124.35      | 128.58   |
| 5   | W     | 708 | ADP  | C5-N7-C8   | 2.67  | 107.64      | 103.45   |
| 5   | H     | 703 | ADP  | C4-C5-N7   | -2.66 | 107.54      | 110.58   |
| 5   | K     | 704 | ADP  | C4-C5-N7   | -2.62 | 107.58      | 110.58   |
| 5   | B     | 701 | ADP  | C6-C5-N7   | 2.60  | 137.09      | 132.09   |
| 5   | E     | 702 | ADP  | C5-N7-C8   | 2.53  | 107.43      | 103.45   |
| 4   | M     | 905 | ASN  | OXT-C-O    | -2.53 | 118.34      | 124.08   |
| 5   | Q     | 706 | ADP  | C6-C5-N7   | 2.51  | 136.93      | 132.09   |
| 5   | Q     | 706 | ADP  | C5-N7-C8   | 2.49  | 107.36      | 103.45   |
| 4   | V     | 908 | ASN  | OD1-CG-CB  | -2.43 | 118.31      | 125.38   |
| 5   | T     | 707 | ADP  | O3B-PB-O2B | 2.42  | 116.89      | 107.80   |
| 5   | B     | 701 | ADP  | C5-N7-C8   | 2.40  | 107.23      | 103.45   |
| 5   | T     | 707 | ADP  | C5-N7-C8   | 2.40  | 107.22      | 103.45   |
| 5   | Q     | 706 | ADP  | C4-N9-C8   | 2.39  | 108.25      | 105.74   |
| 5   | Q     | 706 | ADP  | O3B-PB-O2B | 2.37  | 116.68      | 107.80   |
| 5   | E     | 702 | ADP  | N9-C8-N7   | -2.34 | 110.61      | 113.94   |
| 5   | H     | 703 | ADP  | C4-N9-C8   | 2.30  | 108.15      | 105.74   |
| 5   | W     | 708 | ADP  | C6-C5-N7   | 2.30  | 136.52      | 132.09   |
| 4   | J     | 904 | ASN  | OD1-CG-CB  | -2.29 | 118.71      | 125.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | B     | 701 | ADP  | C4-N9-C8   | 2.28  | 108.13      | 105.74   |
| 5   | T     | 707 | ADP  | C6-C5-N7   | 2.24  | 136.41      | 132.09   |
| 5   | N     | 705 | ADP  | C2-N1-C6   | 2.21  | 122.36      | 118.73   |
| 5   | E     | 702 | ADP  | C6-C5-N7   | 2.20  | 136.34      | 132.09   |
| 5   | W     | 708 | ADP  | C4-N9-C8   | 2.19  | 108.04      | 105.74   |
| 5   | N     | 705 | ADP  | C5-N7-C8   | 2.16  | 106.85      | 103.45   |
| 5   | E     | 702 | ADP  | O3B-PB-O2B | 2.12  | 115.76      | 107.80   |
| 5   | E     | 702 | ADP  | C2-N1-C6   | 2.08  | 122.14      | 118.73   |
| 5   | B     | 701 | ADP  | O4'-C1'-N9 | 2.03  | 112.00      | 108.09   |
| 4   | D     | 902 | ASN  | OXT-C-O    | -2.03 | 119.47      | 124.08   |
| 5   | T     | 707 | ADP  | N9-C8-N7   | -2.03 | 111.06      | 113.94   |

There are no chirality outliers.

All (48) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | B     | 701 | ADP  | PA-O3A-PB-O2B   |
| 5   | B     | 701 | ADP  | O4'-C4'-C5'-O5' |
| 5   | E     | 702 | ADP  | C5'-O5'-PA-O1A  |
| 5   | K     | 704 | ADP  | PA-O3A-PB-O3B   |
| 5   | K     | 704 | ADP  | O4'-C4'-C5'-O5' |
| 5   | N     | 705 | ADP  | C5'-O5'-PA-O1A  |
| 5   | N     | 705 | ADP  | C5'-O5'-PA-O2A  |
| 5   | N     | 705 | ADP  | C5'-O5'-PA-O3A  |
| 5   | Q     | 706 | ADP  | C5'-O5'-PA-O1A  |
| 5   | Q     | 706 | ADP  | C5'-O5'-PA-O2A  |
| 5   | Q     | 706 | ADP  | C5'-O5'-PA-O3A  |
| 5   | T     | 707 | ADP  | C5'-O5'-PA-O2A  |
| 5   | T     | 707 | ADP  | C5'-O5'-PA-O3A  |
| 5   | T     | 707 | ADP  | O4'-C4'-C5'-O5' |
| 5   | W     | 708 | ADP  | PA-O3A-PB-O2B   |
| 5   | W     | 708 | ADP  | O4'-C4'-C5'-O5' |
| 5   | B     | 701 | ADP  | C3'-C4'-C5'-O5' |
| 5   | T     | 707 | ADP  | C3'-C4'-C5'-O5' |
| 5   | W     | 708 | ADP  | C3'-C4'-C5'-O5' |
| 5   | K     | 704 | ADP  | C3'-C4'-C5'-O5' |
| 5   | Q     | 706 | ADP  | O4'-C4'-C5'-O5' |
| 4   | J     | 904 | ASN  | O-C-CA-N        |
| 4   | P     | 906 | ASN  | OXT-C-CA-N      |
| 5   | H     | 703 | ADP  | C5'-O5'-PA-O1A  |
| 5   | H     | 703 | ADP  | C5'-O5'-PA-O2A  |
| 5   | H     | 703 | ADP  | C5'-O5'-PA-O3A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | T     | 707 | ADP  | C5'-O5'-PA-O1A  |
| 5   | Q     | 706 | ADP  | PA-O3A-PB-O1B   |
| 4   | D     | 902 | ASN  | O-C-CA-N        |
| 5   | E     | 702 | ADP  | O4'-C4'-C5'-O5' |
| 4   | J     | 904 | ASN  | OXT-C-CA-N      |
| 4   | D     | 902 | ASN  | OXT-C-CA-N      |
| 5   | K     | 704 | ADP  | PA-O3A-PB-O1B   |
| 5   | B     | 701 | ADP  | PA-O3A-PB-O3B   |
| 5   | H     | 703 | ADP  | PA-O3A-PB-O3B   |
| 5   | T     | 707 | ADP  | PA-O3A-PB-O3B   |
| 4   | G     | 903 | ASN  | OXT-C-CA-N      |
| 4   | M     | 905 | ASN  | OXT-C-CA-N      |
| 5   | N     | 705 | ADP  | O4'-C4'-C5'-O5' |
| 5   | H     | 703 | ADP  | PA-O3A-PB-O1B   |
| 5   | W     | 708 | ADP  | PA-O3A-PB-O1B   |
| 4   | S     | 907 | ASN  | OXT-C-CA-N      |
| 5   | Q     | 706 | ADP  | C3'-C4'-C5'-O5' |
| 4   | G     | 903 | ASN  | O-C-CA-N        |
| 4   | M     | 905 | ASN  | O-C-CA-N        |
| 4   | S     | 907 | ASN  | O-C-CA-N        |
| 5   | E     | 702 | ADP  | PB-O3A-PA-O2A   |
| 4   | A     | 901 | ASN  | OXT-C-CA-N      |

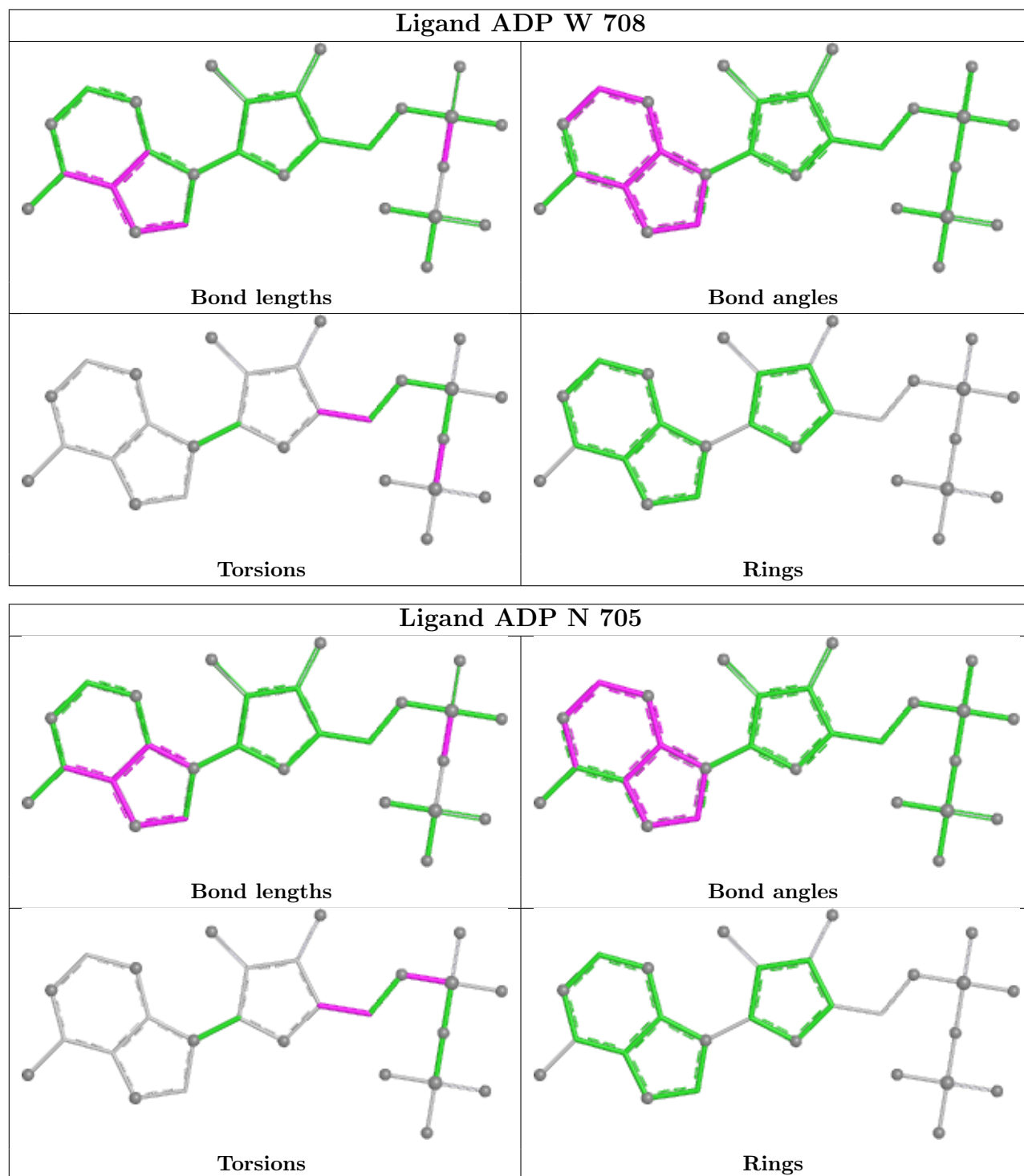
There are no ring outliers.

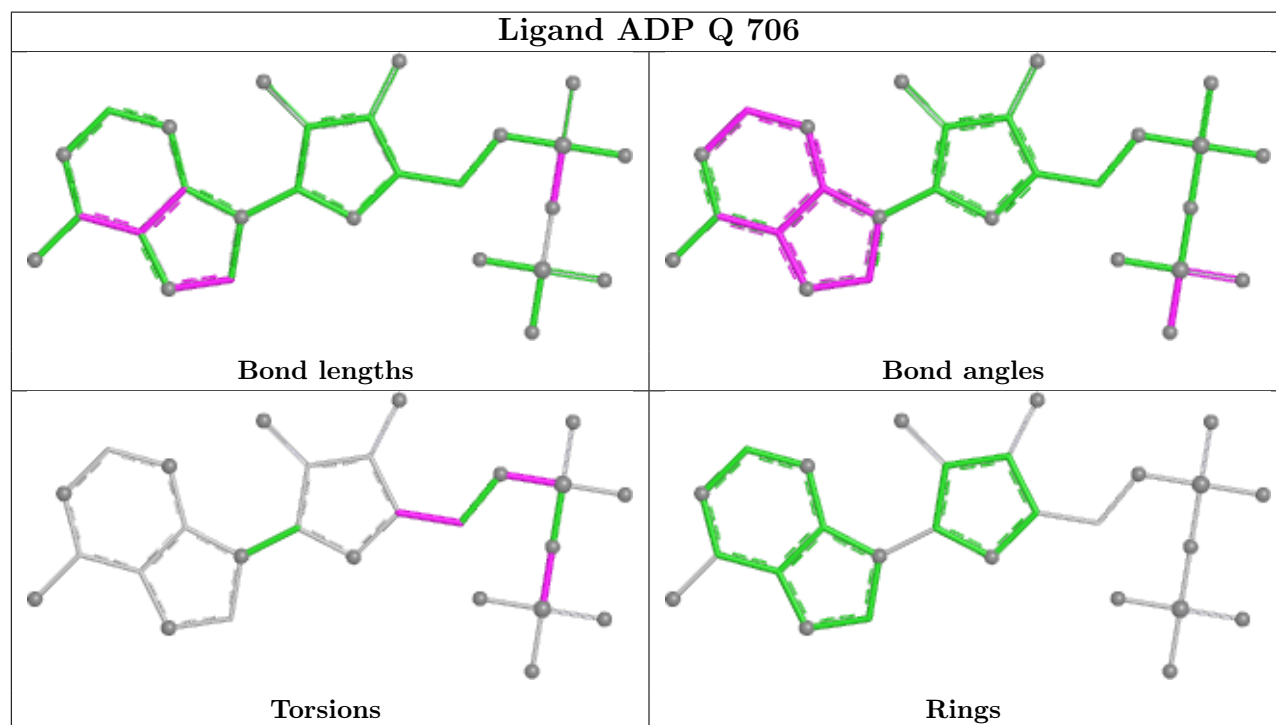
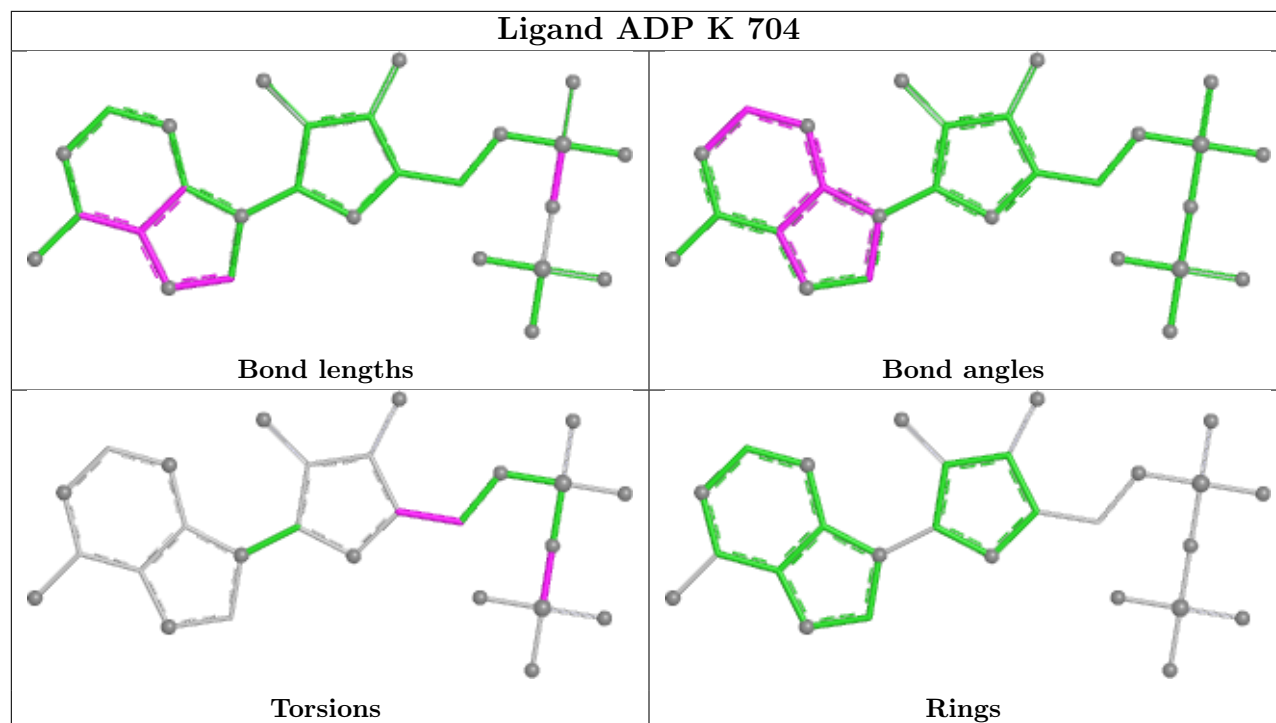
6 monomers are involved in 6 short contacts:

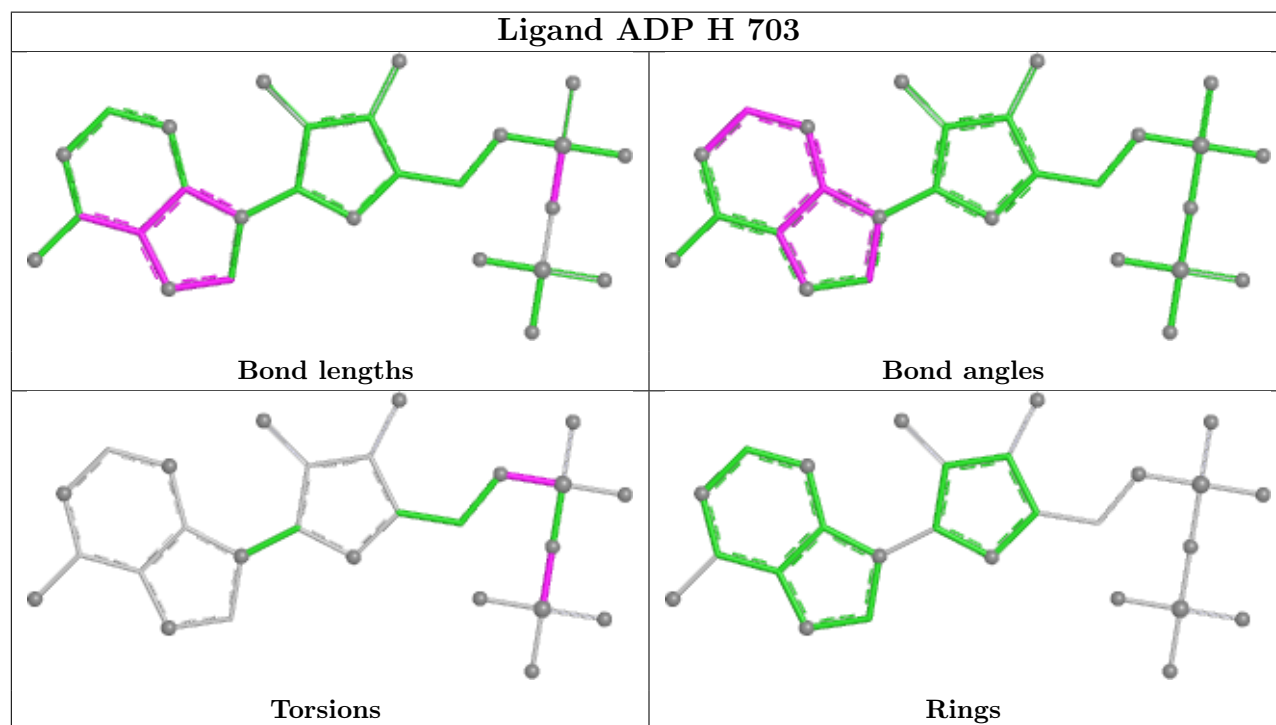
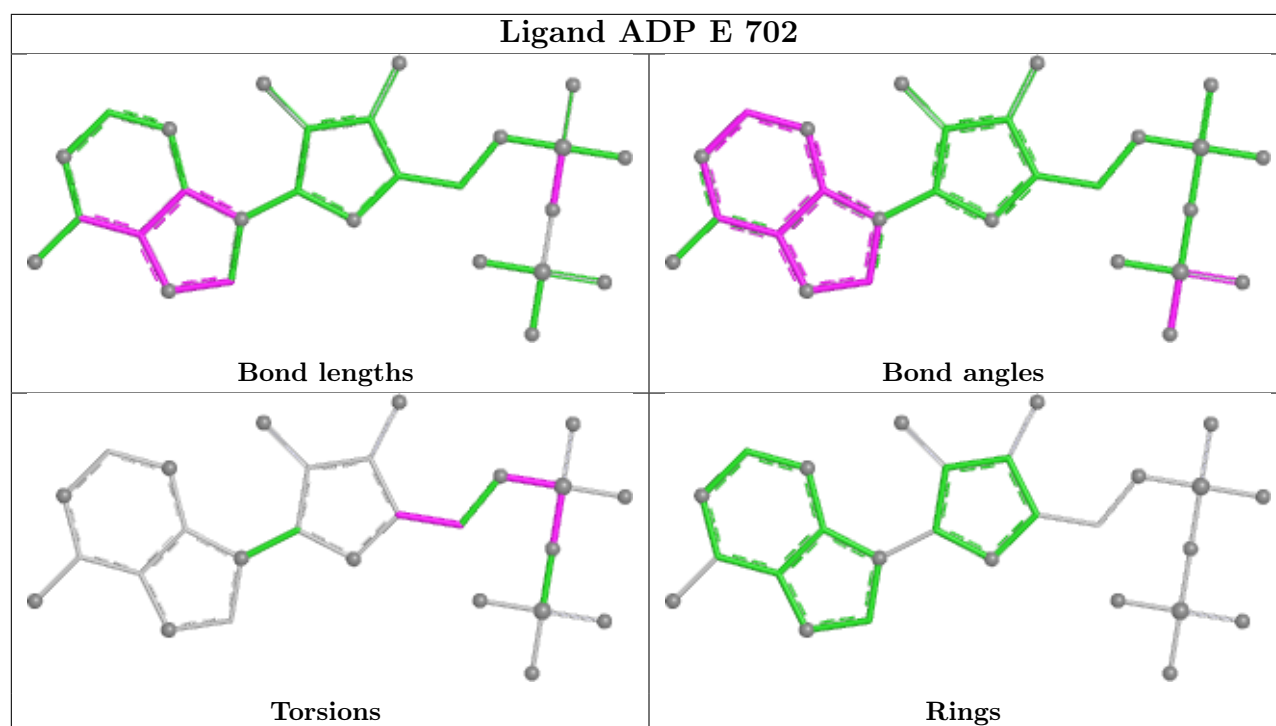
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | P     | 906 | ASN  | 1       | 0            |
| 4   | D     | 902 | ASN  | 1       | 0            |
| 4   | S     | 907 | ASN  | 1       | 0            |
| 4   | A     | 901 | ASN  | 1       | 0            |
| 5   | T     | 707 | ADP  | 1       | 0            |
| 5   | B     | 701 | ADP  | 1       | 0            |

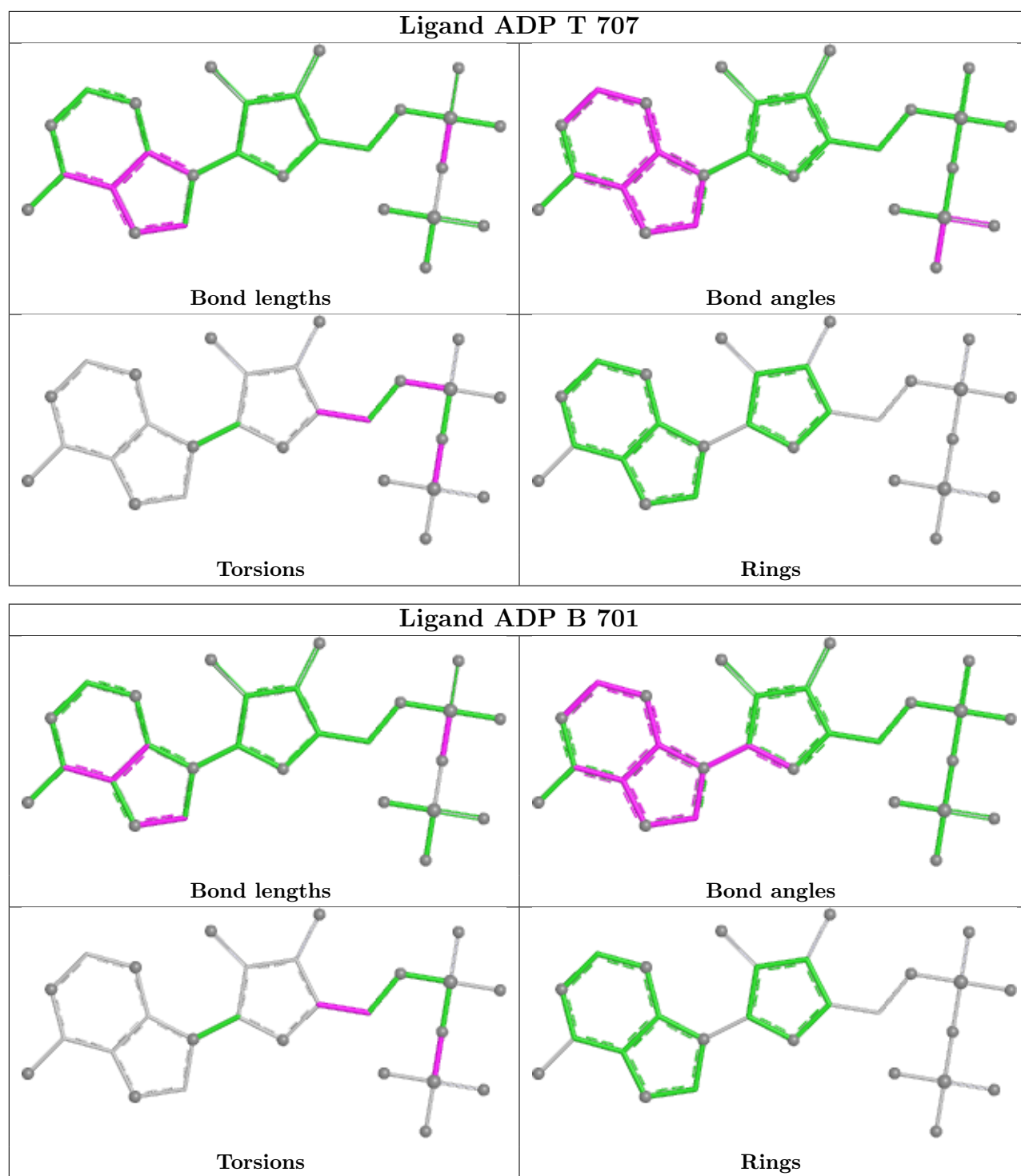
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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     | 478/478 (100%) | -1.22  | 0 100 100 | 23, 44, 71, 79        | 0     |
| 1   | D     | 478/478 (100%) | -1.25  | 0 100 100 | 29, 44, 71, 80        | 0     |
| 1   | G     | 478/478 (100%) | -1.26  | 0 100 100 | 29, 43, 71, 79        | 0     |
| 1   | J     | 478/478 (100%) | -1.26  | 0 100 100 | 28, 43, 71, 79        | 0     |
| 1   | M     | 478/478 (100%) | -1.26  | 0 100 100 | 29, 43, 71, 79        | 0     |
| 1   | P     | 478/478 (100%) | -1.25  | 0 100 100 | 28, 43, 71, 79        | 0     |
| 1   | S     | 478/478 (100%) | -1.24  | 0 100 100 | 29, 44, 71, 79        | 0     |
| 1   | V     | 478/478 (100%) | -1.22  | 0 100 100 | 29, 44, 71, 79        | 0     |
| 2   | B     | 410/478 (85%)  | -1.15  | 0 100 100 | 28, 54, 85, 103       | 0     |
| 2   | E     | 410/478 (85%)  | -1.13  | 0 100 100 | 29, 54, 85, 103       | 0     |
| 2   | H     | 410/478 (85%)  | -1.19  | 0 100 100 | 29, 54, 85, 103       | 0     |
| 2   | K     | 410/478 (85%)  | -1.17  | 0 100 100 | 29, 54, 85, 103       | 0     |
| 2   | N     | 410/478 (85%)  | -1.17  | 0 100 100 | 29, 54, 85, 103       | 0     |
| 2   | Q     | 410/478 (85%)  | -1.18  | 0 100 100 | 28, 54, 85, 103       | 0     |
| 2   | T     | 410/478 (85%)  | -1.18  | 0 100 100 | 28, 54, 85, 103       | 0     |
| 2   | W     | 410/478 (85%)  | -1.16  | 0 100 100 | 29, 54, 85, 103       | 0     |
| 3   | C     | 91/94 (96%)    | -1.22  | 0 100 100 | 39, 50, 64, 68        | 0     |
| 3   | F     | 91/94 (96%)    | -1.21  | 0 100 100 | 39, 50, 64, 67        | 0     |
| 3   | I     | 91/94 (96%)    | -1.24  | 0 100 100 | 39, 50, 64, 68        | 0     |
| 3   | L     | 91/94 (96%)    | -1.22  | 0 100 100 | 39, 50, 64, 67        | 0     |
| 3   | O     | 91/94 (96%)    | -1.19  | 0 100 100 | 39, 50, 64, 68        | 0     |
| 3   | R     | 91/94 (96%)    | -1.21  | 0 100 100 | 39, 50, 64, 67        | 0     |
| 3   | U     | 91/94 (96%)    | -1.20  | 0 100 100 | 39, 50, 64, 68        | 0     |
| 3   | X     | 91/94 (96%)    | -1.25  | 0 100 100 | 39, 50, 64, 68        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| All | All   | 7832/8400 (93%) | -1.21  | 0 100 100 | 23, 47, 79, 103       | 0     |

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

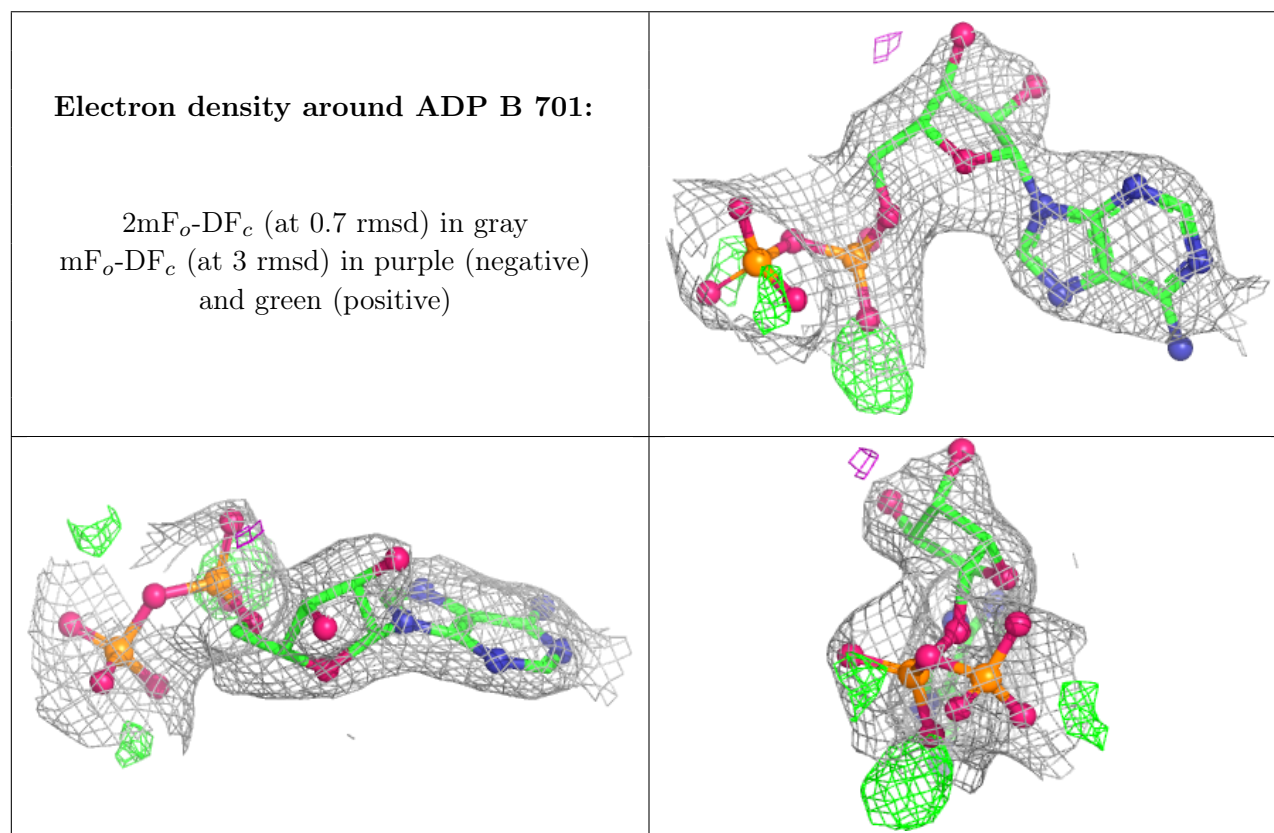
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | MG   | W     | 808 | 1/1   | 0.97 | 0.05 | 18,18,18,18                | 0     |
| 4   | ASN  | D     | 902 | 8/9   | 0.98 | 0.04 | 39,40,40,41                | 0     |
| 4   | ASN  | G     | 903 | 8/9   | 0.98 | 0.06 | 28,30,31,31                | 0     |
| 4   | ASN  | P     | 906 | 8/9   | 0.98 | 0.05 | 28,32,33,34                | 0     |
| 5   | ADP  | B     | 701 | 27/27 | 0.98 | 0.05 | 46,49,65,66                | 27    |
| 5   | ADP  | E     | 702 | 27/27 | 0.98 | 0.05 | 59,60,72,73                | 27    |
| 5   | ADP  | H     | 703 | 27/27 | 0.98 | 0.04 | 44,48,63,65                | 27    |
| 5   | ADP  | K     | 704 | 27/27 | 0.98 | 0.05 | 40,41,64,66                | 27    |
| 5   | ADP  | Q     | 706 | 27/27 | 0.98 | 0.05 | 44,46,65,66                | 27    |
| 5   | ADP  | T     | 707 | 27/27 | 0.98 | 0.05 | 51,52,70,71                | 27    |
| 5   | ADP  | W     | 708 | 27/27 | 0.98 | 0.05 | 48,50,68,70                | 27    |
| 6   | MG   | E     | 802 | 1/1   | 0.98 | 0.03 | 19,19,19,19                | 0     |
| 6   | MG   | H     | 803 | 1/1   | 0.98 | 0.03 | 10,10,10,10                | 0     |
| 6   | MG   | N     | 805 | 1/1   | 0.98 | 0.04 | 16,16,16,16                | 0     |
| 4   | ASN  | A     | 901 | 8/9   | 0.98 | 0.04 | 33,33,36,36                | 0     |
| 4   | ASN  | S     | 907 | 8/9   | 0.99 | 0.03 | 28,32,33,33                | 0     |
| 6   | MG   | B     | 801 | 1/1   | 0.99 | 0.03 | 10,10,10,10                | 0     |
| 4   | ASN  | V     | 908 | 8/9   | 0.99 | 0.04 | 29,30,31,32                | 0     |
| 5   | ADP  | N     | 705 | 27/27 | 0.99 | 0.05 | 49,52,63,65                | 27    |

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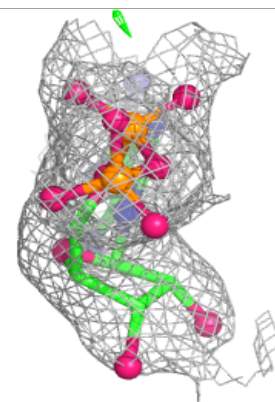
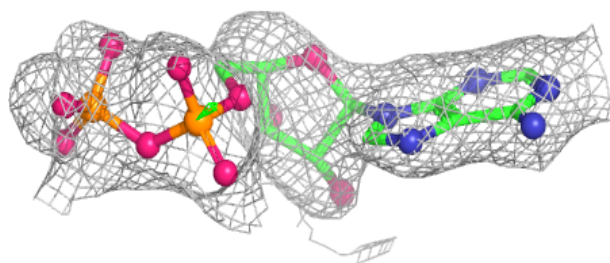
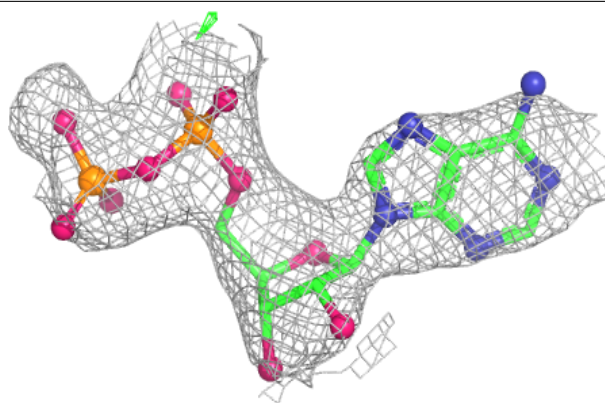
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | MG   | K     | 804 | 1/1   | 0.99 | 0.03 | 11,11,11,11                 | 0     |
| 4   | ASN  | M     | 905 | 8/9   | 0.99 | 0.03 | 32,33,34,36                 | 0     |
| 6   | MG   | Q     | 806 | 1/1   | 0.99 | 0.04 | 21,21,21,21                 | 0     |
| 6   | MG   | T     | 807 | 1/1   | 0.99 | 0.03 | 15,15,15,15                 | 0     |
| 4   | ASN  | J     | 904 | 8/9   | 0.99 | 0.03 | 26,28,29,29                 | 0     |
| 7   | ZN   | B     | 901 | 1/1   | 1.00 | 0.01 | 37,37,37,37                 | 0     |
| 7   | ZN   | E     | 902 | 1/1   | 1.00 | 0.02 | 40,40,40,40                 | 0     |
| 7   | ZN   | H     | 903 | 1/1   | 1.00 | 0.01 | 33,33,33,33                 | 0     |
| 7   | ZN   | K     | 904 | 1/1   | 1.00 | 0.01 | 29,29,29,29                 | 0     |
| 7   | ZN   | N     | 905 | 1/1   | 1.00 | 0.01 | 36,36,36,36                 | 0     |
| 7   | ZN   | Q     | 906 | 1/1   | 1.00 | 0.01 | 30,30,30,30                 | 0     |
| 7   | ZN   | T     | 907 | 1/1   | 1.00 | 0.01 | 37,37,37,37                 | 0     |
| 7   | ZN   | W     | 908 | 1/1   | 1.00 | 0.02 | 33,33,33,33                 | 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.

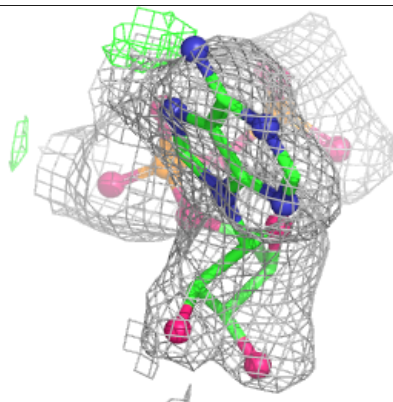
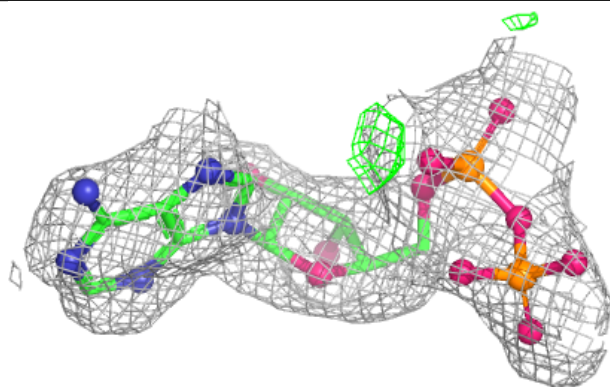
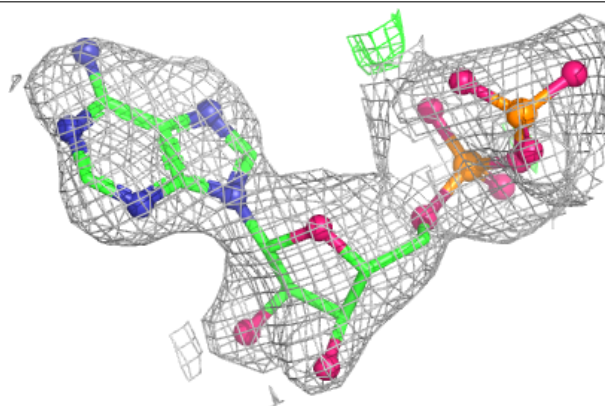


**Electron density around ADP E 702:**

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

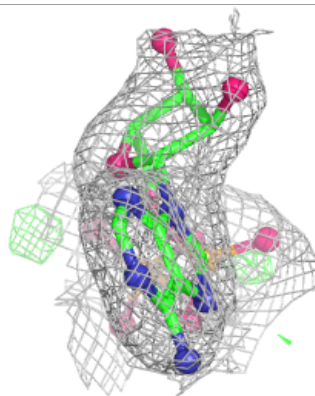
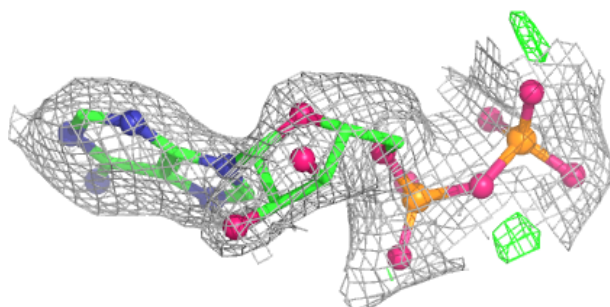
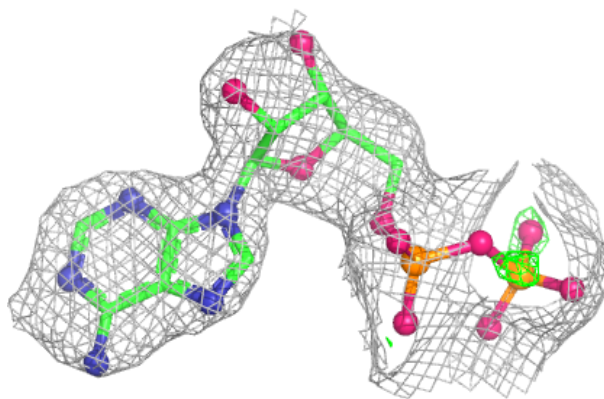
**Electron density around ADP H 703:**

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

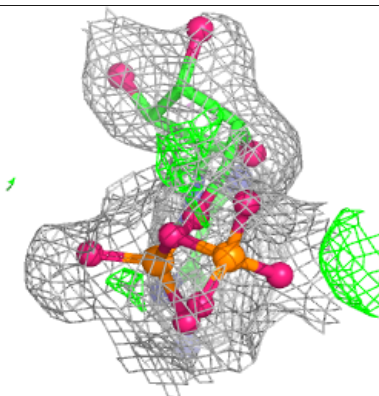
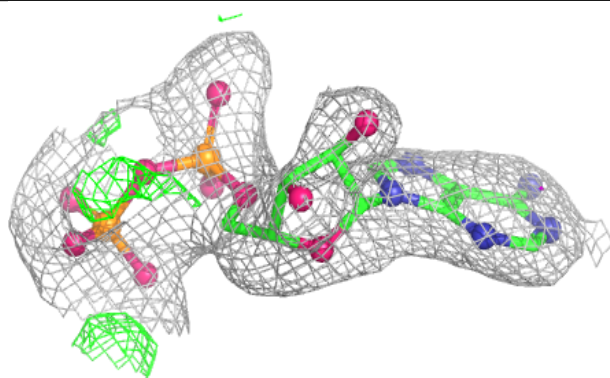
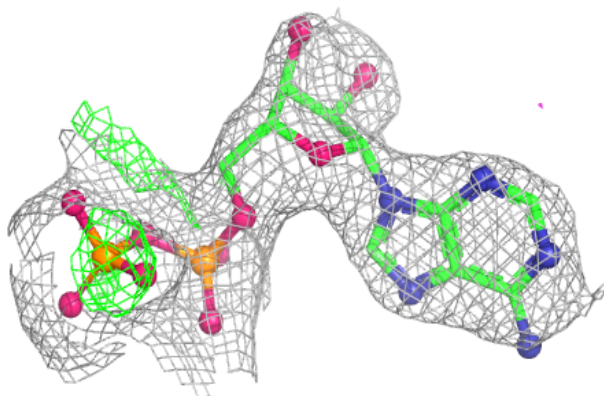


**Electron density around ADP K 704:**

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

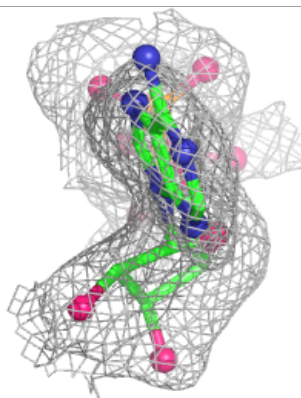
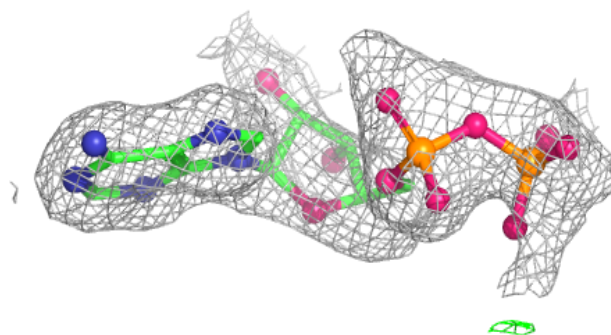
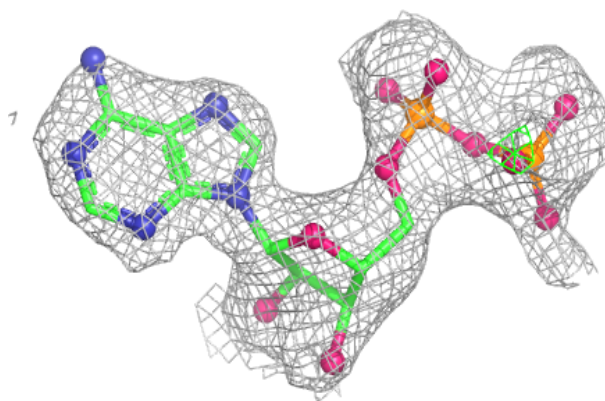
**Electron density around ADP Q 706:**

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

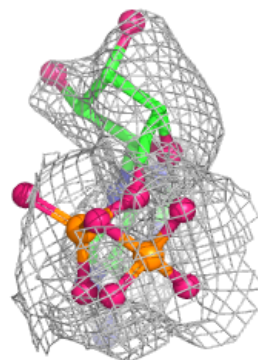
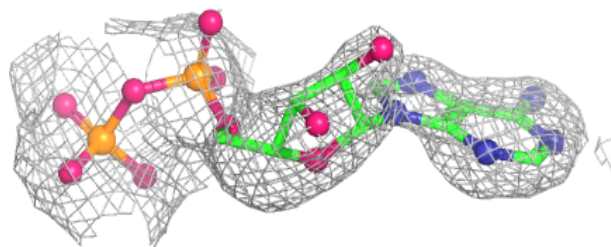
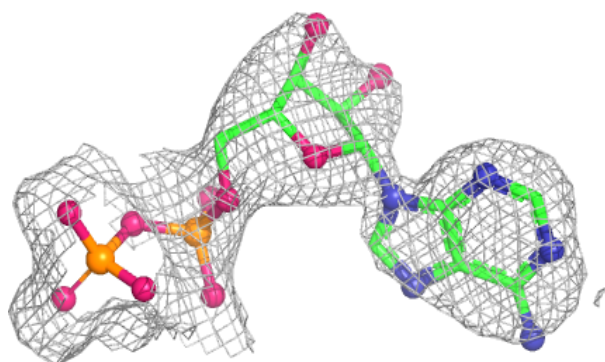


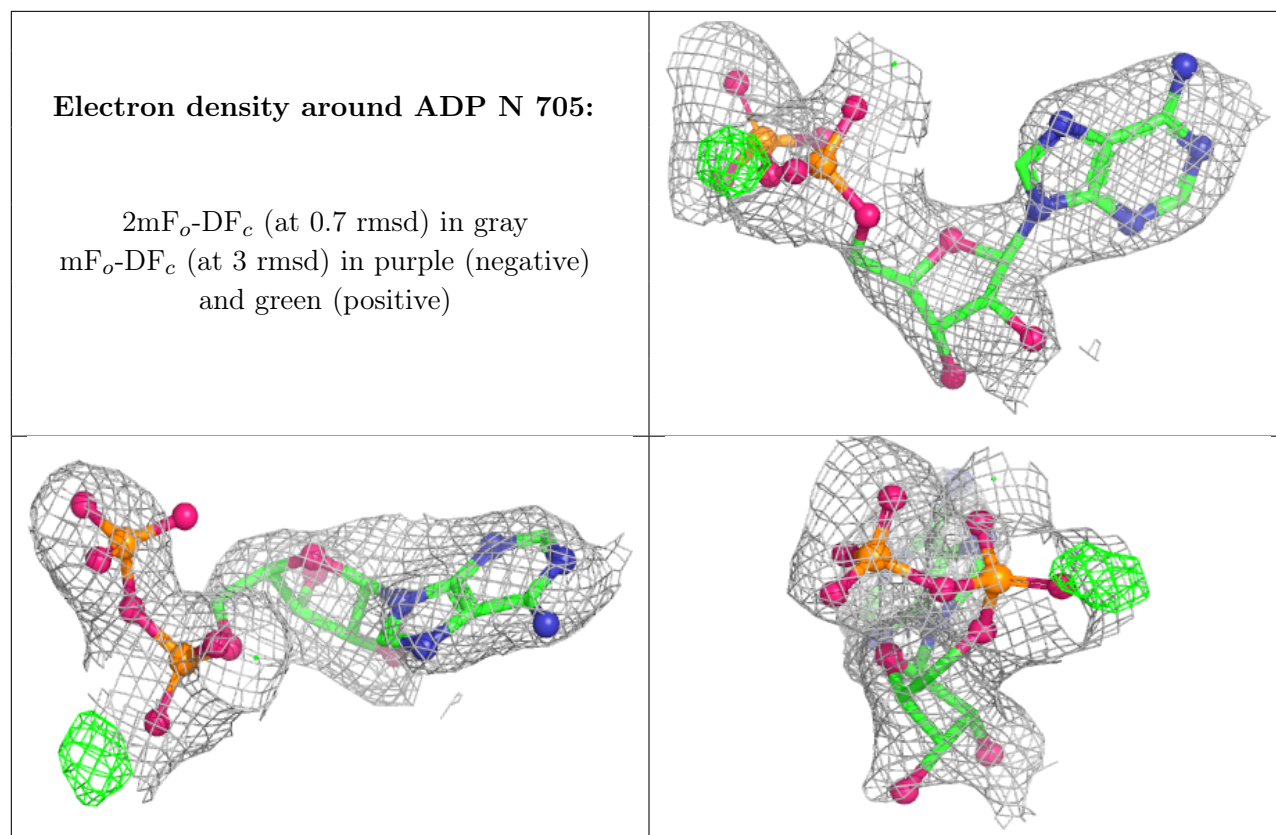
**Electron density around ADP T 707:**

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

**Electron density around ADP W 708:**

$2mF_o-DF_c$  (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.