



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:06 am BST

PDB ID : 4KOD  
Title : Structure of p97 N-D1 R155H mutant in complex with ADP  
Authors : Xia, D.; Tang, W.K.  
Deposited on : 2013-05-11  
Resolution : 2.96 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

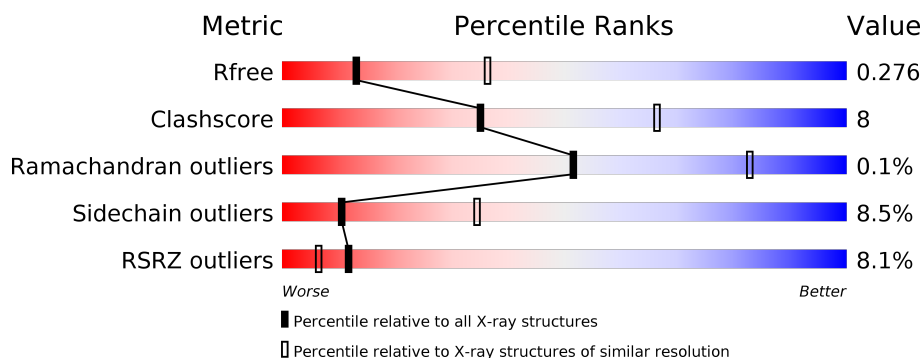
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3104 (3.00-2.92)                                      |
| Clashscore            | 141614                      | 3462 (3.00-2.92)                                      |
| Ramachandran outliers | 138981                      | 3340 (3.00-2.92)                                      |
| Sidechain outliers    | 138945                      | 3343 (3.00-2.92)                                      |
| RSRZ outliers         | 127900                      | 2986 (3.00-2.92)                                      |

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 on 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     | 489    | <div> <div>7%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>  |
| 1   | B     | 489    | <div> <div>4%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>  |
| 1   | C     | 489    | <div> <div>6%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>  |
| 1   | D     | 489    | <div> <div>7%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>  |
| 1   | E     | 489    | <div> <div>12%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div> |
| 1   | F     | 489    | <div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | G     | 489    | <div><div></div><div>6%</div><div>71%</div><div>17%</div><div>•</div><div>11%</div></div>               |
| 1   | H     | 489    | <div><div></div><div>4%</div><div>71%</div><div>16%</div><div>•</div><div>10%</div></div>               |
| 1   | I     | 489    | <div><div></div><div>7%</div><div>71%</div><div>17%</div><div>•</div><div>10%</div></div>               |
| 1   | J     | 489    | <div><div></div><div>3%</div><div>73%</div><div>16%</div><div>•</div><div>9%</div></div>                |
| 1   | K     | 489    | <div><div></div><div>18%</div><div>61%</div><div>23%</div><div>5%</div><div>•</div><div>10%</div></div> |
| 1   | L     | 489    | <div><div></div><div>9%</div><div>71%</div><div>18%</div><div>•</div><div>10%</div></div>               |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41760 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 Transitional endoplasmic reticulum ATPase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3430  | 2154 | 607 | 651 | 18 |         |         |       |
| 1   | B     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3438  | 2158 | 609 | 653 | 18 |         |         |       |
| 1   | C     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3427  | 2152 | 605 | 652 | 18 |         |         |       |
| 1   | D     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3438  | 2158 | 609 | 653 | 18 |         |         |       |
| 1   | E     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3434  | 2157 | 606 | 653 | 18 |         |         |       |
| 1   | F     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3427  | 2152 | 605 | 652 | 18 |         |         |       |
| 1   | G     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3419  | 2148 | 603 | 650 | 18 |         |         |       |
| 1   | H     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3430  | 2154 | 607 | 651 | 18 |         |         |       |
| 1   | I     | 440      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3447  | 2164 | 611 | 654 | 18 |         |         |       |
| 1   | J     | 445      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3486  | 2187 | 619 | 662 | 18 |         |         |       |
| 1   | K     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3427  | 2152 | 605 | 652 | 18 |         |         |       |
| 1   | L     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3465  | 2175 | 615 | 657 | 18 |         |         |       |

There are 108 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| A     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| A     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| B     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| B     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| C     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| C     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| D     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| D     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| E     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| E     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| F     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |

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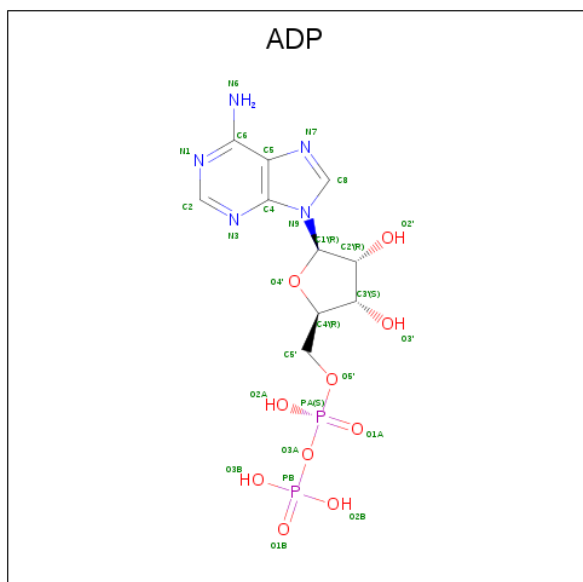
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| F     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| F     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| G     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| G     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| H     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| H     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| I     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| I     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| J     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| J     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| J     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| K     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| K     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 155     | HIS      | ARG    | ENGINEERED MUTATION | UNP P55072 |
| L     | 482     | ARG      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 483     | SER      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 484     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 485     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 486     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 487     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 488     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |
| L     | 489     | HIS      | -      | EXPRESSION TAG      | UNP P55072 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | I     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | K     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | L     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 3   | B     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 3   | C     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 3   | D     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 3   | E     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 3   | F     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 3   | G     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 3   | H     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |

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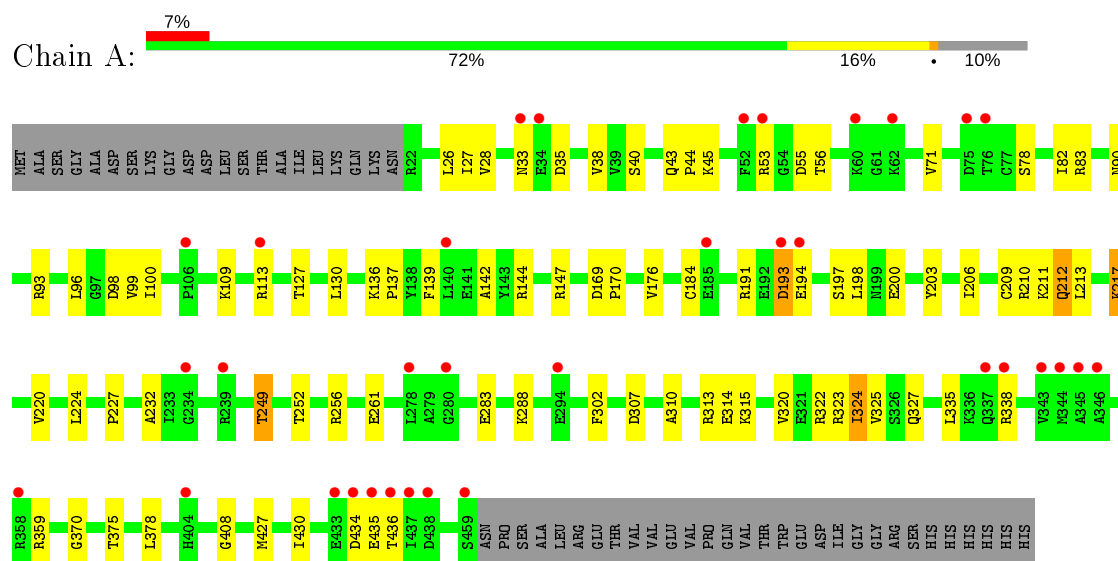
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | I     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | J     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | K     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | L     | 16       | Total<br>16 | O<br>16 | 0       | 0       |

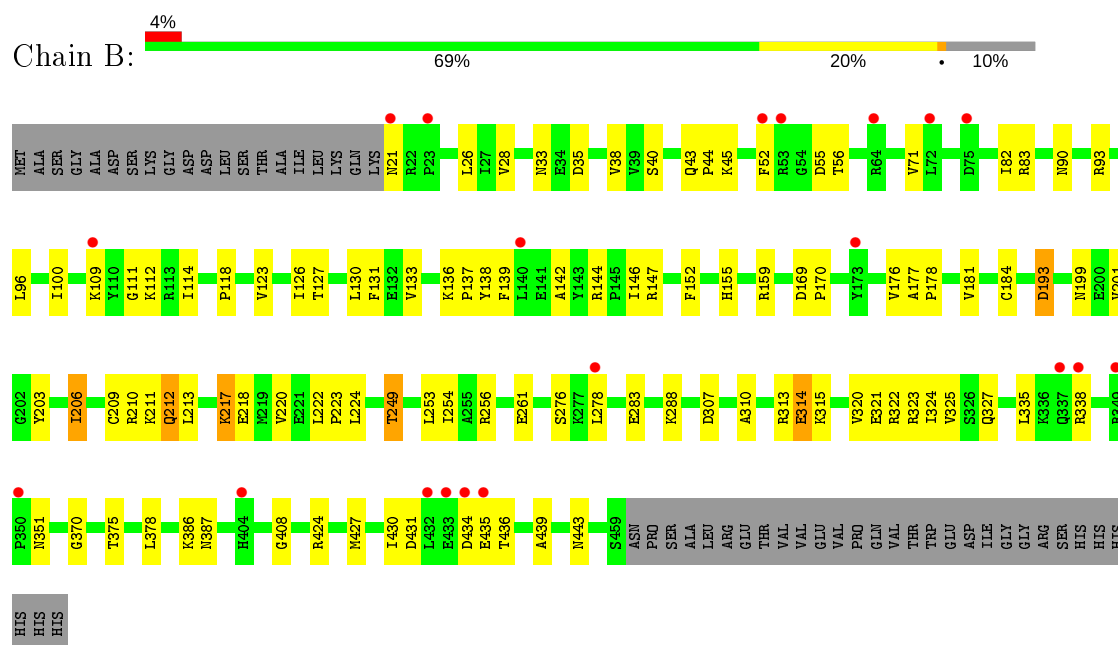
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

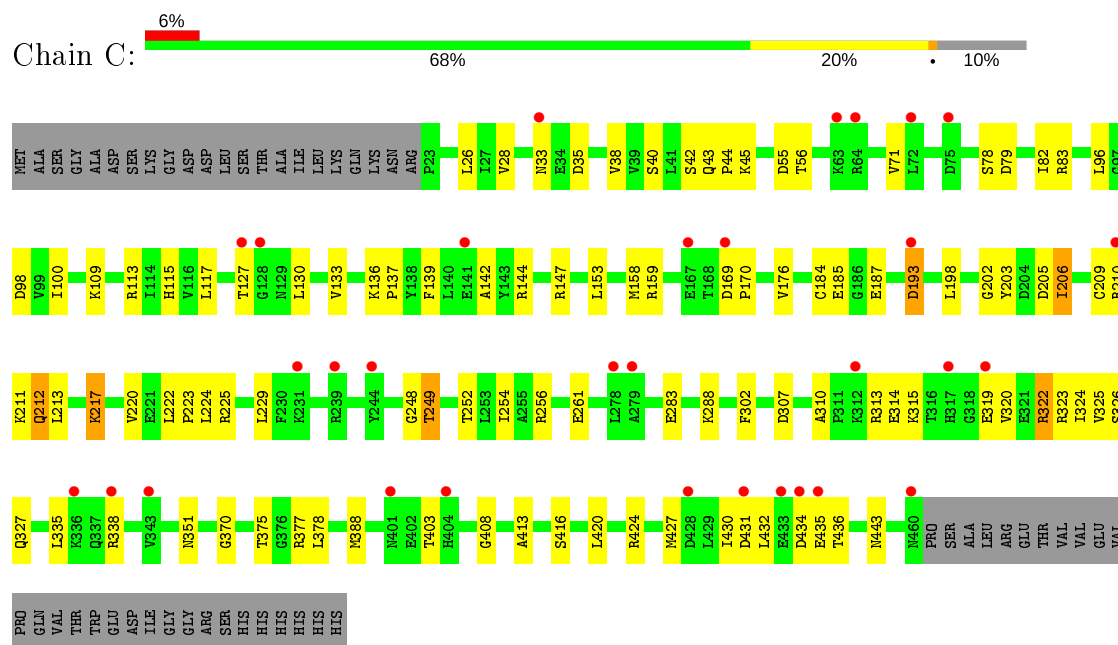
- Molecule 1: Transitional endoplasmic reticulum ATPase



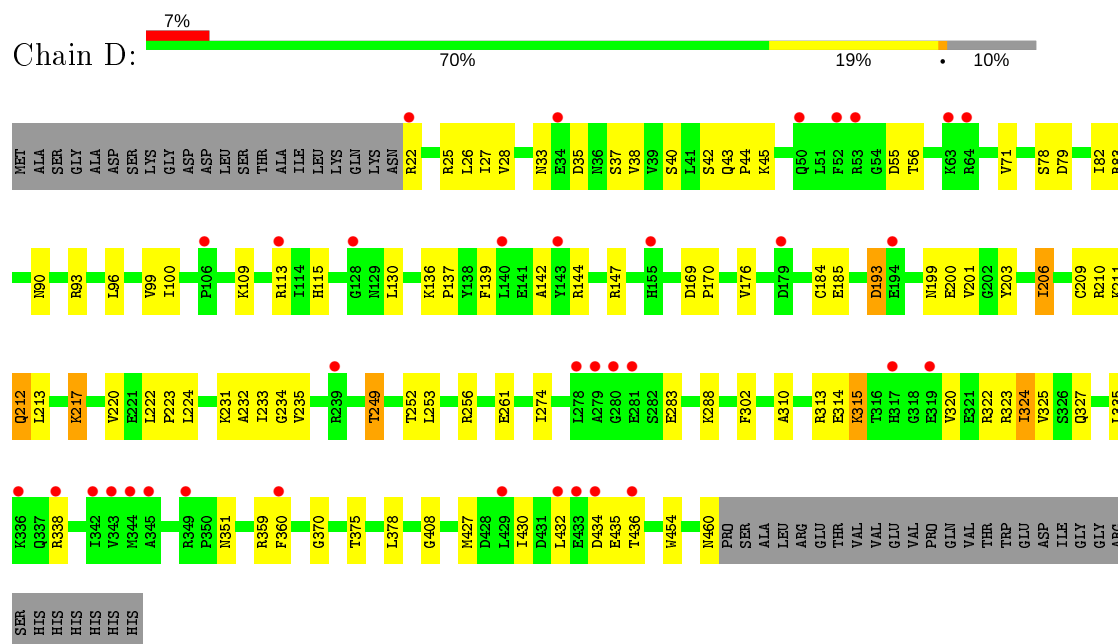
- Molecule 1: Transitional endoplasmic reticulum ATPase



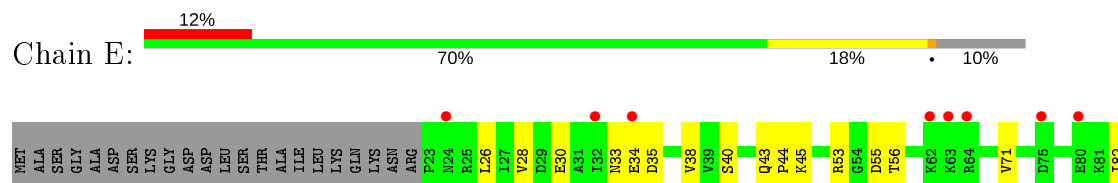
- Molecule 1: Transitional endoplasmic reticulum ATPase

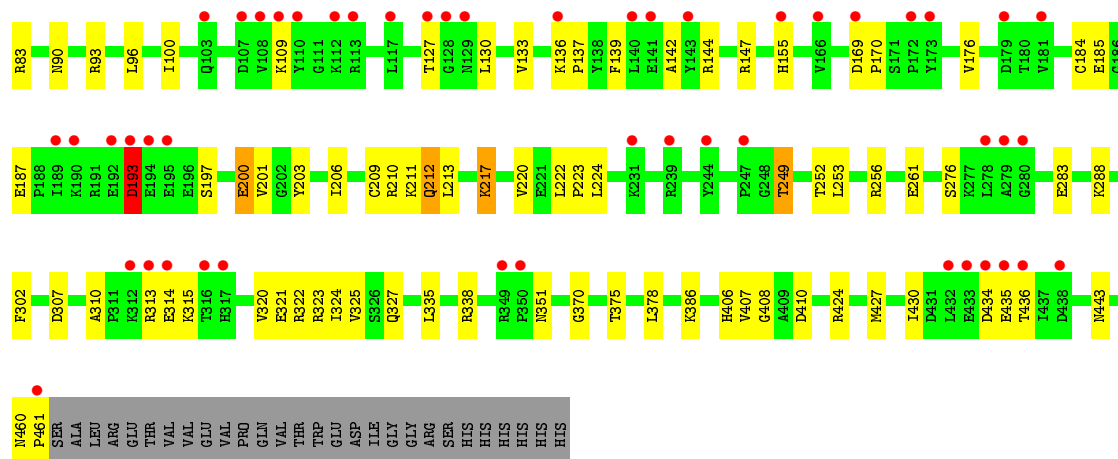


- Molecule 1: Transitional endoplasmic reticulum ATPase

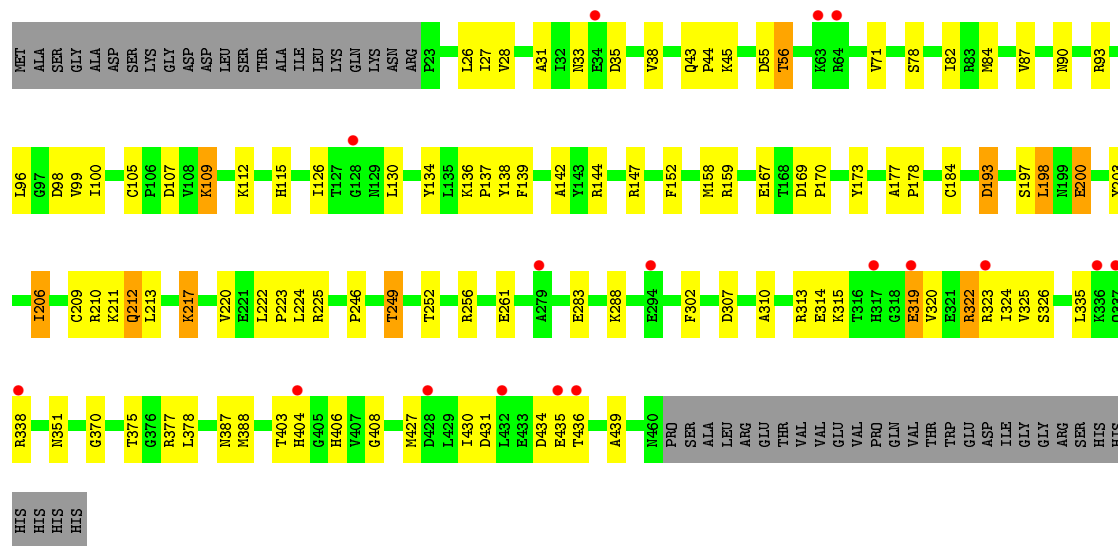


- Molecule 1: Transitional endoplasmic reticulum ATPase

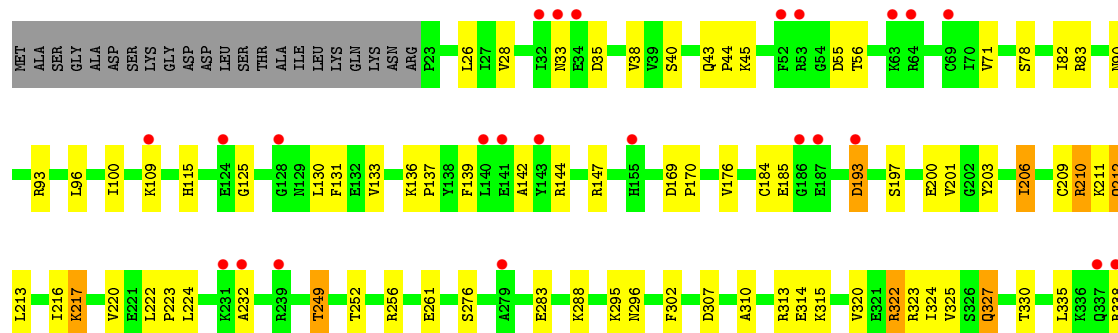


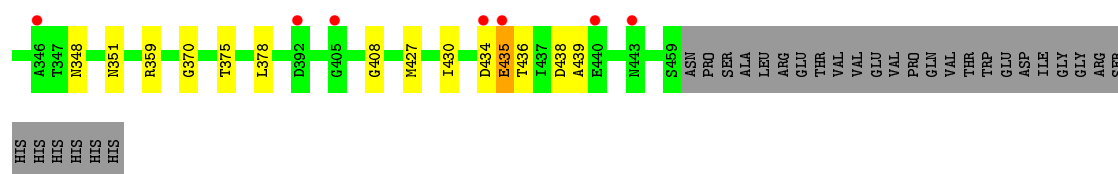


• Molecule 1: Transitional endoplasmic reticulum ATPase

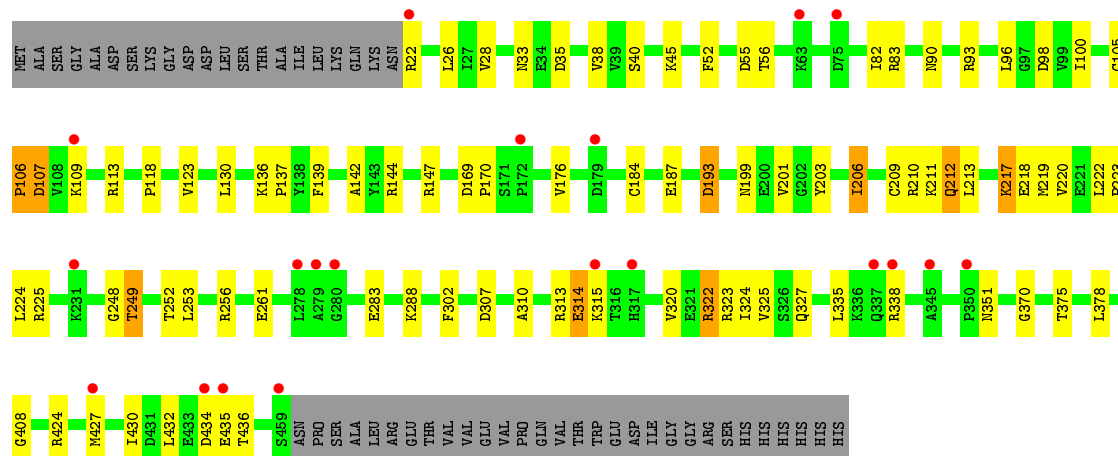


• Molecule 1: Transitional endoplasmic reticulum ATPase

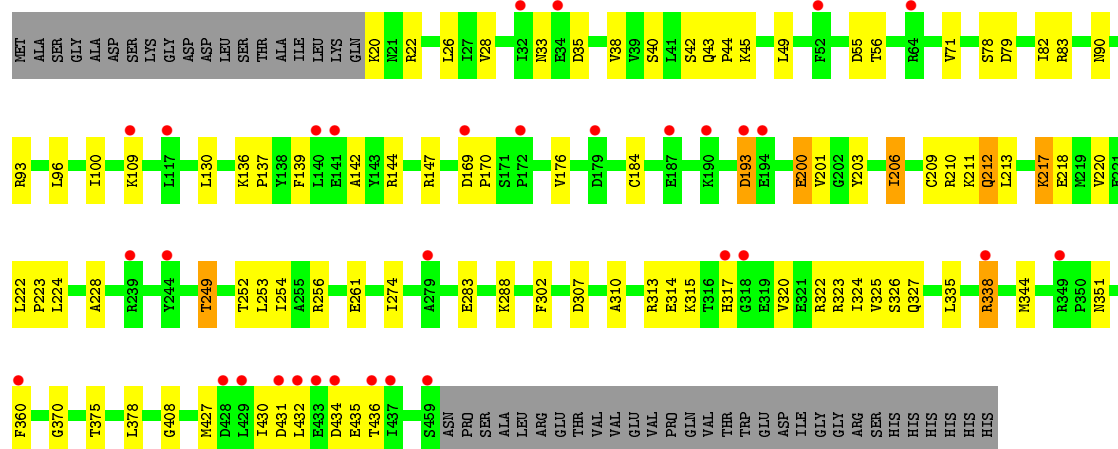




• Molecule 1: Transitional endoplasmic reticulum ATPase

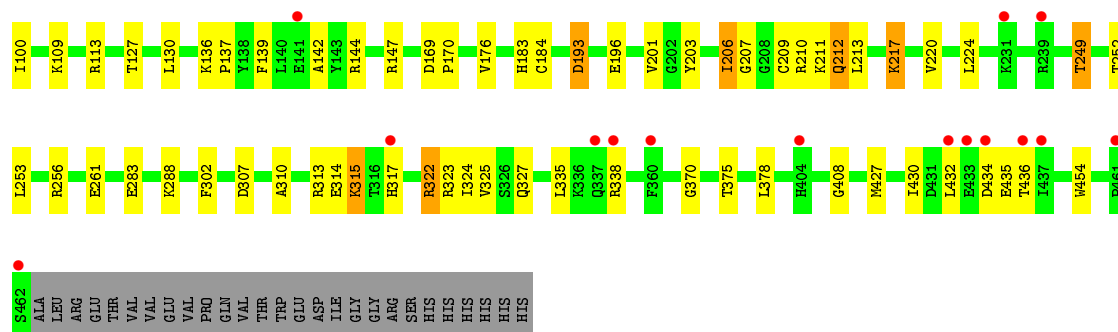


• Molecule 1: Transitional endoplasmic reticulum ATPase

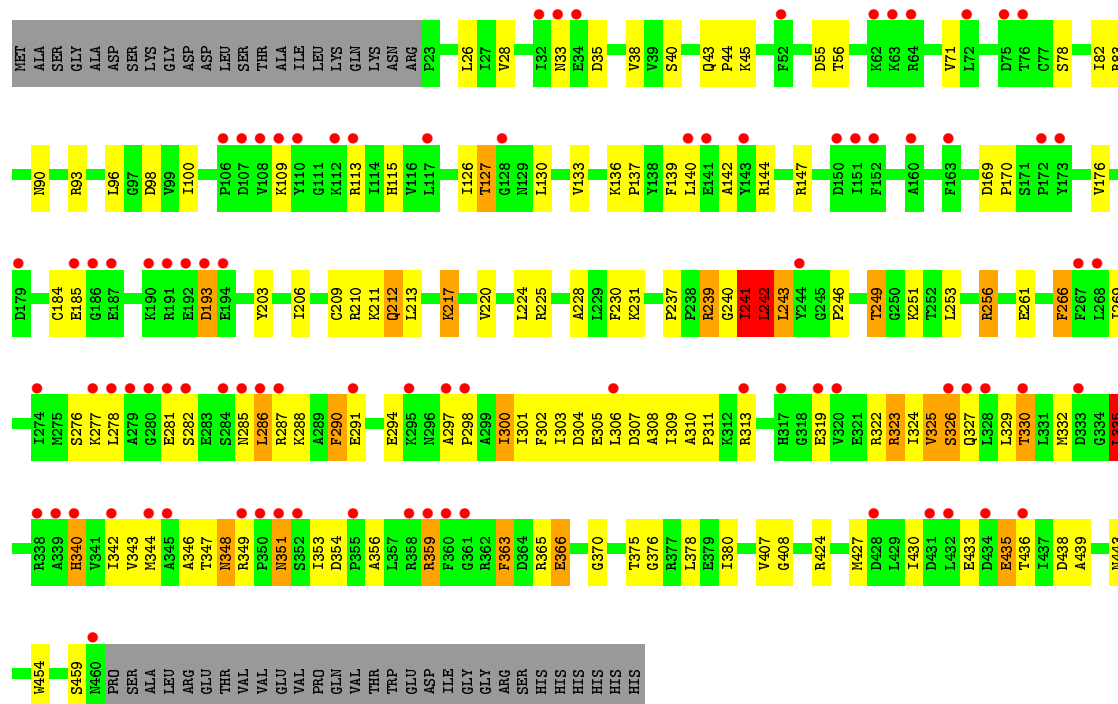


• Molecule 1: Transitional endoplasmic reticulum ATPase

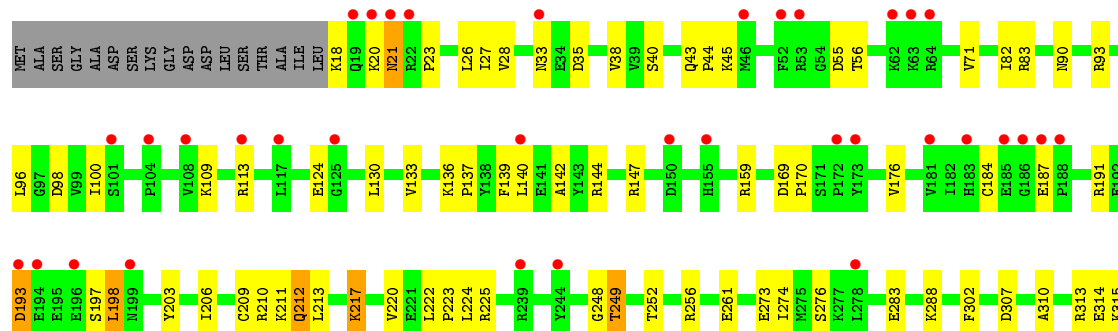


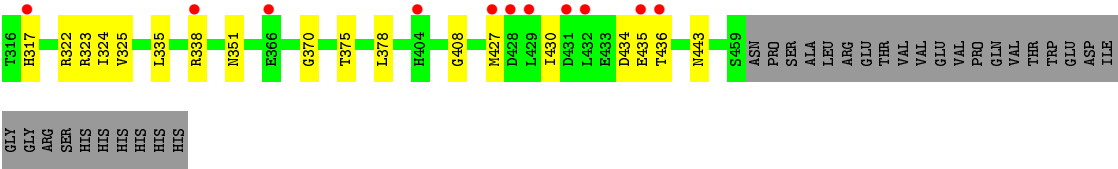


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 146.52Å 170.74Å 256.60Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 21.99 – 2.96<br>21.99 – 2.96                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.0 (21.99-2.96)<br>88.3 (21.99-2.96)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.53 (at 2.94Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0102   | Depositor        |
| R, $R_{free}$   | 0.268 , 0.291<br>0.250 , 0.276                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5937 reflections (5.02%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 66.4  | Xtriage          |
| Anisotropy  | 0.542   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 26.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 41760   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 120.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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     | 0.37         | 0/3484         | 0.63        | 0/4708         |
| 1   | B     | 0.47         | 0/3492         | 0.67        | 0/4719         |
| 1   | C     | 0.38         | 0/3481         | 0.62        | 0/4704         |
| 1   | D     | 0.39         | 0/3492         | 0.64        | 0/4719         |
| 1   | E     | 0.40         | 1/3489 (0.0%)  | 0.68        | 3/4716 (0.1%)  |
| 1   | F     | 0.48         | 0/3481         | 0.70        | 1/4704 (0.0%)  |
| 1   | G     | 0.43         | 2/3473 (0.1%)  | 0.64        | 0/4693         |
| 1   | H     | 0.42         | 0/3484         | 0.66        | 0/4708         |
| 1   | I     | 0.40         | 0/3501         | 0.64        | 2/4730 (0.0%)  |
| 1   | J     | 0.44         | 0/3541         | 0.66        | 0/4784         |
| 1   | K     | 0.44         | 1/3481 (0.0%)  | 0.71        | 2/4704 (0.0%)  |
| 1   | L     | 0.36         | 0/3519         | 0.62        | 0/4753         |
| All | All   | 0.42         | 4/41918 (0.0%) | 0.66        | 8/56642 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | K     | 0                   | 1                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 459 | SER  | C-N    | 8.47  | 1.53        | 1.34     |
| 1   | E     | 193 | ASP  | CB-CG  | -8.24 | 1.34        | 1.51     |
| 1   | G     | 296 | ASN  | CG-ND2 | -6.77 | 1.16        | 1.32     |
| 1   | G     | 296 | ASN  | CG-OD1 | -5.05 | 1.12        | 1.24     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | E     | 193 | ASP  | CB-CG-OD1 | -16.01 | 103.89      | 118.30   |
| 1   | E     | 193 | ASP  | CB-CG-OD2 | 7.36   | 124.93      | 118.30   |
| 1   | I     | 360 | PHE  | CB-CG-CD1 | -5.64  | 116.85      | 120.80   |
| 1   | K     | 242 | LEU  | CA-CB-CG  | 5.54   | 128.04      | 115.30   |
| 1   | F     | 319 | GLU  | CB-CA-C   | -5.48  | 99.43       | 110.40   |
| 1   | E     | 193 | ASP  | CB-CA-C   | -5.25  | 99.90       | 110.40   |
| 1   | K     | 335 | LEU  | CA-CB-CG  | 5.23   | 127.34      | 115.30   |
| 1   | I     | 360 | PHE  | CB-CG-CD2 | 5.11   | 124.38      | 120.80   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | K     | 239 | ARG  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3430  | 0        | 3480     | 44      | 0            |
| 1   | B     | 3438  | 0        | 3486     | 66      | 1            |
| 1   | C     | 3427  | 0        | 3474     | 74      | 0            |
| 1   | D     | 3438  | 0        | 3486     | 61      | 0            |
| 1   | E     | 3434  | 0        | 3481     | 60      | 0            |
| 1   | F     | 3427  | 0        | 3474     | 71      | 1            |
| 1   | G     | 3419  | 0        | 3468     | 55      | 1            |
| 1   | H     | 3430  | 0        | 3480     | 54      | 0            |
| 1   | I     | 3447  | 0        | 3499     | 49      | 1            |
| 1   | J     | 3486  | 0        | 3538     | 46      | 0            |
| 1   | K     | 3427  | 0        | 3474     | 132     | 0            |
| 1   | L     | 3465  | 0        | 3520     | 56      | 0            |
| 2   | A     | 27    | 0        | 12       | 2       | 0            |
| 2   | B     | 27    | 0        | 12       | 2       | 0            |
| 2   | C     | 27    | 0        | 12       | 4       | 0            |
| 2   | D     | 27    | 0        | 12       | 2       | 0            |
| 2   | E     | 27    | 0        | 12       | 2       | 0            |
| 2   | F     | 27    | 0        | 12       | 3       | 0            |
| 2   | G     | 27    | 0        | 12       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | H     | 27    | 0        | 12       | 3       | 0            |
| 2   | I     | 27    | 0        | 12       | 2       | 0            |
| 2   | J     | 27    | 0        | 12       | 2       | 0            |
| 2   | K     | 27    | 0        | 12       | 3       | 0            |
| 2   | L     | 27    | 0        | 12       | 4       | 0            |
| 3   | A     | 14    | 0        | 0        | 2       | 0            |
| 3   | B     | 9     | 0        | 0        | 0       | 0            |
| 3   | C     | 14    | 0        | 0        | 0       | 0            |
| 3   | D     | 17    | 0        | 0        | 1       | 0            |
| 3   | E     | 17    | 0        | 0        | 2       | 0            |
| 3   | F     | 15    | 0        | 0        | 0       | 0            |
| 3   | G     | 11    | 0        | 0        | 4       | 0            |
| 3   | H     | 16    | 0        | 0        | 0       | 0            |
| 3   | I     | 11    | 0        | 0        | 1       | 0            |
| 3   | J     | 17    | 0        | 0        | 2       | 0            |
| 3   | K     | 11    | 0        | 0        | 1       | 0            |
| 3   | L     | 16    | 0        | 0        | 0       | 0            |
| All | All   | 41760 | 0        | 42004    | 681     | 2            |

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 8.

All (681) 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:K:433:GLU:HG3  | 1:K:436:THR:HG21 | 1.29                     | 1.12              |
| 1:C:159:ARG:HD2  | 1:D:232:ALA:O    | 1.53                     | 1.09              |
| 1:B:276:SER:HB3  | 1:F:326:SER:HB3  | 1.33                     | 1.08              |
| 1:C:158:MET:HB2  | 1:D:233:ILE:HG22 | 1.36                     | 1.07              |
| 1:I:209:CYS:HB2  | 1:I:212:GLN:HG2  | 1.36                     | 1.03              |
| 1:K:240:GLY:HA3  | 1:K:363:PHE:CD1  | 1.95                     | 1.02              |
| 1:J:209:CYS:HB2  | 1:J:212:GLN:HG2  | 1.41                     | 1.00              |
| 1:D:209:CYS:HB2  | 1:D:212:GLN:HG2  | 1.52                     | 0.91              |
| 1:B:209:CYS:HB2  | 1:B:212:GLN:HG2  | 1.53                     | 0.90              |
| 1:C:413:ALA:HB2  | 1:D:360:PHE:HE1  | 1.36                     | 0.90              |
| 1:K:256:ARG:HA   | 1:K:266:PHE:CE2  | 2.06                     | 0.89              |
| 1:K:430:ILE:HG22 | 1:K:433:GLU:CB   | 2.03                     | 0.88              |
| 1:L:209:CYS:HB2  | 1:L:212:GLN:HG2  | 1.56                     | 0.88              |
| 1:I:209:CYS:HB2  | 1:I:212:GLN:CG   | 2.03                     | 0.88              |
| 1:E:406:HIS:CD2  | 1:E:461:PRO:HB3  | 2.10                     | 0.87              |
| 1:K:433:GLU:HG3  | 1:K:436:THR:CG2  | 2.05                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:322:ARG:HH22 | 1:J:317:HIS:HB2  | 1.41                     | 0.85              |
| 1:C:209:CYS:HB2  | 1:C:212:GLN:HG2  | 1.59                     | 0.85              |
| 1:G:438:ASP:HA   | 3:G:910:HOH:O    | 1.77                     | 0.84              |
| 1:B:320:VAL:HG21 | 1:F:319:GLU:OE2  | 1.78                     | 0.84              |
| 1:B:276:SER:CB   | 1:F:326:SER:HB3  | 2.06                     | 0.84              |
| 1:K:433:GLU:CG   | 1:K:436:THR:HG21 | 2.07                     | 0.84              |
| 1:K:209:CYS:HB2  | 1:K:212:GLN:HG2  | 1.61                     | 0.83              |
| 1:A:209:CYS:HB2  | 1:A:212:GLN:HG2  | 1.59                     | 0.83              |
| 1:B:276:SER:HA   | 1:F:326:SER:HB2  | 1.59                     | 0.83              |
| 1:K:430:ILE:HG22 | 1:K:433:GLU:HB2  | 1.59                     | 0.82              |
| 1:E:209:CYS:HB2  | 1:E:212:GLN:HG2  | 1.60                     | 0.82              |
| 1:K:298:PRO:HA   | 1:K:340:HIS:O    | 1.80                     | 0.82              |
| 1:K:313:ARG:NH1  | 1:K:325:VAL:O    | 2.13                     | 0.81              |
| 1:K:322:ARG:HA   | 1:K:325:VAL:HB   | 1.63                     | 0.80              |
| 1:K:433:GLU:CG   | 1:K:436:THR:CG2  | 2.59                     | 0.80              |
| 1:G:133:VAL:HG21 | 1:G:439:ALA:HB3  | 1.64                     | 0.79              |
| 1:K:365:ARG:O    | 1:K:365:ARG:HG2  | 1.82                     | 0.78              |
| 1:K:241:ILE:HD11 | 1:K:342:ILE:HG23 | 1.65                     | 0.78              |
| 1:F:403:THR:HB   | 1:F:406:HIS:ND1  | 1.97                     | 0.78              |
| 1:B:431:ASP:HB2  | 1:F:99:VAL:HG11  | 1.65                     | 0.77              |
| 1:K:240:GLY:HA3  | 1:K:363:PHE:CE1  | 2.20                     | 0.77              |
| 1:K:241:ILE:HG12 | 1:K:343:VAL:O    | 1.85                     | 0.76              |
| 1:H:209:CYS:HB2  | 1:H:212:GLN:HG2  | 1.67                     | 0.76              |
| 1:G:232:ALA:O    | 1:L:159:ARG:HD2  | 1.86                     | 0.76              |
| 1:L:139:PHE:HA   | 1:L:142:ALA:HB2  | 1.68                     | 0.75              |
| 1:K:256:ARG:HA   | 1:K:266:PHE:HE2  | 1.52                     | 0.75              |
| 1:I:431:ASP:HB2  | 1:J:99:VAL:HG11  | 1.67                     | 0.75              |
| 1:K:242:LEU:HD22 | 1:K:243:LEU:N    | 2.02                     | 0.74              |
| 1:H:203:TYR:CE2  | 1:H:261:GLU:HG2  | 2.22                     | 0.74              |
| 1:J:203:TYR:CE2  | 1:J:261:GLU:HG2  | 2.23                     | 0.73              |
| 1:C:326:SER:HB3  | 1:E:276:SER:HB3  | 1.71                     | 0.73              |
| 1:F:209:CYS:HB2  | 1:F:212:GLN:HG2  | 1.70                     | 0.73              |
| 1:A:139:PHE:HA   | 1:A:142:ALA:HB2  | 1.70                     | 0.73              |
| 1:C:431:ASP:HB2  | 1:D:99:VAL:CG1   | 2.19                     | 0.73              |
| 1:K:139:PHE:HA   | 1:K:142:ALA:HB2  | 1.71                     | 0.72              |
| 1:K:347:THR:HG22 | 1:K:348:ASN:H    | 1.54                     | 0.72              |
| 1:G:276:SER:HB3  | 1:K:326:SER:HB2  | 1.69                     | 0.72              |
| 1:F:139:PHE:HA   | 1:F:142:ALA:HB2  | 1.71                     | 0.72              |
| 1:I:200:GLU:OE1  | 1:I:201:VAL:N    | 2.19                     | 0.72              |
| 1:C:139:PHE:HA   | 1:C:142:ALA:HB2  | 1.71                     | 0.72              |
| 1:B:201:VAL:HG11 | 1:B:253:LEU:HD12 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:320:VAL:CG2  | 1:F:319:GLU:OE2  | 2.38                     | 0.72              |
| 1:E:193:ASP:OD1  | 1:E:193:ASP:N    | 2.18                     | 0.72              |
| 1:I:139:PHE:HA   | 1:I:142:ALA:HB2  | 1.71                     | 0.72              |
| 1:B:276:SER:HB3  | 1:F:326:SER:CB   | 2.18                     | 0.72              |
| 1:D:139:PHE:HA   | 1:D:142:ALA:HB2  | 1.72                     | 0.72              |
| 1:G:435:GLU:HG2  | 1:K:228:ALA:HB3  | 1.72                     | 0.72              |
| 1:C:432:LEU:HA   | 1:D:25:ARG:HH21  | 1.55                     | 0.71              |
| 1:G:139:PHE:HA   | 1:G:142:ALA:HB2  | 1.70                     | 0.71              |
| 1:H:139:PHE:HA   | 1:H:142:ALA:HB2  | 1.72                     | 0.71              |
| 1:E:139:PHE:HA   | 1:E:142:ALA:HB2  | 1.72                     | 0.71              |
| 1:C:319:GLU:OE2  | 1:E:320:VAL:CG2  | 2.38                     | 0.71              |
| 1:C:416:SER:HA   | 1:D:235:VAL:HG13 | 1.73                     | 0.70              |
| 1:K:433:GLU:CB   | 1:K:436:THR:HG22 | 2.20                     | 0.70              |
| 1:K:242:LEU:HD22 | 1:K:243:LEU:H    | 1.56                     | 0.70              |
| 1:K:363:PHE:HE1  | 1:K:365:ARG:HB3  | 1.56                     | 0.70              |
| 1:J:139:PHE:HA   | 1:J:142:ALA:HB2  | 1.71                     | 0.70              |
| 1:J:201:VAL:HG11 | 1:J:253:LEU:HD12 | 1.72                     | 0.70              |
| 1:E:203:TYR:CE2  | 1:E:261:GLU:HG2  | 2.26                     | 0.70              |
| 1:F:98:ASP:OD1   | 1:F:225:ARG:NH2  | 2.24                     | 0.70              |
| 1:B:276:SER:CB   | 1:F:326:SER:CB   | 2.70                     | 0.69              |
| 1:C:203:TYR:CE2  | 1:C:261:GLU:HG2  | 2.27                     | 0.69              |
| 1:B:139:PHE:HA   | 1:B:142:ALA:HB2  | 1.73                     | 0.68              |
| 1:D:209:CYS:HB2  | 1:D:212:GLN:CG   | 2.22                     | 0.68              |
| 1:C:431:ASP:HB2  | 1:D:99:VAL:HG11  | 1.74                     | 0.68              |
| 1:F:158:MET:HA   | 1:F:387:ASN:O    | 1.93                     | 0.68              |
| 1:F:203:TYR:CE2  | 1:F:261:GLU:HG2  | 2.28                     | 0.68              |
| 1:B:276:SER:CA   | 1:F:326:SER:HB2  | 2.23                     | 0.68              |
| 1:I:326:SER:HB2  | 1:K:276:SER:HB3  | 1.76                     | 0.68              |
| 1:K:241:ILE:HA   | 1:K:365:ARG:NH1  | 2.09                     | 0.68              |
| 1:F:115:HIS:CD2  | 1:F:167:GLU:OE2  | 2.47                     | 0.68              |
| 1:C:158:MET:HB2  | 1:D:233:ILE:CG2  | 2.21                     | 0.67              |
| 1:E:193:ASP:HB3  | 1:G:295:LYS:HE3  | 1.75                     | 0.67              |
| 1:G:133:VAL:HG21 | 1:G:439:ALA:CB   | 2.24                     | 0.67              |
| 1:G:209:CYS:HB2  | 1:G:212:GLN:HG2  | 1.76                     | 0.67              |
| 1:K:127:THR:HB   | 1:K:438:ASP:OD1  | 1.94                     | 0.67              |
| 1:H:106:PRO:HD2  | 1:H:107:ASP:OD1  | 1.93                     | 0.67              |
| 1:A:53:ARG:NH2   | 3:A:909:HOH:O    | 2.26                     | 0.67              |
| 1:I:249:THR:HG21 | 1:I:370:GLY:O    | 1.94                     | 0.67              |
| 1:G:203:TYR:CE2  | 1:G:261:GLU:HG2  | 2.30                     | 0.67              |
| 1:B:278:LEU:HA   | 1:F:323:ARG:NH1  | 2.10                     | 0.66              |
| 1:F:126:ILE:HB   | 1:F:439:ALA:HB2  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:317:HIS:HB2  | 1:J:322:ARG:HH22 | 1.61                     | 0.66              |
| 1:K:287:ARG:HA   | 1:K:290:PHE:HB2  | 1.76                     | 0.66              |
| 1:J:249:THR:HG21 | 1:J:370:GLY:O    | 1.95                     | 0.66              |
| 1:K:240:GLY:O    | 1:K:241:ILE:HD12 | 1.94                     | 0.66              |
| 1:F:249:THR:HG21 | 1:F:370:GLY:O    | 1.97                     | 0.65              |
| 1:I:203:TYR:CE2  | 1:I:261:GLU:HG2  | 2.32                     | 0.65              |
| 1:B:276:SER:CA   | 1:F:326:SER:CB   | 2.74                     | 0.65              |
| 1:L:203:TYR:CE2  | 1:L:261:GLU:HG2  | 2.30                     | 0.65              |
| 1:C:249:THR:HG21 | 1:C:370:GLY:O    | 1.96                     | 0.65              |
| 1:C:432:LEU:HA   | 1:D:25:ARG:NH2   | 2.12                     | 0.64              |
| 1:H:432:LEU:HD21 | 1:L:21:ASN:HD22  | 1.61                     | 0.64              |
| 1:K:203:TYR:CE2  | 1:K:261:GLU:HG2  | 2.32                     | 0.64              |
| 1:L:98:ASP:OD1   | 1:L:225:ARG:NH2  | 2.31                     | 0.64              |
| 1:K:136:LYS:HB3  | 1:K:137:PRO:HD3  | 1.80                     | 0.64              |
| 1:E:249:THR:HG21 | 1:E:370:GLY:O    | 1.98                     | 0.64              |
| 1:H:249:THR:HG21 | 1:H:370:GLY:O    | 1.97                     | 0.64              |
| 1:A:249:THR:HG21 | 1:A:370:GLY:O    | 1.98                     | 0.63              |
| 1:B:209:CYS:HB2  | 1:B:212:GLN:CG   | 2.24                     | 0.63              |
| 1:C:413:ALA:HB2  | 1:D:360:PHE:CE1  | 2.26                     | 0.63              |
| 1:E:187:GLU:HG3  | 1:L:124:GLU:HG2  | 1.80                     | 0.63              |
| 1:A:136:LYS:HB3  | 1:A:137:PRO:HD3  | 1.81                     | 0.63              |
| 1:J:209:CYS:HB2  | 1:J:212:GLN:CG   | 2.21                     | 0.62              |
| 1:B:136:LYS:HB3  | 1:B:137:PRO:HD3  | 1.81                     | 0.62              |
| 1:D:136:LYS:HB3  | 1:D:137:PRO:HD3  | 1.81                     | 0.62              |
| 1:F:136:LYS:HB3  | 1:F:137:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:249:THR:HG21 | 1:B:370:GLY:O    | 1.99                     | 0.62              |
| 1:C:158:MET:O    | 1:D:234:GLY:N    | 2.32                     | 0.62              |
| 1:E:136:LYS:HB3  | 1:E:137:PRO:HD3  | 1.82                     | 0.62              |
| 1:A:203:TYR:CE2  | 1:A:261:GLU:HG2  | 2.35                     | 0.62              |
| 1:C:136:LYS:HB3  | 1:C:137:PRO:HD3  | 1.81                     | 0.62              |
| 1:D:201:VAL:HG11 | 1:D:253:LEU:HD11 | 1.82                     | 0.62              |
| 1:L:249:THR:HG21 | 1:L:370:GLY:O    | 1.99                     | 0.62              |
| 1:G:283:GLU:OE2  | 1:G:323:ARG:HG2  | 2.00                     | 0.61              |
| 1:E:133:VAL:HG13 | 1:E:443:ASN:HB2  | 1.82                     | 0.61              |
| 1:G:249:THR:HG21 | 1:G:370:GLY:O    | 1.99                     | 0.61              |
| 1:C:222:LEU:HD11 | 1:E:424:ARG:HG3  | 1.83                     | 0.61              |
| 1:H:136:LYS:HB3  | 1:H:137:PRO:HD3  | 1.82                     | 0.61              |
| 1:K:306:LEU:HA   | 1:K:346:ALA:O    | 2.01                     | 0.61              |
| 1:A:434:ASP:HA   | 1:A:436:THR:H    | 1.66                     | 0.61              |
| 1:E:406:HIS:CD2  | 1:E:461:PRO:CB   | 2.84                     | 0.61              |
| 1:J:136:LYS:HB3  | 1:J:137:PRO:HD3  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:322:ARG:CZ   | 1:E:321:GLU:OE1  | 2.49                     | 0.61              |
| 1:G:136:LYS:HB3  | 1:G:137:PRO:HD3  | 1.82                     | 0.61              |
| 1:B:203:TYR:CE2  | 1:B:261:GLU:HG2  | 2.37                     | 0.60              |
| 1:K:249:THR:HG21 | 1:K:370:GLY:O    | 2.01                     | 0.60              |
| 1:E:213:LEU:O    | 1:E:217:LYS:HG3  | 2.02                     | 0.60              |
| 1:H:206:ILE:CD1  | 1:H:209:CYS:SG   | 2.89                     | 0.60              |
| 1:J:283:GLU:OE2  | 1:J:323:ARG:HG2  | 2.02                     | 0.60              |
| 1:F:158:MET:N    | 1:F:387:ASN:O    | 2.34                     | 0.60              |
| 1:G:232:ALA:O    | 1:L:159:ARG:CD   | 2.50                     | 0.60              |
| 1:J:201:VAL:HG11 | 1:J:253:LEU:CD1  | 2.31                     | 0.60              |
| 1:L:209:CYS:HB2  | 1:L:212:GLN:CG   | 2.30                     | 0.60              |
| 1:K:433:GLU:HB3  | 1:K:436:THR:HG22 | 1.83                     | 0.59              |
| 1:I:136:LYS:HB3  | 1:I:137:PRO:HD3  | 1.84                     | 0.59              |
| 1:G:327:GLN:HE21 | 1:L:276:SER:HB2  | 1.67                     | 0.59              |
| 1:H:434:ASP:HA   | 1:H:436:THR:H    | 1.67                     | 0.59              |
| 1:D:249:THR:HG21 | 1:D:370:GLY:O    | 2.01                     | 0.59              |
| 1:K:302:PHE:HA   | 1:K:344:MET:O    | 2.02                     | 0.59              |
| 1:I:222:LEU:HD11 | 1:K:424:ARG:HG3  | 1.84                     | 0.59              |
| 1:G:359:ARG:NH2  | 2:L:800:ADP:O3B  | 2.36                     | 0.59              |
| 1:E:434:ASP:HA   | 1:E:436:THR:H    | 1.68                     | 0.58              |
| 1:I:434:ASP:HA   | 1:I:436:THR:H    | 1.68                     | 0.58              |
| 1:B:434:ASP:HA   | 1:B:436:THR:H    | 1.69                     | 0.58              |
| 1:L:136:LYS:HB3  | 1:L:137:PRO:HD3  | 1.85                     | 0.58              |
| 1:B:276:SER:O    | 1:F:323:ARG:HG3  | 2.03                     | 0.58              |
| 1:D:283:GLU:OE2  | 1:D:323:ARG:HG2  | 2.03                     | 0.58              |
| 1:A:209:CYS:HB2  | 1:A:212:GLN:CG   | 2.32                     | 0.58              |
| 1:C:283:GLU:OE2  | 1:C:323:ARG:HG2  | 2.04                     | 0.58              |
| 1:F:434:ASP:HA   | 1:F:436:THR:H    | 1.69                     | 0.58              |
| 1:D:434:ASP:HA   | 1:D:436:THR:H    | 1.69                     | 0.57              |
| 1:E:283:GLU:OE2  | 1:E:323:ARG:HG2  | 2.04                     | 0.57              |
| 1:J:206:ILE:HG13 | 1:J:207:GLY:N    | 2.18                     | 0.57              |
| 1:J:434:ASP:HA   | 1:J:436:THR:H    | 1.68                     | 0.57              |
| 1:A:283:GLU:OE2  | 1:A:323:ARG:HG2  | 2.04                     | 0.57              |
| 1:C:213:LEU:O    | 1:C:217:LYS:HG3  | 2.05                     | 0.57              |
| 1:K:301:ILE:HD12 | 1:K:343:VAL:HG22 | 1.87                     | 0.57              |
| 1:A:213:LEU:O    | 1:A:217:LYS:HG3  | 2.04                     | 0.57              |
| 1:D:35:ASP:HB3   | 1:D:38:VAL:HG12  | 1.87                     | 0.57              |
| 1:K:285:ASN:HD21 | 1:K:288:LYS:HD2  | 1.69                     | 0.57              |
| 1:F:213:LEU:O    | 1:F:217:LYS:HG3  | 2.05                     | 0.57              |
| 1:L:35:ASP:HB3   | 1:L:38:VAL:HG12  | 1.88                     | 0.56              |
| 1:G:434:ASP:HA   | 1:G:436:THR:H    | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:241:ILE:CD1  | 1:K:342:ILE:HG23 | 2.32                     | 0.56              |
| 1:K:213:LEU:O    | 1:K:217:LYS:HG3  | 2.05                     | 0.56              |
| 1:E:201:VAL:HG11 | 1:E:253:LEU:HD12 | 1.88                     | 0.56              |
| 1:F:82:ILE:HG21  | 1:F:100:ILE:HD11 | 1.87                     | 0.56              |
| 1:C:434:ASP:HA   | 1:C:436:THR:H    | 1.70                     | 0.56              |
| 1:F:158:MET:CA   | 1:F:387:ASN:O    | 2.54                     | 0.56              |
| 1:L:434:ASP:HA   | 1:L:436:THR:H    | 1.69                     | 0.56              |
| 1:J:35:ASP:HB3   | 1:J:38:VAL:HG12  | 1.86                     | 0.56              |
| 1:I:220:VAL:HB   | 1:I:224:LEU:HD12 | 1.88                     | 0.56              |
| 1:L:20:LYS:C     | 1:L:21:ASN:OD1   | 2.44                     | 0.56              |
| 1:E:35:ASP:HB3   | 1:E:38:VAL:HG12  | 1.88                     | 0.56              |
| 1:G:193:ASP:OD1  | 1:G:193:ASP:N    | 2.39                     | 0.56              |
| 1:I:35:ASP:HB3   | 1:I:38:VAL:HG12  | 1.88                     | 0.56              |
| 1:C:209:CYS:HB2  | 1:C:212:GLN:CG   | 2.34                     | 0.56              |
| 1:K:347:THR:CG2  | 1:K:348:ASN:H    | 2.19                     | 0.56              |
| 1:E:220:VAL:HB   | 1:E:224:LEU:HD12 | 1.88                     | 0.56              |
| 1:D:201:VAL:HG11 | 1:D:253:LEU:CD1  | 2.36                     | 0.55              |
| 1:E:53:ARG:N     | 3:E:905:HOH:O    | 2.38                     | 0.55              |
| 1:K:35:ASP:HB3   | 1:K:38:VAL:HG12  | 1.88                     | 0.55              |
| 1:L:213:LEU:O    | 1:L:217:LYS:HG3  | 2.05                     | 0.55              |
| 1:L:220:VAL:HB   | 1:L:224:LEU:HD12 | 1.88                     | 0.55              |
| 1:B:142:ALA:HB1  | 1:B:144:ARG:HG3  | 1.88                     | 0.55              |
| 1:C:133:VAL:HG13 | 1:C:443:ASN:HB2  | 1.87                     | 0.55              |
| 1:K:285:ASN:ND2  | 1:K:288:LYS:HB3  | 2.21                     | 0.55              |
| 1:A:220:VAL:HB   | 1:A:224:LEU:HD12 | 1.88                     | 0.55              |
| 1:D:220:VAL:HB   | 1:D:224:LEU:HD12 | 1.88                     | 0.55              |
| 1:J:220:VAL:HB   | 1:J:224:LEU:HD12 | 1.88                     | 0.55              |
| 1:B:201:VAL:HG11 | 1:B:253:LEU:CD1  | 2.35                     | 0.55              |
| 1:K:297:ALA:HB1  | 1:K:340:HIS:O    | 2.07                     | 0.55              |
| 1:F:158:MET:HG2  | 1:F:388:MET:HB3  | 1.88                     | 0.55              |
| 1:H:220:VAL:HB   | 1:H:224:LEU:HD12 | 1.89                     | 0.55              |
| 1:J:21:ASN:HA    | 1:J:22:ARG:HG2   | 1.88                     | 0.55              |
| 1:K:306:LEU:HA   | 1:K:347:THR:HA   | 1.88                     | 0.55              |
| 1:K:304:ASP:HA   | 1:K:346:ALA:HB3  | 1.89                     | 0.55              |
| 1:B:220:VAL:HB   | 1:B:224:LEU:HD12 | 1.88                     | 0.55              |
| 1:G:206:ILE:HD11 | 1:G:209:CYS:SG   | 2.47                     | 0.55              |
| 1:K:301:ILE:HB   | 1:K:343:VAL:HG13 | 1.88                     | 0.55              |
| 1:I:218:GLU:OE1  | 1:K:454:TRP:HZ2  | 1.88                     | 0.55              |
| 1:B:213:LEU:O    | 1:B:217:LYS:HG3  | 2.07                     | 0.55              |
| 1:C:319:GLU:OE2  | 1:E:320:VAL:HG21 | 2.07                     | 0.55              |
| 1:F:283:GLU:OE2  | 1:F:323:ARG:HG2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:98:ASP:OD1   | 1:C:225:ARG:NH2  | 2.39                     | 0.54              |
| 1:D:193:ASP:N    | 1:D:193:ASP:OD1  | 2.40                     | 0.54              |
| 1:B:133:VAL:HG13 | 1:B:443:ASN:HB2  | 1.89                     | 0.54              |
| 1:G:125:GLY:HA2  | 1:K:231:LYS:HB3  | 1.89                     | 0.54              |
| 1:B:169:ASP:HB3  | 1:B:170:PRO:HD3  | 1.88                     | 0.54              |
| 1:F:142:ALA:HB1  | 1:F:144:ARG:HG3  | 1.90                     | 0.54              |
| 1:K:193:ASP:OD1  | 1:K:193:ASP:N    | 2.39                     | 0.54              |
| 1:A:35:ASP:HB3   | 1:A:38:VAL:HG12  | 1.88                     | 0.54              |
| 1:B:35:ASP:HB3   | 1:B:38:VAL:HG12  | 1.90                     | 0.54              |
| 1:C:35:ASP:HB3   | 1:C:38:VAL:HG12  | 1.89                     | 0.54              |
| 1:F:206:ILE:O    | 1:F:206:ILE:CG1  | 2.54                     | 0.54              |
| 1:G:35:ASP:HB3   | 1:G:38:VAL:HG12  | 1.87                     | 0.54              |
| 1:H:35:ASP:HB3   | 1:H:38:VAL:HG12  | 1.89                     | 0.54              |
| 1:H:218:GLU:OE1  | 1:J:454:TRP:HZ2  | 1.91                     | 0.54              |
| 1:K:209:CYS:HB2  | 1:K:212:GLN:CG   | 2.35                     | 0.54              |
| 1:C:222:LEU:HD11 | 1:E:424:ARG:CG   | 2.37                     | 0.54              |
| 1:G:220:VAL:HB   | 1:G:224:LEU:HD12 | 1.88                     | 0.54              |
| 1:I:432:LEU:HD23 | 1:J:21:ASN:HB2   | 1.90                     | 0.54              |
| 1:K:300:ILE:HD11 | 1:K:344:MET:HG3  | 1.90                     | 0.54              |
| 1:L:283:GLU:OE2  | 1:L:323:ARG:HG2  | 2.08                     | 0.54              |
| 1:E:187:GLU:CG   | 1:L:124:GLU:HG2  | 2.38                     | 0.54              |
| 1:G:322:ARG:HH22 | 1:L:317:HIS:HB2  | 1.73                     | 0.54              |
| 1:F:220:VAL:HB   | 1:F:224:LEU:HD12 | 1.90                     | 0.53              |
| 1:H:213:LEU:O    | 1:H:217:LYS:HG3  | 2.08                     | 0.53              |
| 1:G:213:LEU:O    | 1:G:217:LYS:HG3  | 2.09                     | 0.53              |
| 1:H:434:ASP:HA   | 1:H:436:THR:N    | 2.24                     | 0.53              |
| 1:H:26:LEU:HD21  | 1:H:45:LYS:HE2   | 1.90                     | 0.53              |
| 1:K:220:VAL:HB   | 1:K:224:LEU:HD12 | 1.91                     | 0.53              |
| 1:K:322:ARG:CA   | 1:K:325:VAL:HB   | 2.36                     | 0.53              |
| 1:J:249:THR:N    | 2:J:800:ADP:O2B  | 2.42                     | 0.53              |
| 1:C:193:ASP:N    | 1:C:193:ASP:OD1  | 2.42                     | 0.53              |
| 1:D:203:TYR:CE2  | 1:D:261:GLU:HG2  | 2.43                     | 0.53              |
| 1:E:209:CYS:HB2  | 1:E:212:GLN:CG   | 2.33                     | 0.53              |
| 1:F:197:SER:HB3  | 1:F:200:GLU:HG3  | 1.90                     | 0.53              |
| 1:I:283:GLU:OE2  | 1:I:323:ARG:HG2  | 2.09                     | 0.53              |
| 1:A:434:ASP:HA   | 1:A:436:THR:N    | 2.24                     | 0.53              |
| 1:F:169:ASP:HB3  | 1:F:170:PRO:HD3  | 1.91                     | 0.53              |
| 1:C:220:VAL:HB   | 1:C:224:LEU:HD12 | 1.89                     | 0.53              |
| 1:F:35:ASP:HB3   | 1:F:38:VAL:HG12  | 1.90                     | 0.53              |
| 1:K:300:ILE:HG13 | 1:K:342:ILE:O    | 2.08                     | 0.53              |
| 1:C:82:ILE:HG21  | 1:C:100:ILE:HD11 | 1.91                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:125:GLY:HA3 | 1:K:231:LYS:O    | 2.09                     | 0.53              |
| 1:B:55:ASP:O    | 1:B:71:VAL:HG12  | 2.09                     | 0.52              |
| 1:F:26:LEU:HD21 | 1:F:45:LYS:HE2   | 1.91                     | 0.52              |
| 1:H:82:ILE:HG21 | 1:H:100:ILE:HD11 | 1.91                     | 0.52              |
| 1:H:424:ARG:HG3 | 1:L:222:LEU:HD11 | 1.91                     | 0.52              |
| 1:J:193:ASP:OD1 | 1:J:193:ASP:N    | 2.42                     | 0.52              |
| 1:K:282:SER:O   | 1:K:324:ILE:HG21 | 2.09                     | 0.52              |
| 1:I:326:SER:CB  | 1:K:276:SER:HB3  | 2.38                     | 0.52              |
| 1:D:434:ASP:HA  | 1:D:436:THR:N    | 2.24                     | 0.52              |
| 1:E:434:ASP:HA  | 1:E:436:THR:N    | 2.24                     | 0.52              |
| 1:J:434:ASP:HA  | 1:J:436:THR:N    | 2.24                     | 0.52              |
| 1:K:436:THR:O   | 1:K:436:THR:HG23 | 2.07                     | 0.52              |
| 1:B:434:ASP:HA  | 1:B:436:THR:N    | 2.25                     | 0.52              |
| 1:I:193:ASP:OD1 | 1:I:193:ASP:N    | 2.41                     | 0.52              |
| 1:K:82:ILE:HG21 | 1:K:100:ILE:HD11 | 1.92                     | 0.52              |
| 1:F:90:ASN:O    | 1:F:93:ARG:NH1   | 2.43                     | 0.52              |
| 1:I:434:ASP:HA  | 1:I:436:THR:N    | 2.24                     | 0.52              |
| 1:A:227:PRO:HD2 | 3:A:906:HOH:O    | 2.10                     | 0.52              |
| 1:I:432:LEU:CD2 | 1:J:21:ASN:HB2   | 2.39                     | 0.52              |
| 1:J:82:ILE:HG21 | 1:J:100:ILE:HD11 | 1.91                     | 0.52              |
| 1:H:219:MET:HE2 | 3:J:917:HOH:O    | 2.09                     | 0.51              |
| 1:L:434:ASP:HA  | 1:L:436:THR:N    | 2.26                     | 0.51              |
| 1:A:82:ILE:HG21 | 1:A:100:ILE:HD11 | 1.92                     | 0.51              |
| 1:F:434:ASP:HA  | 1:F:436:THR:N    | 2.26                     | 0.51              |
| 1:H:106:PRO:HD2 | 1:H:107:ASP:H    | 1.75                     | 0.51              |
| 1:I:130:LEU:H   | 1:I:130:LEU:HD23 | 1.75                     | 0.51              |
| 1:B:249:THR:N   | 2:B:800:ADP:O2B  | 2.44                     | 0.51              |
| 1:I:213:LEU:O   | 1:I:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:C:139:PHE:CE1 | 1:C:176:VAL:HG11 | 2.46                     | 0.51              |
| 1:D:139:PHE:CE1 | 1:D:176:VAL:HG11 | 2.46                     | 0.51              |
| 1:G:310:ALA:HA  | 1:G:325:VAL:HG22 | 1.93                     | 0.51              |
| 1:H:139:PHE:CE1 | 1:H:176:VAL:HG11 | 2.46                     | 0.51              |
| 1:K:139:PHE:CE1 | 1:K:176:VAL:HG11 | 2.46                     | 0.51              |
| 1:L:193:ASP:OD1 | 1:L:193:ASP:N    | 2.43                     | 0.51              |
| 1:D:82:ILE:HG21 | 1:D:100:ILE:HD11 | 1.92                     | 0.51              |
| 1:B:283:GLU:OE2 | 1:B:323:ARG:HG2  | 2.10                     | 0.51              |
| 1:B:310:ALA:HA  | 1:B:325:VAL:HG22 | 1.93                     | 0.51              |
| 1:D:310:ALA:HA  | 1:D:325:VAL:HG22 | 1.92                     | 0.51              |
| 1:C:249:THR:N   | 2:C:800:ADP:O2B  | 2.44                     | 0.51              |
| 1:E:155:HIS:HB3 | 1:E:386:LYS:O    | 2.10                     | 0.51              |
| 1:I:338:ARG:HD2 | 3:I:901:HOH:O    | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:305:GLU:HG2  | 1:K:308:ALA:CB   | 2.40                     | 0.51              |
| 1:L:133:VAL:HG13 | 1:L:443:ASN:HB2  | 1.93                     | 0.51              |
| 1:A:193:ASP:N    | 1:A:193:ASP:OD1  | 2.42                     | 0.50              |
| 1:A:307:ASP:N    | 1:A:307:ASP:OD1  | 2.43                     | 0.50              |
| 1:E:82:ILE:HG21  | 1:E:100:ILE:HD11 | 1.92                     | 0.50              |
| 1:G:434:ASP:HA   | 1:G:436:THR:N    | 2.26                     | 0.50              |
| 1:H:206:ILE:HD11 | 1:H:209:CYS:SG   | 2.51                     | 0.50              |
| 1:K:241:ILE:HG12 | 1:K:343:VAL:C    | 2.31                     | 0.50              |
| 1:B:139:PHE:CE1  | 1:B:176:VAL:HG11 | 2.46                     | 0.50              |
| 1:B:193:ASP:N    | 1:B:193:ASP:OD1  | 2.44                     | 0.50              |
| 1:C:322:ARG:NE   | 1:E:321:GLU:OE1  | 2.44                     | 0.50              |
| 1:C:222:LEU:HD11 | 1:E:424:ARG:HH11 | 1.76                     | 0.50              |
| 1:F:310:ALA:HA   | 1:F:325:VAL:HG22 | 1.93                     | 0.50              |
| 1:G:82:ILE:HG21  | 1:G:100:ILE:HD11 | 1.92                     | 0.50              |
| 1:A:169:ASP:HB3  | 1:A:170:PRO:HD3  | 1.93                     | 0.50              |
| 1:E:169:ASP:HB3  | 1:E:170:PRO:HD3  | 1.94                     | 0.50              |
| 1:L:55:ASP:O     | 1:L:71:VAL:HG12  | 2.12                     | 0.50              |
| 1:A:194:GLU:HB2  | 1:K:193:ASP:OD2  | 2.11                     | 0.50              |
| 1:C:434:ASP:HA   | 1:C:436:THR:N    | 2.27                     | 0.50              |
| 1:J:310:ALA:HA   | 1:J:325:VAL:HG22 | 1.94                     | 0.50              |
| 1:H:106:PRO:CD   | 1:H:107:ASP:H    | 2.24                     | 0.50              |
| 1:H:52:PHE:O     | 1:H:55:ASP:HB2   | 2.12                     | 0.50              |
| 1:I:26:LEU:HD21  | 1:I:45:LYS:HE2   | 1.92                     | 0.50              |
| 1:K:408:GLY:HA3  | 2:K:800:ADP:N7   | 2.27                     | 0.50              |
| 1:C:169:ASP:HB3  | 1:C:170:PRO:HD3  | 1.94                     | 0.50              |
| 1:J:213:LEU:O    | 1:J:217:LYS:HG3  | 2.12                     | 0.50              |
| 1:L:169:ASP:HB3  | 1:L:170:PRO:HD3  | 1.94                     | 0.50              |
| 1:A:142:ALA:HB1  | 1:A:144:ARG:HG3  | 1.94                     | 0.50              |
| 1:F:377:ARG:NE   | 1:F:403:THR:O    | 2.45                     | 0.50              |
| 1:H:206:ILE:HG13 | 1:H:206:ILE:O    | 2.12                     | 0.50              |
| 1:K:430:ILE:HG22 | 1:K:433:GLU:HB3  | 1.92                     | 0.49              |
| 1:C:310:ALA:HA   | 1:C:325:VAL:HG22 | 1.94                     | 0.49              |
| 1:F:130:LEU:H    | 1:F:130:LEU:HD23 | 1.78                     | 0.49              |
| 1:B:424:ARG:HG3  | 1:F:222:LEU:HD11 | 1.95                     | 0.49              |
| 1:H:314:GLU:HB2  | 1:J:315:LYS:NZ   | 2.27                     | 0.49              |
| 1:K:305:GLU:CG   | 1:K:308:ALA:HA   | 2.42                     | 0.49              |
| 1:K:26:LEU:HD21  | 1:K:45:LYS:HE2   | 1.93                     | 0.49              |
| 1:C:326:SER:HB2  | 1:E:276:SER:HA   | 1.94                     | 0.49              |
| 1:I:307:ASP:N    | 1:I:307:ASP:OD1  | 2.44                     | 0.49              |
| 1:J:142:ALA:HB1  | 1:J:144:ARG:HG3  | 1.93                     | 0.49              |
| 1:K:305:GLU:HG3  | 1:K:308:ALA:HA   | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:201:VAL:HG11 | 1:I:253:LEU:HD12 | 1.95                     | 0.49              |
| 1:K:365:ARG:O    | 1:K:365:ARG:CG   | 2.56                     | 0.49              |
| 1:D:213:LEU:O    | 1:D:217:LYS:HG3  | 2.11                     | 0.49              |
| 1:G:169:ASP:HB3  | 1:G:170:PRO:HD3  | 1.94                     | 0.49              |
| 1:J:26:LEU:HD21  | 1:J:45:LYS:HE2   | 1.94                     | 0.49              |
| 1:L:40:SER:HB2   | 1:L:83:ARG:HB2   | 1.95                     | 0.49              |
| 1:A:26:LEU:HD21  | 1:A:45:LYS:HE2   | 1.93                     | 0.49              |
| 1:E:139:PHE:CE1  | 1:E:176:VAL:HG11 | 2.47                     | 0.49              |
| 1:H:310:ALA:HA   | 1:H:325:VAL:HG22 | 1.94                     | 0.49              |
| 1:B:278:LEU:HA   | 1:F:323:ARG:HH11 | 1.75                     | 0.49              |
| 1:I:249:THR:N    | 2:I:800:ADP:O2B  | 2.46                     | 0.49              |
| 2:C:800:ADP:O3B  | 1:D:359:ARG:NH2  | 2.46                     | 0.49              |
| 1:E:142:ALA:HB1  | 1:E:144:ARG:HG3  | 1.95                     | 0.49              |
| 1:F:408:GLY:HA3  | 2:F:800:ADP:N7   | 2.28                     | 0.49              |
| 1:G:133:VAL:HG11 | 1:G:439:ALA:HB1  | 1.94                     | 0.49              |
| 1:K:169:ASP:HB3  | 1:K:170:PRO:HD3  | 1.95                     | 0.49              |
| 1:A:310:ALA:HA   | 1:A:325:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:142:ALA:HB1  | 1:D:144:ARG:HG3  | 1.95                     | 0.49              |
| 1:F:56:THR:OG1   | 1:F:105:CYS:O    | 2.30                     | 0.49              |
| 1:H:169:ASP:HB3  | 1:H:170:PRO:HD3  | 1.95                     | 0.49              |
| 1:K:40:SER:HB2   | 1:K:83:ARG:HB2   | 1.95                     | 0.49              |
| 1:B:26:LEU:HD21  | 1:B:45:LYS:HE2   | 1.94                     | 0.48              |
| 1:H:283:GLU:OE2  | 1:H:323:ARG:HG2  | 2.13                     | 0.48              |
| 1:K:126:ILE:HB   | 1:K:439:ALA:HB2  | 1.94                     | 0.48              |
| 1:H:408:GLY:HA3  | 2:H:800:ADP:N7   | 2.28                     | 0.48              |
| 1:L:249:THR:N    | 2:L:800:ADP:O2B  | 2.47                     | 0.48              |
| 1:B:130:LEU:HD23 | 1:B:130:LEU:H    | 1.78                     | 0.48              |
| 1:B:427:MET:HA   | 1:B:430:ILE:HD12 | 1.95                     | 0.48              |
| 1:C:252:THR:HA   | 1:C:302:PHE:CE2  | 2.48                     | 0.48              |
| 1:I:82:ILE:HG21  | 1:I:100:ILE:HD11 | 1.94                     | 0.48              |
| 1:I:90:ASN:O     | 1:I:93:ARG:NH1   | 2.46                     | 0.48              |
| 1:K:306:LEU:HD23 | 1:K:346:ALA:HB1  | 1.95                     | 0.48              |
| 1:A:249:THR:N    | 2:A:800:ADP:O2B  | 2.46                     | 0.48              |
| 1:B:40:SER:HB2   | 1:B:83:ARG:HB2   | 1.94                     | 0.48              |
| 1:E:310:ALA:HA   | 1:E:325:VAL:HG22 | 1.95                     | 0.48              |
| 1:I:169:ASP:HB3  | 1:I:170:PRO:HD3  | 1.95                     | 0.48              |
| 1:L:90:ASN:O     | 1:L:93:ARG:NH1   | 2.45                     | 0.48              |
| 1:A:191:ARG:NH1  | 1:A:197:SER:HA   | 2.29                     | 0.48              |
| 1:J:169:ASP:HB3  | 1:J:170:PRO:HD3  | 1.94                     | 0.48              |
| 1:K:313:ARG:HD3  | 1:K:325:VAL:HG13 | 1.95                     | 0.48              |
| 1:B:206:ILE:CD1  | 1:B:254:ILE:HG12 | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:249:THR:N    | 2:F:800:ADP:O2B  | 2.46                     | 0.48              |
| 1:G:130:LEU:H    | 1:G:130:LEU:HD23 | 1.78                     | 0.48              |
| 1:G:55:ASP:O     | 1:G:71:VAL:HG12  | 2.14                     | 0.48              |
| 1:H:98:ASP:OD1   | 1:H:225:ARG:NH2  | 2.45                     | 0.48              |
| 1:I:142:ALA:HB1  | 1:I:144:ARG:HG3  | 1.95                     | 0.48              |
| 1:J:130:LEU:H    | 1:J:130:LEU:HD23 | 1.78                     | 0.48              |
| 1:K:130:LEU:HD23 | 1:K:130:LEU:H    | 1.79                     | 0.48              |
| 1:L:82:ILE:HG21  | 1:L:100:ILE:HD11 | 1.96                     | 0.48              |
| 1:C:153:LEU:HD13 | 1:C:198:LEU:HB2  | 1.94                     | 0.48              |
| 1:G:26:LEU:HD21  | 1:G:45:LYS:HE2   | 1.96                     | 0.48              |
| 1:I:408:GLY:HA3  | 2:I:800:ADP:N7   | 2.29                     | 0.48              |
| 1:K:286:LEU:O    | 1:K:290:PHE:CD1  | 2.67                     | 0.48              |
| 1:K:347:THR:HG22 | 1:K:348:ASN:N    | 2.23                     | 0.48              |
| 1:G:249:THR:N    | 2:G:800:ADP:O2B  | 2.46                     | 0.48              |
| 1:I:139:PHE:CE1  | 1:I:176:VAL:HG11 | 2.49                     | 0.48              |
| 1:J:183:HIS:HB3  | 3:J:909:HOH:O    | 2.14                     | 0.48              |
| 1:K:266:PHE:CD1  | 1:K:300:ILE:HG22 | 2.49                     | 0.48              |
| 1:I:310:ALA:HA   | 1:I:325:VAL:HG22 | 1.95                     | 0.48              |
| 1:C:26:LEU:HD21  | 1:C:45:LYS:HE2   | 1.95                     | 0.48              |
| 1:D:169:ASP:HB3  | 1:D:170:PRO:HD3  | 1.95                     | 0.48              |
| 1:K:142:ALA:HB1  | 1:K:144:ARG:HG3  | 1.96                     | 0.48              |
| 1:K:230:PHE:CE1  | 1:K:237:PRO:HG3  | 2.49                     | 0.48              |
| 1:L:26:LEU:HD21  | 1:L:45:LYS:HE2   | 1.95                     | 0.48              |
| 1:D:130:LEU:HD23 | 1:D:130:LEU:H    | 1.78                     | 0.47              |
| 1:F:138:TYR:CE2  | 1:F:152:PHE:CD2  | 3.02                     | 0.47              |
| 1:A:408:GLY:HA3  | 2:A:800:ADP:N7   | 2.29                     | 0.47              |
| 1:A:427:MET:HA   | 1:A:430:ILE:HD12 | 1.96                     | 0.47              |
| 1:D:427:MET:HA   | 1:D:430:ILE:HD12 | 1.97                     | 0.47              |
| 1:E:55:ASP:O     | 1:E:71:VAL:HG12  | 2.14                     | 0.47              |
| 1:F:87:VAL:HA    | 1:F:198:LEU:HD11 | 1.95                     | 0.47              |
| 1:K:241:ILE:HD11 | 1:K:342:ILE:HD12 | 1.95                     | 0.47              |
| 1:G:408:GLY:HA3  | 2:G:800:ADP:N7   | 2.28                     | 0.47              |
| 1:B:408:GLY:HA3  | 2:B:800:ADP:N7   | 2.30                     | 0.47              |
| 1:E:26:LEU:HD21  | 1:E:45:LYS:HE2   | 1.95                     | 0.47              |
| 1:E:34:GLU:N     | 3:E:909:HOH:O    | 2.27                     | 0.47              |
| 1:F:109:LYS:NZ   | 1:F:173:TYR:O    | 2.47                     | 0.47              |
| 1:F:203:TYR:CD2  | 1:F:261:GLU:HG2  | 2.50                     | 0.47              |
| 1:H:130:LEU:H    | 1:H:130:LEU:HD23 | 1.79                     | 0.47              |
| 1:C:427:MET:HA   | 1:C:430:ILE:HD12 | 1.97                     | 0.47              |
| 1:E:249:THR:N    | 2:E:800:ADP:O2B  | 2.47                     | 0.47              |
| 1:K:98:ASP:OD1   | 1:K:225:ARG:NH2  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:130:LEU:H    | 1:A:130:LEU:HD23 | 1.80                     | 0.47              |
| 1:A:139:PHE:CE1  | 1:A:176:VAL:HG11 | 2.50                     | 0.47              |
| 1:A:232:ALA:O    | 1:F:159:ARG:NE   | 2.48                     | 0.47              |
| 1:J:139:PHE:CE1  | 1:J:176:VAL:HG11 | 2.49                     | 0.47              |
| 1:K:306:LEU:HB3  | 1:K:347:THR:HA   | 1.97                     | 0.47              |
| 1:C:408:GLY:HA3  | 2:C:800:ADP:N7   | 2.30                     | 0.47              |
| 1:B:126:ILE:HB   | 1:B:439:ALA:HB2  | 1.95                     | 0.47              |
| 1:D:252:THR:HA   | 1:D:302:PHE:CE2  | 2.50                     | 0.47              |
| 1:D:408:GLY:HA3  | 2:D:800:ADP:N7   | 2.30                     | 0.47              |
| 1:E:185:GLU:OE2  | 1:L:187:GLU:OE1  | 2.33                     | 0.47              |
| 1:K:269:ILE:HG23 | 1:K:269:ILE:O    | 2.15                     | 0.47              |
| 1:L:408:GLY:HA3  | 2:L:800:ADP:N7   | 2.29                     | 0.47              |
| 1:I:222:LEU:HD11 | 1:K:424:ARG:CG   | 2.45                     | 0.47              |
| 1:L:310:ALA:HA   | 1:L:325:VAL:HG22 | 1.96                     | 0.47              |
| 1:G:142:ALA:HB1  | 1:G:144:ARG:HG3  | 1.96                     | 0.46              |
| 1:J:427:MET:HA   | 1:J:430:ILE:HD12 | 1.97                     | 0.46              |
| 1:L:139:PHE:CE1  | 1:L:176:VAL:HG11 | 2.50                     | 0.46              |
| 1:L:427:MET:HA   | 1:L:430:ILE:HD12 | 1.97                     | 0.46              |
| 1:C:55:ASP:O     | 1:C:71:VAL:HG12  | 2.15                     | 0.46              |
| 1:K:348:ASN:N    | 1:K:348:ASN:ND2  | 2.63                     | 0.46              |
| 1:D:55:ASP:O     | 1:D:71:VAL:HG12  | 2.15                     | 0.46              |
| 1:F:307:ASP:N    | 1:F:307:ASP:OD1  | 2.47                     | 0.46              |
| 1:C:130:LEU:H    | 1:C:130:LEU:HD23 | 1.81                     | 0.46              |
| 1:E:130:LEU:H    | 1:E:130:LEU:HD23 | 1.80                     | 0.46              |
| 1:F:427:MET:HA   | 1:F:430:ILE:HD12 | 1.97                     | 0.46              |
| 1:H:106:PRO:CD   | 1:H:107:ASP:N    | 2.76                     | 0.46              |
| 1:I:427:MET:HA   | 1:I:430:ILE:HD12 | 1.97                     | 0.46              |
| 1:K:430:ILE:CG2  | 1:K:433:GLU:CB   | 2.87                     | 0.46              |
| 1:D:26:LEU:HD21  | 1:D:45:LYS:HE2   | 1.97                     | 0.46              |
| 1:G:139:PHE:CE1  | 1:G:176:VAL:HG11 | 2.50                     | 0.46              |
| 1:K:269:ILE:O    | 1:K:303:ILE:HA   | 2.16                     | 0.46              |
| 1:C:142:ALA:HB1  | 1:C:144:ARG:HG3  | 1.97                     | 0.46              |
| 1:E:408:GLY:HA3  | 2:E:800:ADP:N7   | 2.31                     | 0.46              |
| 1:F:206:ILE:O    | 1:F:206:ILE:HG12 | 2.15                     | 0.46              |
| 1:K:239:ARG:HD3  | 1:K:342:ILE:CD1  | 2.45                     | 0.46              |
| 1:K:427:MET:HA   | 1:K:430:ILE:HD12 | 1.97                     | 0.46              |
| 1:K:433:GLU:CB   | 1:K:436:THR:CG2  | 2.88                     | 0.46              |
| 1:E:427:MET:HA   | 1:E:430:ILE:HD12 | 1.98                     | 0.46              |
| 1:B:82:ILE:HG21  | 1:B:100:ILE:HD11 | 1.98                     | 0.46              |
| 1:B:206:ILE:HD13 | 1:B:254:ILE:HG12 | 1.98                     | 0.46              |
| 1:D:40:SER:HB2   | 1:D:83:ARG:HB2   | 1.99                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:319:GLU:OE2  | 1:E:320:VAL:HG23 | 2.14                     | 0.45              |
| 1:D:249:THR:N    | 2:D:800:ADP:O2B  | 2.48                     | 0.45              |
| 1:L:137:PRO:HA   | 1:L:140:LEU:CD2  | 2.46                     | 0.45              |
| 1:K:266:PHE:CD1  | 1:K:300:ILE:CG2  | 2.99                     | 0.45              |
| 1:K:313:ARG:CZ   | 1:K:329:LEU:HD11 | 2.47                     | 0.45              |
| 1:H:201:VAL:HG11 | 1:H:253:LEU:HD12 | 1.97                     | 0.45              |
| 1:K:354:ASP:OD2  | 1:K:356:ALA:HB3  | 2.17                     | 0.45              |
| 1:L:140:LEU:O    | 1:L:140:LEU:HD12 | 2.15                     | 0.45              |
| 1:L:27:ILE:HA    | 1:L:98:ASP:O     | 2.16                     | 0.45              |
| 1:A:40:SER:HB2   | 1:A:83:ARG:HB2   | 1.98                     | 0.45              |
| 1:C:202:GLY:O    | 1:C:205:ASP:HB2  | 2.16                     | 0.45              |
| 1:E:252:THR:HA   | 1:E:302:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:55:ASP:O     | 1:A:71:VAL:HG12  | 2.16                     | 0.45              |
| 1:C:322:ARG:NH2  | 1:E:321:GLU:OE1  | 2.50                     | 0.45              |
| 1:F:320:VAL:HG22 | 1:F:323:ARG:NH2  | 2.32                     | 0.45              |
| 1:H:427:MET:HA   | 1:H:430:ILE:HD12 | 1.99                     | 0.45              |
| 1:J:408:GLY:HA3  | 2:J:800:ADP:N7   | 2.31                     | 0.45              |
| 1:G:320:VAL:N    | 1:K:319:GLU:OE2  | 2.50                     | 0.45              |
| 1:C:307:ASP:N    | 1:C:307:ASP:OD1  | 2.50                     | 0.45              |
| 1:H:307:ASP:OD1  | 1:H:307:ASP:N    | 2.48                     | 0.45              |
| 1:A:90:ASN:O     | 1:A:93:ARG:NH1   | 2.49                     | 0.45              |
| 1:J:307:ASP:OD1  | 1:J:307:ASP:N    | 2.49                     | 0.45              |
| 3:G:908:HOH:O    | 1:K:359:ARG:CG   | 2.65                     | 0.45              |
| 1:L:248:GLY:N    | 2:L:800:ADP:O3B  | 2.43                     | 0.45              |
| 1:D:90:ASN:O     | 1:D:93:ARG:NH1   | 2.50                     | 0.45              |
| 1:F:193:ASP:N    | 1:F:193:ASP:OD1  | 2.48                     | 0.45              |
| 1:F:43:GLN:N     | 1:F:44:PRO:HD2   | 2.32                     | 0.45              |
| 1:B:218:GLU:OE1  | 1:D:454:TRP:HZ2  | 2.00                     | 0.45              |
| 1:H:22:ARG:HG2   | 1:J:432:LEU:HG   | 1.98                     | 0.45              |
| 1:K:322:ARG:HA   | 1:K:325:VAL:CB   | 2.41                     | 0.45              |
| 1:C:431:ASP:HB3  | 1:D:27:ILE:HD11  | 1.99                     | 0.44              |
| 1:F:55:ASP:O     | 1:F:71:VAL:HG12  | 2.17                     | 0.44              |
| 1:K:242:LEU:O    | 1:K:366:GLU:HA   | 2.17                     | 0.44              |
| 1:C:159:ARG:NH2  | 1:D:231:LYS:O    | 2.49                     | 0.44              |
| 1:L:142:ALA:HB1  | 1:L:144:ARG:HG3  | 1.99                     | 0.44              |
| 1:L:43:GLN:N     | 1:L:44:PRO:HD2   | 2.32                     | 0.44              |
| 1:C:158:MET:HG2  | 1:C:388:MET:HB3  | 2.00                     | 0.44              |
| 1:C:222:LEU:CD1  | 1:E:424:ARG:HH11 | 2.30                     | 0.44              |
| 1:K:376:GLY:O    | 1:K:380:ILE:HG12 | 2.18                     | 0.44              |
| 1:B:139:PHE:CD1  | 1:B:176:VAL:HG11 | 2.52                     | 0.44              |
| 1:D:43:GLN:N     | 1:D:44:PRO:HD2   | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:SER:O    | 1:E:200:GLU:HB2  | 2.17                     | 0.44              |
| 1:G:427:MET:HA   | 1:G:430:ILE:HD12 | 1.99                     | 0.44              |
| 1:E:307:ASP:OD1  | 1:E:307:ASP:N    | 2.48                     | 0.44              |
| 1:G:40:SER:HB2   | 1:G:83:ARG:HB2   | 1.99                     | 0.44              |
| 1:J:40:SER:HB2   | 1:J:83:ARG:HB2   | 1.99                     | 0.44              |
| 3:G:908:HOH:O    | 1:K:359:ARG:HG3  | 2.16                     | 0.44              |
| 1:K:90:ASN:O     | 1:K:93:ARG:NH1   | 2.50                     | 0.44              |
| 1:L:307:ASP:N    | 1:L:307:ASP:OD1  | 2.50                     | 0.44              |
| 1:A:359:ARG:NH2  | 2:F:800:ADP:O3B  | 2.51                     | 0.44              |
| 1:B:276:SER:HA   | 1:F:326:SER:CB   | 2.35                     | 0.44              |
| 1:B:307:ASP:OD1  | 1:B:307:ASP:N    | 2.50                     | 0.44              |
| 1:F:112:LYS:HD2  | 1:F:169:ASP:OD2  | 2.18                     | 0.44              |
| 1:G:197:SER:O    | 1:G:200:GLU:HB2  | 2.18                     | 0.44              |
| 1:H:118:PRO:HB2  | 1:H:123:VAL:HG11 | 1.99                     | 0.44              |
| 1:H:222:LEU:N    | 1:H:223:PRO:HD2  | 2.32                     | 0.44              |
| 1:L:130:LEU:H    | 1:L:130:LEU:HD23 | 1.82                     | 0.44              |
| 1:C:420:LEU:HG   | 1:D:235:VAL:HG11 | 2.00                     | 0.44              |
| 1:F:252:THR:HA   | 1:F:302:PHE:CE2  | 2.53                     | 0.44              |
| 1:F:31:ALA:HB2   | 1:F:84:MET:C     | 2.38                     | 0.44              |
| 1:K:133:VAL:HG13 | 1:K:443:ASN:HB2  | 2.00                     | 0.44              |
| 1:K:347:THR:CG2  | 1:K:348:ASN:N    | 2.81                     | 0.44              |
| 1:B:21:ASN:CA    | 1:D:432:LEU:HG   | 2.47                     | 0.43              |
| 1:E:43:GLN:N     | 1:E:44:PRO:HD2   | 2.33                     | 0.43              |
| 1:H:139:PHE:CD1  | 1:H:176:VAL:HG11 | 2.53                     | 0.43              |
| 1:K:249:THR:N    | 2:K:800:ADP:O2B  | 2.51                     | 0.43              |
| 1:G:43:GLN:N     | 1:G:44:PRO:HD2   | 2.33                     | 0.43              |
| 1:H:142:ALA:HB1  | 1:H:144:ARG:HG3  | 2.00                     | 0.43              |
| 1:K:286:LEU:HD21 | 1:K:287:ARG:HH21 | 1.81                     | 0.43              |
| 1:B:114:ILE:HD11 | 1:B:146:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:155:HIS:HB3  | 1:B:386:LYS:O    | 2.18                     | 0.43              |
| 1:F:27:ILE:HA    | 1:F:98:ASP:O     | 2.19                     | 0.43              |
| 1:K:285:ASN:ND2  | 1:K:288:LYS:CB   | 2.81                     | 0.43              |
| 1:K:251:LYS:NZ   | 1:K:348:ASN:HB3  | 2.32                     | 0.43              |
| 1:C:222:LEU:N    | 1:C:223:PRO:HD2  | 2.33                     | 0.43              |
| 1:D:206:ILE:O    | 1:D:206:ILE:CG1  | 2.61                     | 0.43              |
| 1:K:140:LEU:HD12 | 3:K:905:HOH:O    | 2.18                     | 0.43              |
| 1:E:90:ASN:O     | 1:E:93:ARG:NH1   | 2.51                     | 0.43              |
| 1:H:249:THR:N    | 2:H:800:ADP:O2B  | 2.52                     | 0.43              |
| 1:G:276:SER:O    | 1:K:323:ARG:O    | 2.36                     | 0.43              |
| 1:E:40:SER:HB2   | 1:E:83:ARG:HB2   | 2.01                     | 0.43              |
| 1:H:320:VAL:HG22 | 1:H:323:ARG:NH2  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:248:GLY:N    | 2:H:800:ADP:O3B  | 2.43                     | 0.43              |
| 1:B:222:LEU:N    | 1:B:223:PRO:HD2  | 2.32                     | 0.43              |
| 1:B:314:GLU:HB2  | 1:D:315:LYS:NZ   | 2.34                     | 0.43              |
| 1:E:320:VAL:HG22 | 1:E:323:ARG:NH2  | 2.34                     | 0.43              |
| 1:H:113:ARG:HB3  | 1:H:169:ASP:HB2  | 2.00                     | 0.43              |
| 1:L:191:ARG:NH1  | 1:L:197:SER:HA   | 2.34                     | 0.43              |
| 1:C:117:LEU:HD13 | 1:H:187:GLU:HG3  | 2.00                     | 0.43              |
| 1:H:40:SER:HB2   | 1:H:83:ARG:HB2   | 2.01                     | 0.43              |
| 1:K:239:ARG:HB3  | 1:K:335:LEU:HD12 | 2.01                     | 0.43              |
| 1:K:55:ASP:O     | 1:K:71:VAL:HG12  | 2.18                     | 0.43              |
| 1:C:229:LEU:CD1  | 1:E:427:MET:HE3  | 2.49                     | 0.43              |
| 1:I:222:LEU:N    | 1:I:223:PRO:HD2  | 2.34                     | 0.43              |
| 1:K:302:PHE:CZ   | 1:K:346:ALA:HB2  | 2.53                     | 0.43              |
| 1:D:42:SER:OG    | 1:D:79:ASP:HA    | 2.19                     | 0.42              |
| 1:J:43:GLN:N     | 1:J:44:PRO:HD2   | 2.34                     | 0.42              |
| 1:J:55:ASP:O     | 1:J:71:VAL:HG12  | 2.19                     | 0.42              |
| 1:K:43:GLN:N     | 1:K:44:PRO:HD2   | 2.34                     | 0.42              |
| 1:A:43:GLN:N     | 1:A:44:PRO:HD2   | 2.34                     | 0.42              |
| 1:C:206:ILE:HD13 | 1:C:254:ILE:HG12 | 2.01                     | 0.42              |
| 1:C:424:ARG:HG3  | 1:D:222:LEU:HD11 | 2.02                     | 0.42              |
| 1:I:176:VAL:O    | 1:I:176:VAL:HG13 | 2.20                     | 0.42              |
| 1:K:242:LEU:CD1  | 1:K:363:PHE:HE2  | 2.32                     | 0.42              |
| 1:K:433:GLU:CA   | 1:K:436:THR:HG22 | 2.48                     | 0.42              |
| 1:B:159:ARG:C    | 1:B:387:ASN:OD1  | 2.58                     | 0.42              |
| 1:B:177:ALA:HB1  | 1:B:178:PRO:HD2  | 2.01                     | 0.42              |
| 1:D:199:ASN:O    | 1:D:200:GLU:C    | 2.57                     | 0.42              |
| 1:D:222:LEU:N    | 1:D:223:PRO:HD2  | 2.34                     | 0.42              |
| 1:E:30:GLU:OE2   | 1:E:217:LYS:HE2  | 2.19                     | 0.42              |
| 1:G:222:LEU:N    | 1:G:223:PRO:HD2  | 2.34                     | 0.42              |
| 1:I:252:THR:HA   | 1:I:302:PHE:CE2  | 2.54                     | 0.42              |
| 1:I:55:ASP:O     | 1:I:71:VAL:HG12  | 2.20                     | 0.42              |
| 1:K:115:HIS:HE1  | 1:K:185:GLU:HB2  | 1.85                     | 0.42              |
| 1:B:111:GLY:HA2  | 1:B:170:PRO:CD   | 2.50                     | 0.42              |
| 1:F:177:ALA:HB1  | 1:F:178:PRO:HD2  | 2.01                     | 0.42              |
| 1:I:43:GLN:N     | 1:I:44:PRO:HD2   | 2.34                     | 0.42              |
| 1:G:115:HIS:HE1  | 1:G:185:GLU:HB2  | 1.85                     | 0.42              |
| 1:G:307:ASP:N    | 1:G:307:ASP:OD1  | 2.52                     | 0.42              |
| 1:I:40:SER:HB2   | 1:I:83:ARG:HB2   | 2.01                     | 0.42              |
| 1:J:252:THR:HA   | 1:J:302:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:27:ILE:HD11  | 1:F:431:ASP:HB3  | 2.01                     | 0.42              |
| 1:C:187:GLU:HB2  | 1:H:187:GLU:HB2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:252:THR:HA   | 1:H:302:PHE:CE2  | 2.55                     | 0.42              |
| 1:K:246:PRO:O    | 1:K:249:THR:OG1  | 2.38                     | 0.42              |
| 1:G:330:THR:OG1  | 1:L:273:GLU:HA   | 2.19                     | 0.42              |
| 1:A:252:THR:HA   | 1:A:302:PHE:CE2  | 2.54                     | 0.42              |
| 1:C:229:LEU:HD12 | 1:E:427:MET:HE1  | 2.01                     | 0.42              |
| 1:C:40:SER:HB2   | 1:C:83:ARG:HB2   | 2.01                     | 0.42              |
| 1:I:42:SER:OG    | 1:I:79:ASP:HA    | 2.20                     | 0.42              |
| 1:F:126:ILE:CB   | 1:F:439:ALA:HB2  | 2.47                     | 0.42              |
| 1:B:320:VAL:HG22 | 1:B:323:ARG:NH2  | 2.34                     | 0.42              |
| 1:C:377:ARG:NE   | 1:C:403:THR:O    | 2.53                     | 0.42              |
| 1:D:203:TYR:CE2  | 1:D:217:LYS:HD2  | 2.55                     | 0.42              |
| 1:A:99:VAL:HG11  | 1:F:431:ASP:HB2  | 2.02                     | 0.42              |
| 1:I:302:PHE:HA   | 1:I:344:MET:O    | 2.20                     | 0.42              |
| 1:J:203:TYR:CD2  | 1:J:261:GLU:HG2  | 2.54                     | 0.42              |
| 1:K:253:LEU:HD22 | 2:K:800:ADP:H2'  | 2.01                     | 0.42              |
| 1:L:20:LYS:CB    | 1:L:21:ASN:OD1   | 2.68                     | 0.42              |
| 1:A:324:ILE:HG22 | 1:A:325:VAL:N    | 2.35                     | 0.41              |
| 1:C:42:SER:OG    | 1:C:79:ASP:HA    | 2.20                     | 0.41              |
| 1:G:252:THR:HA   | 1:G:302:PHE:CE2  | 2.55                     | 0.41              |
| 1:H:90:ASN:O     | 1:H:93:ARG:NH1   | 2.53                     | 0.41              |
| 1:J:90:ASN:O     | 1:J:93:ARG:NH1   | 2.53                     | 0.41              |
| 1:K:310:ALA:N    | 1:K:311:PRO:HD3  | 2.35                     | 0.41              |
| 1:L:198:LEU:HD22 | 1:L:198:LEU:HA   | 1.81                     | 0.41              |
| 1:F:222:LEU:N    | 1:F:223:PRO:HD2  | 2.35                     | 0.41              |
| 1:G:320:VAL:HG22 | 1:G:323:ARG:NH2  | 2.35                     | 0.41              |
| 1:K:212:GLN:CD   | 1:K:212:GLN:H    | 2.24                     | 0.41              |
| 1:J:42:SER:OG    | 1:J:79:ASP:HA    | 2.19                     | 0.41              |
| 1:B:112:LYS:O    | 1:B:181:VAL:N    | 2.52                     | 0.41              |
| 1:D:113:ARG:HB3  | 1:D:169:ASP:HB2  | 2.03                     | 0.41              |
| 1:B:118:PRO:HB2  | 1:B:123:VAL:HG11 | 2.02                     | 0.41              |
| 1:B:321:GLU:OE1  | 1:F:322:ARG:CZ   | 2.68                     | 0.41              |
| 1:B:90:ASN:O     | 1:B:93:ARG:NH1   | 2.54                     | 0.41              |
| 1:C:320:VAL:HG22 | 1:C:323:ARG:NH2  | 2.36                     | 0.41              |
| 1:D:324:ILE:HG22 | 1:D:325:VAL:N    | 2.36                     | 0.41              |
| 1:F:35:ASP:HB3   | 1:F:38:VAL:CG1   | 2.49                     | 0.41              |
| 1:G:176:VAL:O    | 1:G:176:VAL:HG13 | 2.20                     | 0.41              |
| 1:G:232:ALA:O    | 1:L:159:ARG:NE   | 2.53                     | 0.41              |
| 1:H:193:ASP:N    | 1:H:193:ASP:OD1  | 2.53                     | 0.41              |
| 1:L:113:ARG:HB3  | 1:L:169:ASP:HB2  | 2.01                     | 0.41              |
| 1:D:115:HIS:HE1  | 1:D:185:GLU:HB2  | 1.84                     | 0.41              |
| 1:G:90:ASN:O     | 1:G:93:ARG:NH1   | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:176:VAL:HG13 | 1:K:176:VAL:O    | 2.21                     | 0.41              |
| 1:C:43:GLN:N     | 1:C:44:PRO:HD2   | 2.35                     | 0.41              |
| 1:F:134:TYR:O    | 1:F:137:PRO:HD2  | 2.21                     | 0.41              |
| 1:G:131:PHE:CD1  | 1:G:131:PHE:C    | 2.94                     | 0.41              |
| 1:L:252:THR:HA   | 1:L:302:PHE:CE2  | 2.56                     | 0.41              |
| 1:I:274:ILE:HD13 | 1:I:274:ILE:HA   | 1.95                     | 0.41              |
| 1:A:113:ARG:HB3  | 1:A:169:ASP:HB2  | 2.03                     | 0.41              |
| 1:A:176:VAL:O    | 1:A:176:VAL:HG13 | 2.20                     | 0.41              |
| 1:B:176:VAL:O    | 1:B:176:VAL:HG13 | 2.20                     | 0.41              |
| 1:G:212:GLN:O    | 1:G:216:ILE:HG12 | 2.21                     | 0.41              |
| 1:G:348:ASN:HB2  | 3:G:902:HOH:O    | 2.21                     | 0.41              |
| 1:H:176:VAL:O    | 1:H:176:VAL:HG13 | 2.21                     | 0.41              |
| 1:H:35:ASP:HB3   | 1:H:38:VAL:CG1   | 2.49                     | 0.41              |
| 1:K:348:ASN:N    | 1:K:348:ASN:HD22 | 2.19                     | 0.41              |
| 1:L:35:ASP:HB3   | 1:L:38:VAL:CG1   | 2.50                     | 0.41              |
| 1:A:320:VAL:HG22 | 1:A:323:ARG:NH2  | 2.35                     | 0.41              |
| 1:D:37:SER:HA    | 3:D:914:HOH:O    | 2.21                     | 0.41              |
| 1:I:206:ILE:HD13 | 1:I:254:ILE:HG12 | 2.03                     | 0.41              |
| 1:L:139:PHE:CD1  | 1:L:176:VAL:HG11 | 2.56                     | 0.41              |
| 1:L:20:LYS:C     | 1:L:21:ASN:CG    | 2.79                     | 0.41              |
| 1:L:222:LEU:N    | 1:L:223:PRO:HD2  | 2.35                     | 0.41              |
| 1:B:43:GLN:N     | 1:B:44:PRO:HD2   | 2.35                     | 0.40              |
| 1:C:115:HIS:HE1  | 1:C:185:GLU:HB2  | 1.86                     | 0.40              |
| 1:I:320:VAL:HG22 | 1:I:323:ARG:NH2  | 2.36                     | 0.40              |
| 1:J:113:ARG:HB3  | 1:J:169:ASP:HB2  | 2.03                     | 0.40              |
| 1:K:297:ALA:HB1  | 1:K:298:PRO:HA   | 2.02                     | 0.40              |
| 1:A:27:ILE:HA    | 1:A:98:ASP:O     | 2.22                     | 0.40              |
| 1:D:139:PHE:CD1  | 1:D:176:VAL:HG11 | 2.55                     | 0.40              |
| 1:D:274:ILE:HD13 | 1:D:274:ILE:HA   | 1.95                     | 0.40              |
| 1:I:228:ALA:CB   | 1:K:435:GLU:HG2  | 2.52                     | 0.40              |
| 1:K:113:ARG:HB3  | 1:K:169:ASP:HB2  | 2.03                     | 0.40              |
| 1:K:239:ARG:HD3  | 1:K:342:ILE:HG13 | 2.03                     | 0.40              |
| 1:K:351:ASN:HD22 | 1:K:351:ASN:N    | 2.19                     | 0.40              |
| 1:B:131:PHE:CD1  | 1:B:131:PHE:C    | 2.94                     | 0.40              |
| 1:D:320:VAL:HG22 | 1:D:323:ARG:NH2  | 2.36                     | 0.40              |
| 1:J:35:ASP:HB3   | 1:J:38:VAL:CG1   | 2.50                     | 0.40              |
| 1:K:327:GLN:HA   | 1:K:330:THR:HG22 | 2.03                     | 0.40              |
| 1:L:274:ILE:HA   | 1:L:274:ILE:HD13 | 1.96                     | 0.40              |
| 1:A:139:PHE:CD1  | 1:A:176:VAL:HG11 | 2.57                     | 0.40              |
| 1:A:197:SER:O    | 1:A:200:GLU:HB2  | 2.21                     | 0.40              |
| 1:B:138:TYR:CE2  | 1:B:152:PHE:CD2  | 3.10                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:326:SER:HB3  | 1:E:276:SER:CB   | 2.45                     | 0.40              |
| 1:C:248:GLY:N    | 2:C:800:ADP:O3B  | 2.44                     | 0.40              |
| 1:E:222:LEU:N    | 1:E:223:PRO:HD2  | 2.35                     | 0.40              |
| 1:E:407:VAL:O    | 1:E:410:ASP:HB2  | 2.21                     | 0.40              |
| 1:H:203:TYR:CD2  | 1:H:261:GLU:HG2  | 2.55                     | 0.40              |
| 1:K:249:THR:HA   | 1:K:407:VAL:HG22 | 2.04                     | 0.40              |
| 1:C:113:ARG:HB3  | 1:C:169:ASP:HB2  | 2.03                     | 0.40              |
| 1:C:222:LEU:HD12 | 1:C:222:LEU:H    | 1.85                     | 0.40              |
| 1:K:286:LEU:CD2  | 1:K:287:ARG:HH21 | 2.34                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:F:404:HIS:CG | 1:G:210:ARG:NH1[3_645] | 1.92                     | 0.28              |
| 1:B:52:PHE:CZ  | 1:I:49:LEU:O[4_455]    | 2.09                     | 0.11              |

## 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     | 436/489 (89%) | 419 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | B     | 437/489 (89%) | 416 (95%) | 21 (5%) | 0        | 100         | 100 |
| 1   | C     | 436/489 (89%) | 418 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | D     | 437/489 (89%) | 417 (95%) | 20 (5%) | 0        | 100         | 100 |
| 1   | E     | 437/489 (89%) | 418 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | F     | 436/489 (89%) | 417 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | G     | 435/489 (89%) | 418 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | H     | 436/489 (89%) | 416 (95%) | 19 (4%) | 1 (0%)   | 47          | 79  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | I     | 438/489 (90%)   | 418 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | J     | 443/489 (91%)   | 425 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | K     | 436/489 (89%)   | 398 (91%)  | 35 (8%)  | 3 (1%)   | 22          | 56  |
| 1   | L     | 440/489 (90%)   | 419 (95%)  | 20 (4%)  | 1 (0%)   | 47          | 79  |
| All | All   | 5247/5868 (89%) | 4999 (95%) | 243 (5%) | 5 (0%)   | 51          | 83  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 23  | PRO  |
| 1   | K     | 241 | ILE  |
| 1   | K     | 277 | LYS  |
| 1   | K     | 359 | ARG  |
| 1   | H     | 106 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 375/418 (90%) | 345 (92%) | 30 (8%)  | 12          | 37 |
| 1   | B     | 376/418 (90%) | 346 (92%) | 30 (8%)  | 12          | 37 |
| 1   | C     | 375/418 (90%) | 345 (92%) | 30 (8%)  | 12          | 37 |
| 1   | D     | 376/418 (90%) | 345 (92%) | 31 (8%)  | 11          | 36 |
| 1   | E     | 376/418 (90%) | 345 (92%) | 31 (8%)  | 11          | 36 |
| 1   | F     | 375/418 (90%) | 343 (92%) | 32 (8%)  | 10          | 34 |
| 1   | G     | 374/418 (90%) | 344 (92%) | 30 (8%)  | 12          | 37 |
| 1   | H     | 375/418 (90%) | 344 (92%) | 31 (8%)  | 11          | 35 |
| 1   | I     | 377/418 (90%) | 345 (92%) | 32 (8%)  | 10          | 34 |
| 1   | J     | 382/418 (91%) | 349 (91%) | 33 (9%)  | 10          | 34 |
| 1   | K     | 375/418 (90%) | 329 (88%) | 46 (12%) | 4           | 18 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | L     | 379/418 (91%)   | 349 (92%)  | 30 (8%)  | 12          | 37 |
| All | All   | 4515/5016 (90%) | 4129 (92%) | 386 (8%) | 10          | 34 |

All (386) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | VAL  |
| 1   | A     | 33  | ASN  |
| 1   | A     | 56  | THR  |
| 1   | A     | 78  | SER  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 109 | LYS  |
| 1   | A     | 127 | THR  |
| 1   | A     | 147 | ARG  |
| 1   | A     | 184 | CYS  |
| 1   | A     | 193 | ASP  |
| 1   | A     | 198 | LEU  |
| 1   | A     | 206 | ILE  |
| 1   | A     | 210 | ARG  |
| 1   | A     | 211 | LYS  |
| 1   | A     | 212 | GLN  |
| 1   | A     | 217 | LYS  |
| 1   | A     | 249 | THR  |
| 1   | A     | 256 | ARG  |
| 1   | A     | 288 | LYS  |
| 1   | A     | 313 | ARG  |
| 1   | A     | 314 | GLU  |
| 1   | A     | 315 | LYS  |
| 1   | A     | 322 | ARG  |
| 1   | A     | 324 | ILE  |
| 1   | A     | 327 | GLN  |
| 1   | A     | 335 | LEU  |
| 1   | A     | 338 | ARG  |
| 1   | A     | 375 | THR  |
| 1   | A     | 378 | LEU  |
| 1   | A     | 435 | GLU  |
| 1   | B     | 28  | VAL  |
| 1   | B     | 33  | ASN  |
| 1   | B     | 56  | THR  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 109 | LYS  |
| 1   | B     | 127 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 147 | ARG  |
| 1   | B     | 184 | CYS  |
| 1   | B     | 193 | ASP  |
| 1   | B     | 199 | ASN  |
| 1   | B     | 206 | ILE  |
| 1   | B     | 210 | ARG  |
| 1   | B     | 211 | LYS  |
| 1   | B     | 212 | GLN  |
| 1   | B     | 217 | LYS  |
| 1   | B     | 249 | THR  |
| 1   | B     | 256 | ARG  |
| 1   | B     | 288 | LYS  |
| 1   | B     | 313 | ARG  |
| 1   | B     | 314 | GLU  |
| 1   | B     | 315 | LYS  |
| 1   | B     | 322 | ARG  |
| 1   | B     | 324 | ILE  |
| 1   | B     | 327 | GLN  |
| 1   | B     | 335 | LEU  |
| 1   | B     | 338 | ARG  |
| 1   | B     | 351 | ASN  |
| 1   | B     | 375 | THR  |
| 1   | B     | 378 | LEU  |
| 1   | B     | 435 | GLU  |
| 1   | C     | 28  | VAL  |
| 1   | C     | 33  | ASN  |
| 1   | C     | 56  | THR  |
| 1   | C     | 78  | SER  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 109 | LYS  |
| 1   | C     | 127 | THR  |
| 1   | C     | 147 | ARG  |
| 1   | C     | 184 | CYS  |
| 1   | C     | 193 | ASP  |
| 1   | C     | 206 | ILE  |
| 1   | C     | 210 | ARG  |
| 1   | C     | 211 | LYS  |
| 1   | C     | 212 | GLN  |
| 1   | C     | 217 | LYS  |
| 1   | C     | 249 | THR  |
| 1   | C     | 256 | ARG  |
| 1   | C     | 288 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 313 | ARG  |
| 1   | C     | 314 | GLU  |
| 1   | C     | 315 | LYS  |
| 1   | C     | 322 | ARG  |
| 1   | C     | 324 | ILE  |
| 1   | C     | 327 | GLN  |
| 1   | C     | 335 | LEU  |
| 1   | C     | 338 | ARG  |
| 1   | C     | 351 | ASN  |
| 1   | C     | 375 | THR  |
| 1   | C     | 378 | LEU  |
| 1   | C     | 435 | GLU  |
| 1   | D     | 22  | ARG  |
| 1   | D     | 28  | VAL  |
| 1   | D     | 33  | ASN  |
| 1   | D     | 56  | THR  |
| 1   | D     | 78  | SER  |
| 1   | D     | 96  | LEU  |
| 1   | D     | 109 | LYS  |
| 1   | D     | 147 | ARG  |
| 1   | D     | 184 | CYS  |
| 1   | D     | 193 | ASP  |
| 1   | D     | 206 | ILE  |
| 1   | D     | 210 | ARG  |
| 1   | D     | 211 | LYS  |
| 1   | D     | 212 | GLN  |
| 1   | D     | 217 | LYS  |
| 1   | D     | 249 | THR  |
| 1   | D     | 256 | ARG  |
| 1   | D     | 288 | LYS  |
| 1   | D     | 313 | ARG  |
| 1   | D     | 314 | GLU  |
| 1   | D     | 315 | LYS  |
| 1   | D     | 322 | ARG  |
| 1   | D     | 324 | ILE  |
| 1   | D     | 327 | GLN  |
| 1   | D     | 335 | LEU  |
| 1   | D     | 338 | ARG  |
| 1   | D     | 351 | ASN  |
| 1   | D     | 375 | THR  |
| 1   | D     | 378 | LEU  |
| 1   | D     | 435 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 460 | ASN  |
| 1   | E     | 28  | VAL  |
| 1   | E     | 33  | ASN  |
| 1   | E     | 56  | THR  |
| 1   | E     | 96  | LEU  |
| 1   | E     | 109 | LYS  |
| 1   | E     | 127 | THR  |
| 1   | E     | 147 | ARG  |
| 1   | E     | 184 | CYS  |
| 1   | E     | 193 | ASP  |
| 1   | E     | 200 | GLU  |
| 1   | E     | 206 | ILE  |
| 1   | E     | 210 | ARG  |
| 1   | E     | 211 | LYS  |
| 1   | E     | 212 | GLN  |
| 1   | E     | 217 | LYS  |
| 1   | E     | 249 | THR  |
| 1   | E     | 256 | ARG  |
| 1   | E     | 288 | LYS  |
| 1   | E     | 313 | ARG  |
| 1   | E     | 314 | GLU  |
| 1   | E     | 315 | LYS  |
| 1   | E     | 322 | ARG  |
| 1   | E     | 324 | ILE  |
| 1   | E     | 327 | GLN  |
| 1   | E     | 335 | LEU  |
| 1   | E     | 338 | ARG  |
| 1   | E     | 351 | ASN  |
| 1   | E     | 375 | THR  |
| 1   | E     | 378 | LEU  |
| 1   | E     | 435 | GLU  |
| 1   | E     | 460 | ASN  |
| 1   | F     | 28  | VAL  |
| 1   | F     | 33  | ASN  |
| 1   | F     | 56  | THR  |
| 1   | F     | 78  | SER  |
| 1   | F     | 96  | LEU  |
| 1   | F     | 107 | ASP  |
| 1   | F     | 109 | LYS  |
| 1   | F     | 147 | ARG  |
| 1   | F     | 184 | CYS  |
| 1   | F     | 193 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 198 | LEU  |
| 1   | F     | 200 | GLU  |
| 1   | F     | 206 | ILE  |
| 1   | F     | 210 | ARG  |
| 1   | F     | 211 | LYS  |
| 1   | F     | 212 | GLN  |
| 1   | F     | 217 | LYS  |
| 1   | F     | 246 | PRO  |
| 1   | F     | 249 | THR  |
| 1   | F     | 256 | ARG  |
| 1   | F     | 288 | LYS  |
| 1   | F     | 313 | ARG  |
| 1   | F     | 314 | GLU  |
| 1   | F     | 315 | LYS  |
| 1   | F     | 322 | ARG  |
| 1   | F     | 324 | ILE  |
| 1   | F     | 335 | LEU  |
| 1   | F     | 338 | ARG  |
| 1   | F     | 351 | ASN  |
| 1   | F     | 375 | THR  |
| 1   | F     | 378 | LEU  |
| 1   | F     | 435 | GLU  |
| 1   | G     | 28  | VAL  |
| 1   | G     | 33  | ASN  |
| 1   | G     | 56  | THR  |
| 1   | G     | 78  | SER  |
| 1   | G     | 96  | LEU  |
| 1   | G     | 109 | LYS  |
| 1   | G     | 147 | ARG  |
| 1   | G     | 184 | CYS  |
| 1   | G     | 193 | ASP  |
| 1   | G     | 201 | VAL  |
| 1   | G     | 206 | ILE  |
| 1   | G     | 210 | ARG  |
| 1   | G     | 211 | LYS  |
| 1   | G     | 212 | GLN  |
| 1   | G     | 217 | LYS  |
| 1   | G     | 249 | THR  |
| 1   | G     | 256 | ARG  |
| 1   | G     | 288 | LYS  |
| 1   | G     | 313 | ARG  |
| 1   | G     | 314 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 315 | LYS  |
| 1   | G     | 322 | ARG  |
| 1   | G     | 324 | ILE  |
| 1   | G     | 327 | GLN  |
| 1   | G     | 335 | LEU  |
| 1   | G     | 338 | ARG  |
| 1   | G     | 351 | ASN  |
| 1   | G     | 375 | THR  |
| 1   | G     | 378 | LEU  |
| 1   | G     | 435 | GLU  |
| 1   | H     | 28  | VAL  |
| 1   | H     | 33  | ASN  |
| 1   | H     | 56  | THR  |
| 1   | H     | 96  | LEU  |
| 1   | H     | 105 | CYS  |
| 1   | H     | 107 | ASP  |
| 1   | H     | 109 | LYS  |
| 1   | H     | 147 | ARG  |
| 1   | H     | 184 | CYS  |
| 1   | H     | 193 | ASP  |
| 1   | H     | 199 | ASN  |
| 1   | H     | 206 | ILE  |
| 1   | H     | 210 | ARG  |
| 1   | H     | 211 | LYS  |
| 1   | H     | 212 | GLN  |
| 1   | H     | 217 | LYS  |
| 1   | H     | 249 | THR  |
| 1   | H     | 256 | ARG  |
| 1   | H     | 288 | LYS  |
| 1   | H     | 313 | ARG  |
| 1   | H     | 314 | GLU  |
| 1   | H     | 315 | LYS  |
| 1   | H     | 322 | ARG  |
| 1   | H     | 324 | ILE  |
| 1   | H     | 327 | GLN  |
| 1   | H     | 335 | LEU  |
| 1   | H     | 338 | ARG  |
| 1   | H     | 351 | ASN  |
| 1   | H     | 375 | THR  |
| 1   | H     | 378 | LEU  |
| 1   | H     | 435 | GLU  |
| 1   | I     | 20  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 22  | ARG  |
| 1   | I     | 28  | VAL  |
| 1   | I     | 33  | ASN  |
| 1   | I     | 56  | THR  |
| 1   | I     | 78  | SER  |
| 1   | I     | 96  | LEU  |
| 1   | I     | 109 | LYS  |
| 1   | I     | 147 | ARG  |
| 1   | I     | 184 | CYS  |
| 1   | I     | 193 | ASP  |
| 1   | I     | 200 | GLU  |
| 1   | I     | 206 | ILE  |
| 1   | I     | 210 | ARG  |
| 1   | I     | 211 | LYS  |
| 1   | I     | 212 | GLN  |
| 1   | I     | 217 | LYS  |
| 1   | I     | 249 | THR  |
| 1   | I     | 256 | ARG  |
| 1   | I     | 288 | LYS  |
| 1   | I     | 313 | ARG  |
| 1   | I     | 314 | GLU  |
| 1   | I     | 315 | LYS  |
| 1   | I     | 322 | ARG  |
| 1   | I     | 324 | ILE  |
| 1   | I     | 327 | GLN  |
| 1   | I     | 335 | LEU  |
| 1   | I     | 338 | ARG  |
| 1   | I     | 351 | ASN  |
| 1   | I     | 375 | THR  |
| 1   | I     | 378 | LEU  |
| 1   | I     | 435 | GLU  |
| 1   | J     | 18  | LYS  |
| 1   | J     | 20  | LYS  |
| 1   | J     | 21  | ASN  |
| 1   | J     | 28  | VAL  |
| 1   | J     | 33  | ASN  |
| 1   | J     | 56  | THR  |
| 1   | J     | 78  | SER  |
| 1   | J     | 96  | LEU  |
| 1   | J     | 109 | LYS  |
| 1   | J     | 127 | THR  |
| 1   | J     | 147 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 184 | CYS  |
| 1   | J     | 193 | ASP  |
| 1   | J     | 196 | GLU  |
| 1   | J     | 206 | ILE  |
| 1   | J     | 210 | ARG  |
| 1   | J     | 211 | LYS  |
| 1   | J     | 212 | GLN  |
| 1   | J     | 217 | LYS  |
| 1   | J     | 249 | THR  |
| 1   | J     | 256 | ARG  |
| 1   | J     | 288 | LYS  |
| 1   | J     | 313 | ARG  |
| 1   | J     | 314 | GLU  |
| 1   | J     | 315 | LYS  |
| 1   | J     | 322 | ARG  |
| 1   | J     | 324 | ILE  |
| 1   | J     | 327 | GLN  |
| 1   | J     | 335 | LEU  |
| 1   | J     | 338 | ARG  |
| 1   | J     | 375 | THR  |
| 1   | J     | 378 | LEU  |
| 1   | J     | 435 | GLU  |
| 1   | K     | 28  | VAL  |
| 1   | K     | 33  | ASN  |
| 1   | K     | 56  | THR  |
| 1   | K     | 78  | SER  |
| 1   | K     | 96  | LEU  |
| 1   | K     | 109 | LYS  |
| 1   | K     | 127 | THR  |
| 1   | K     | 147 | ARG  |
| 1   | K     | 184 | CYS  |
| 1   | K     | 193 | ASP  |
| 1   | K     | 206 | ILE  |
| 1   | K     | 210 | ARG  |
| 1   | K     | 211 | LYS  |
| 1   | K     | 212 | GLN  |
| 1   | K     | 217 | LYS  |
| 1   | K     | 241 | ILE  |
| 1   | K     | 242 | LEU  |
| 1   | K     | 243 | LEU  |
| 1   | K     | 249 | THR  |
| 1   | K     | 256 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 266 | PHE  |
| 1   | K     | 278 | LEU  |
| 1   | K     | 281 | GLU  |
| 1   | K     | 286 | LEU  |
| 1   | K     | 290 | PHE  |
| 1   | K     | 291 | GLU  |
| 1   | K     | 294 | GLU  |
| 1   | K     | 300 | ILE  |
| 1   | K     | 307 | ASP  |
| 1   | K     | 309 | ILE  |
| 1   | K     | 323 | ARG  |
| 1   | K     | 325 | VAL  |
| 1   | K     | 326 | SER  |
| 1   | K     | 330 | THR  |
| 1   | K     | 332 | MET  |
| 1   | K     | 335 | LEU  |
| 1   | K     | 340 | HIS  |
| 1   | K     | 348 | ASN  |
| 1   | K     | 349 | ARG  |
| 1   | K     | 351 | ASN  |
| 1   | K     | 353 | ILE  |
| 1   | K     | 363 | PHE  |
| 1   | K     | 366 | GLU  |
| 1   | K     | 375 | THR  |
| 1   | K     | 378 | LEU  |
| 1   | K     | 435 | GLU  |
| 1   | L     | 18  | LYS  |
| 1   | L     | 21  | ASN  |
| 1   | L     | 28  | VAL  |
| 1   | L     | 33  | ASN  |
| 1   | L     | 56  | THR  |
| 1   | L     | 96  | LEU  |
| 1   | L     | 109 | LYS  |
| 1   | L     | 147 | ARG  |
| 1   | L     | 184 | CYS  |
| 1   | L     | 193 | ASP  |
| 1   | L     | 198 | LEU  |
| 1   | L     | 206 | ILE  |
| 1   | L     | 210 | ARG  |
| 1   | L     | 211 | LYS  |
| 1   | L     | 212 | GLN  |
| 1   | L     | 217 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 249 | THR  |
| 1   | L     | 256 | ARG  |
| 1   | L     | 288 | LYS  |
| 1   | L     | 313 | ARG  |
| 1   | L     | 314 | GLU  |
| 1   | L     | 315 | LYS  |
| 1   | L     | 322 | ARG  |
| 1   | L     | 324 | ILE  |
| 1   | L     | 335 | LEU  |
| 1   | L     | 338 | ARG  |
| 1   | L     | 351 | ASN  |
| 1   | L     | 375 | THR  |
| 1   | L     | 378 | LEU  |
| 1   | L     | 435 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | ASN  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 212 | GLN  |
| 1   | A     | 327 | GLN  |
| 1   | A     | 348 | ASN  |
| 1   | B     | 33  | ASN  |
| 1   | B     | 115 | HIS  |
| 1   | B     | 199 | ASN  |
| 1   | B     | 212 | GLN  |
| 1   | B     | 327 | GLN  |
| 1   | B     | 348 | ASN  |
| 1   | C     | 33  | ASN  |
| 1   | C     | 199 | ASN  |
| 1   | C     | 212 | GLN  |
| 1   | C     | 348 | ASN  |
| 1   | D     | 33  | ASN  |
| 1   | D     | 115 | HIS  |
| 1   | D     | 327 | GLN  |
| 1   | D     | 348 | ASN  |
| 1   | E     | 33  | ASN  |
| 1   | E     | 212 | GLN  |
| 1   | E     | 327 | GLN  |
| 1   | E     | 348 | ASN  |
| 1   | F     | 33  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 115 | HIS  |
| 1   | F     | 183 | HIS  |
| 1   | F     | 212 | GLN  |
| 1   | F     | 348 | ASN  |
| 1   | G     | 212 | GLN  |
| 1   | G     | 327 | GLN  |
| 1   | G     | 348 | ASN  |
| 1   | H     | 33  | ASN  |
| 1   | H     | 212 | GLN  |
| 1   | H     | 327 | GLN  |
| 1   | H     | 348 | ASN  |
| 1   | I     | 33  | ASN  |
| 1   | I     | 327 | GLN  |
| 1   | I     | 348 | ASN  |
| 1   | J     | 33  | ASN  |
| 1   | J     | 212 | GLN  |
| 1   | J     | 317 | HIS  |
| 1   | J     | 327 | GLN  |
| 1   | J     | 348 | ASN  |
| 1   | K     | 33  | ASN  |
| 1   | K     | 348 | ASN  |
| 1   | K     | 351 | ASN  |
| 1   | L     | 33  | ASN  |
| 1   | L     | 50  | GLN  |
| 1   | L     | 212 | GLN  |
| 1   | L     | 327 | GLN  |
| 1   | L     | 348 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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 |
| 2   | ADP  | L     | 800 | -    | 24,29,29     | 0.91 | 1 (4%)   | 29,45,45    | 1.46 | 4 (13%)  |
| 2   | ADP  | B     | 800 | -    | 24,29,29     | 0.99 | 1 (4%)   | 29,45,45    | 1.49 | 4 (13%)  |
| 2   | ADP  | C     | 800 | -    | 24,29,29     | 0.93 | 1 (4%)   | 29,45,45    | 1.43 | 4 (13%)  |
| 2   | ADP  | A     | 800 | -    | 24,29,29     | 0.89 | 1 (4%)   | 29,45,45    | 1.50 | 4 (13%)  |
| 2   | ADP  | G     | 800 | -    | 24,29,29     | 0.97 | 1 (4%)   | 29,45,45    | 1.41 | 4 (13%)  |
| 2   | ADP  | J     | 800 | -    | 24,29,29     | 1.15 | 2 (8%)   | 29,45,45    | 1.46 | 3 (10%)  |
| 2   | ADP  | E     | 800 | -    | 24,29,29     | 0.95 | 1 (4%)   | 29,45,45    | 1.44 | 3 (10%)  |
| 2   | ADP  | K     | 800 | -    | 24,29,29     | 0.83 | 1 (4%)   | 29,45,45    | 1.55 | 4 (13%)  |
| 2   | ADP  | I     | 800 | -    | 24,29,29     | 0.94 | 1 (4%)   | 29,45,45    | 1.50 | 4 (13%)  |
| 2   | ADP  | F     | 800 | -    | 24,29,29     | 0.97 | 1 (4%)   | 29,45,45    | 1.52 | 4 (13%)  |
| 2   | ADP  | D     | 800 | -    | 24,29,29     | 1.02 | 2 (8%)   | 29,45,45    | 1.53 | 5 (17%)  |
| 2   | ADP  | H     | 800 | -    | 24,29,29     | 0.87 | 0        | 29,45,45    | 1.46 | 3 (10%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ADP  | L     | 800 | -    | -       | 3/12/32/32 | 0/3/3/3 |
| 2   | ADP  | B     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | C     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | A     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | G     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | J     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | E     | 800 | -    | -       | 3/12/32/32 | 0/3/3/3 |
| 2   | ADP  | K     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ADP  | I     | 800 | -    | -       | 3/12/32/32 | 0/3/3/3 |
| 2   | ADP  | F     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | D     | 800 | -    | -       | 4/12/32/32 | 0/3/3/3 |
| 2   | ADP  | H     | 800 | -    | -       | 2/12/32/32 | 0/3/3/3 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | J     | 800 | ADP  | C2'-C1' | -2.61 | 1.49        | 1.53     |
| 2   | D     | 800 | ADP  | C5-C4   | 2.52  | 1.47        | 1.40     |
| 2   | L     | 800 | ADP  | C5-C4   | 2.49  | 1.47        | 1.40     |
| 2   | G     | 800 | ADP  | C5-C4   | 2.40  | 1.47        | 1.40     |
| 2   | J     | 800 | ADP  | C5-C4   | 2.36  | 1.47        | 1.40     |
| 2   | C     | 800 | ADP  | C5-C4   | 2.30  | 1.47        | 1.40     |
| 2   | F     | 800 | ADP  | C5-C4   | 2.28  | 1.47        | 1.40     |
| 2   | E     | 800 | ADP  | C5-C4   | 2.26  | 1.46        | 1.40     |
| 2   | B     | 800 | ADP  | C5-C4   | 2.13  | 1.46        | 1.40     |
| 2   | D     | 800 | ADP  | C2'-C1' | -2.06 | 1.50        | 1.53     |
| 2   | K     | 800 | ADP  | C5-C4   | 2.04  | 1.46        | 1.40     |
| 2   | I     | 800 | ADP  | C5-C4   | 2.03  | 1.46        | 1.40     |
| 2   | A     | 800 | ADP  | C5-C4   | 2.02  | 1.46        | 1.40     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 800 | ADP  | C3'-C2'-C1' | 3.94  | 106.91      | 100.98   |
| 2   | E     | 800 | ADP  | PA-O3A-PB   | -3.84 | 119.66      | 132.83   |
| 2   | D     | 800 | ADP  | PA-O3A-PB   | -3.82 | 119.72      | 132.83   |
| 2   | J     | 800 | ADP  | PA-O3A-PB   | -3.80 | 119.80      | 132.83   |
| 2   | H     | 800 | ADP  | N3-C2-N1    | -3.79 | 122.76      | 128.68   |
| 2   | F     | 800 | ADP  | PA-O3A-PB   | -3.76 | 119.93      | 132.83   |
| 2   | A     | 800 | ADP  | N3-C2-N1    | -3.69 | 122.91      | 128.68   |
| 2   | I     | 800 | ADP  | N3-C2-N1    | -3.67 | 122.94      | 128.68   |
| 2   | A     | 800 | ADP  | PA-O3A-PB   | -3.62 | 120.42      | 132.83   |
| 2   | B     | 800 | ADP  | PA-O3A-PB   | -3.59 | 120.52      | 132.83   |
| 2   | J     | 800 | ADP  | C3'-C2'-C1' | 3.53  | 106.29      | 100.98   |
| 2   | B     | 800 | ADP  | N3-C2-N1    | -3.47 | 123.26      | 128.68   |
| 2   | L     | 800 | ADP  | N3-C2-N1    | -3.46 | 123.26      | 128.68   |
| 2   | D     | 800 | ADP  | C3'-C2'-C1' | 3.42  | 106.12      | 100.98   |
| 2   | L     | 800 | ADP  | C3'-C2'-C1' | 3.42  | 106.12      | 100.98   |
| 2   | I     | 800 | ADP  | PA-O3A-PB   | -3.37 | 121.27      | 132.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 800 | ADP  | PA-O3A-PB   | -3.34 | 121.37      | 132.83   |
| 2   | D     | 800 | ADP  | N3-C2-N1    | -3.34 | 123.46      | 128.68   |
| 2   | G     | 800 | ADP  | N3-C2-N1    | -3.31 | 123.51      | 128.68   |
| 2   | K     | 800 | ADP  | PA-O3A-PB   | -3.30 | 121.50      | 132.83   |
| 2   | H     | 800 | ADP  | C3'-C2'-C1' | 3.27  | 105.90      | 100.98   |
| 2   | I     | 800 | ADP  | C3'-C2'-C1' | 3.27  | 105.90      | 100.98   |
| 2   | E     | 800 | ADP  | C3'-C2'-C1' | 3.23  | 105.84      | 100.98   |
| 2   | E     | 800 | ADP  | N3-C2-N1    | -3.21 | 123.66      | 128.68   |
| 2   | C     | 800 | ADP  | C3'-C2'-C1' | 3.19  | 105.79      | 100.98   |
| 2   | C     | 800 | ADP  | N3-C2-N1    | -3.19 | 123.70      | 128.68   |
| 2   | J     | 800 | ADP  | N3-C2-N1    | -3.19 | 123.70      | 128.68   |
| 2   | G     | 800 | ADP  | PA-O3A-PB   | -3.17 | 121.96      | 132.83   |
| 2   | C     | 800 | ADP  | PA-O3A-PB   | -3.14 | 122.06      | 132.83   |
| 2   | L     | 800 | ADP  | PA-O3A-PB   | -3.12 | 122.11      | 132.83   |
| 2   | B     | 800 | ADP  | C3'-C2'-C1' | 3.11  | 105.66      | 100.98   |
| 2   | K     | 800 | ADP  | N3-C2-N1    | -3.10 | 123.84      | 128.68   |
| 2   | F     | 800 | ADP  | N3-C2-N1    | -3.09 | 123.85      | 128.68   |
| 2   | K     | 800 | ADP  | C4-C5-N7    | -3.07 | 106.20      | 109.40   |
| 2   | G     | 800 | ADP  | C3'-C2'-C1' | 3.05  | 105.58      | 100.98   |
| 2   | K     | 800 | ADP  | C3'-C2'-C1' | 3.04  | 105.56      | 100.98   |
| 2   | A     | 800 | ADP  | C3'-C2'-C1' | 3.02  | 105.52      | 100.98   |
| 2   | G     | 800 | ADP  | C4-C5-N7    | -2.58 | 106.71      | 109.40   |
| 2   | C     | 800 | ADP  | C4-C5-N7    | -2.50 | 106.80      | 109.40   |
| 2   | I     | 800 | ADP  | C4-C5-N7    | -2.43 | 106.87      | 109.40   |
| 2   | B     | 800 | ADP  | C4-C5-N7    | -2.34 | 106.96      | 109.40   |
| 2   | D     | 800 | ADP  | C2-N1-C6    | 2.34  | 122.75      | 118.75   |
| 2   | D     | 800 | ADP  | C4-C5-N7    | -2.32 | 106.98      | 109.40   |
| 2   | F     | 800 | ADP  | C4-C5-N7    | -2.29 | 107.01      | 109.40   |
| 2   | L     | 800 | ADP  | C2-N1-C6    | 2.13  | 122.40      | 118.75   |
| 2   | A     | 800 | ADP  | C4-C5-N7    | -2.09 | 107.22      | 109.40   |

There are no chirality outliers.

All (43) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | J     | 800 | ADP  | C5'-O5'-PA-O1A |
| 2   | F     | 800 | ADP  | C5'-O5'-PA-O1A |
| 2   | J     | 800 | ADP  | C5'-O5'-PA-O3A |
| 2   | F     | 800 | ADP  | C5'-O5'-PA-O3A |
| 2   | D     | 800 | ADP  | C5'-O5'-PA-O3A |
| 2   | L     | 800 | ADP  | C5'-O5'-PA-O1A |
| 2   | B     | 800 | ADP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 800 | ADP  | C5'-O5'-PA-O3A  |
| 2   | A     | 800 | ADP  | C5'-O5'-PA-O3A  |
| 2   | G     | 800 | ADP  | C5'-O5'-PA-O3A  |
| 2   | K     | 800 | ADP  | C5'-O5'-PA-O3A  |
| 2   | L     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | B     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | C     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | A     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | G     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | J     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | E     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | K     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | I     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | F     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | D     | 800 | ADP  | PB-O3A-PA-O1A   |
| 2   | B     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | C     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | A     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | G     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | E     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | K     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | I     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | D     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | H     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 2   | L     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | B     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | C     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | A     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | G     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | J     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | E     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | K     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | I     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | F     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | D     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | H     | 800 | ADP  | O4'-C4'-C5'-O5' |

There are no ring outliers.

12 monomers are involved in 31 short contacts:

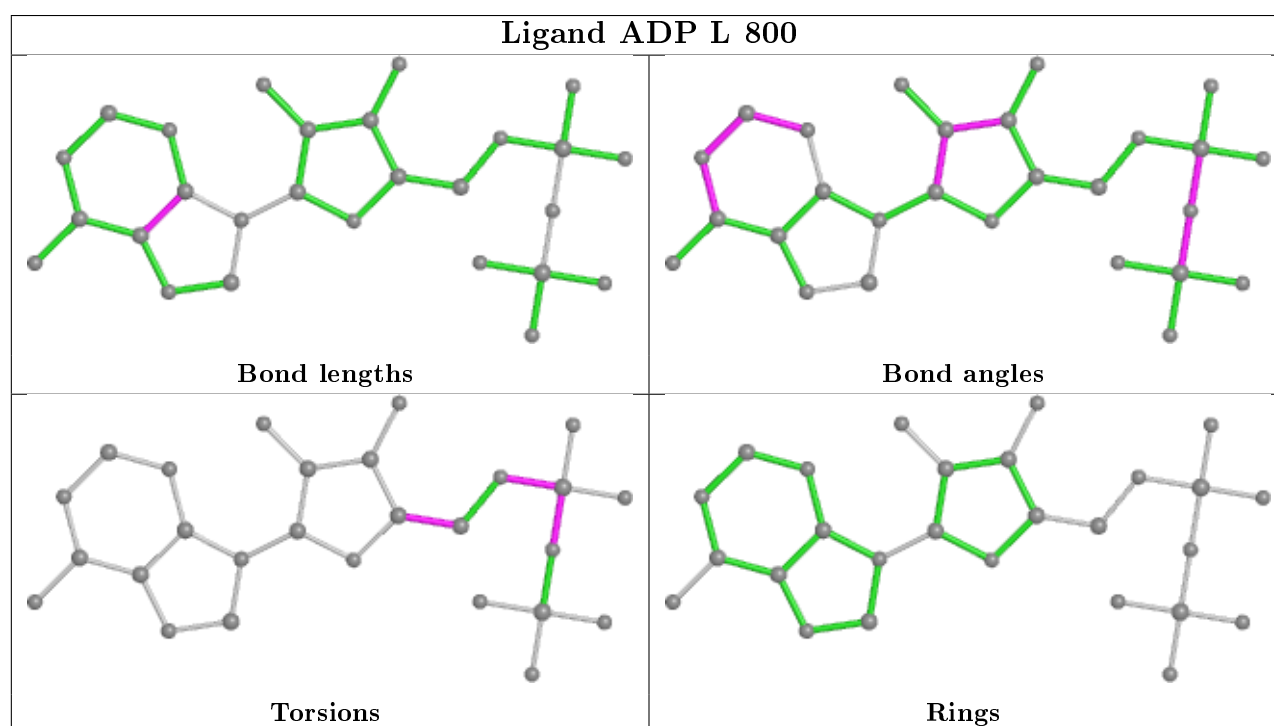
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | L     | 800 | ADP  | 4       | 0            |

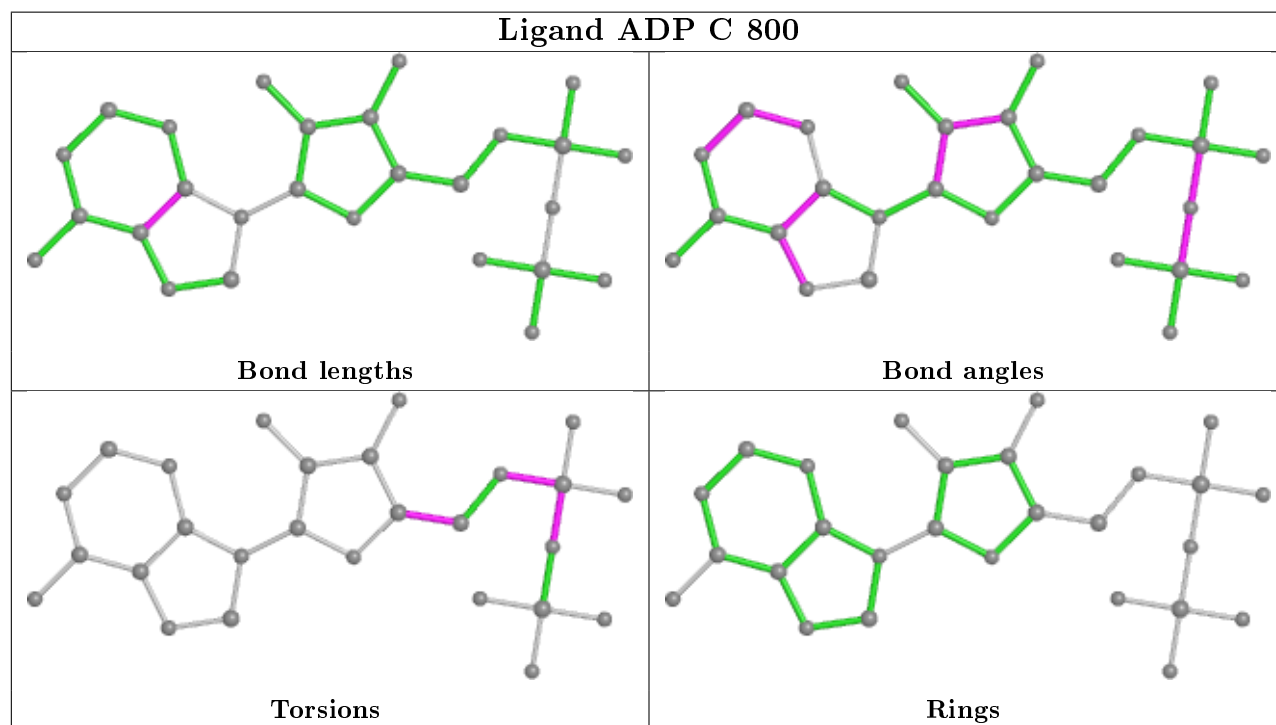
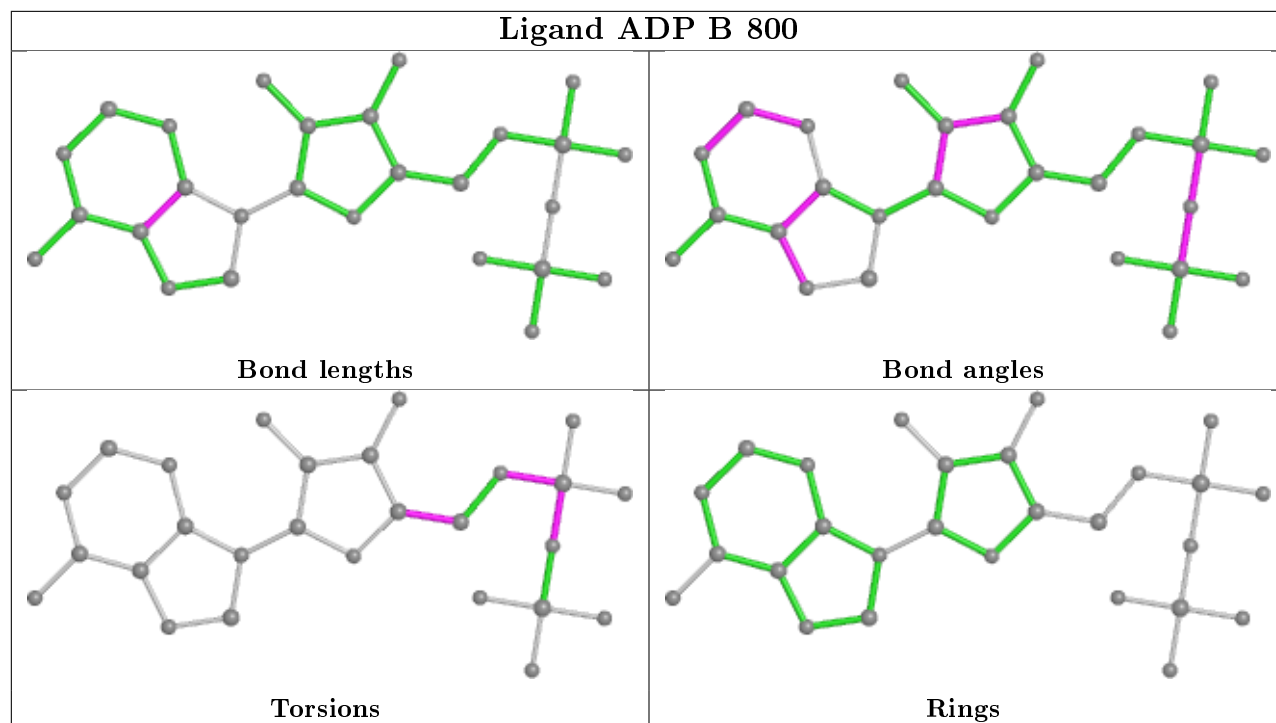
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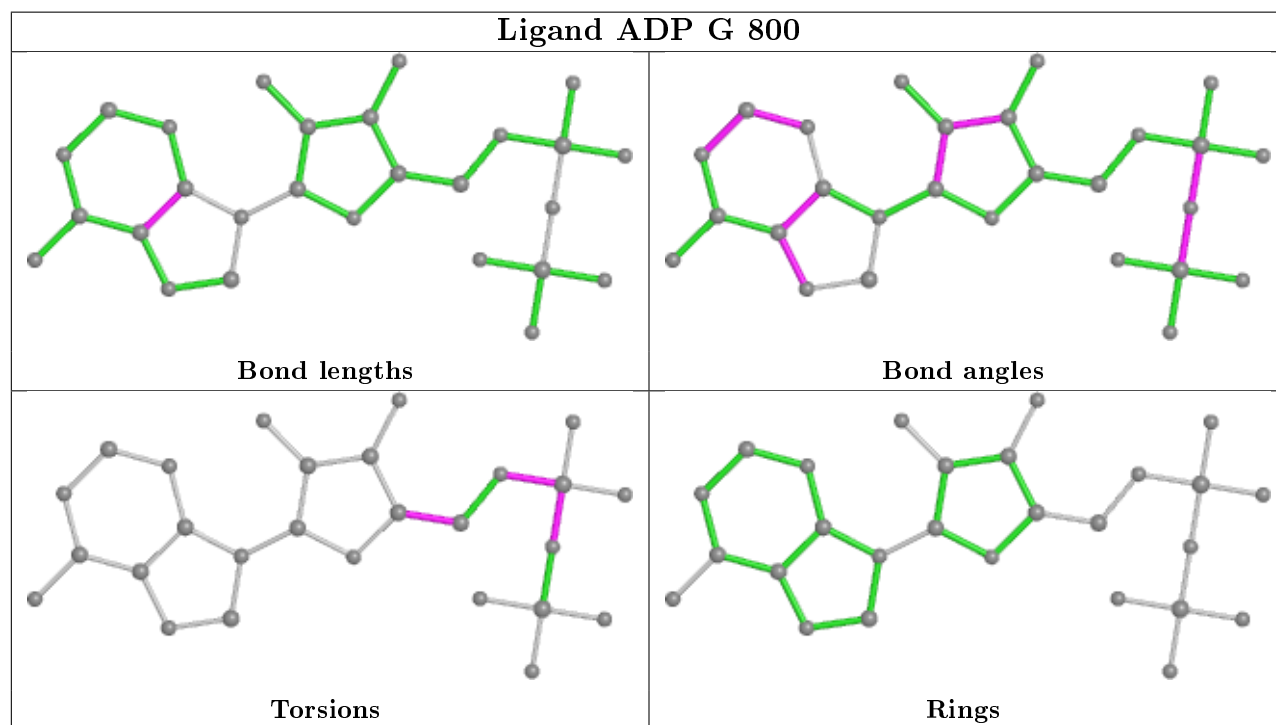
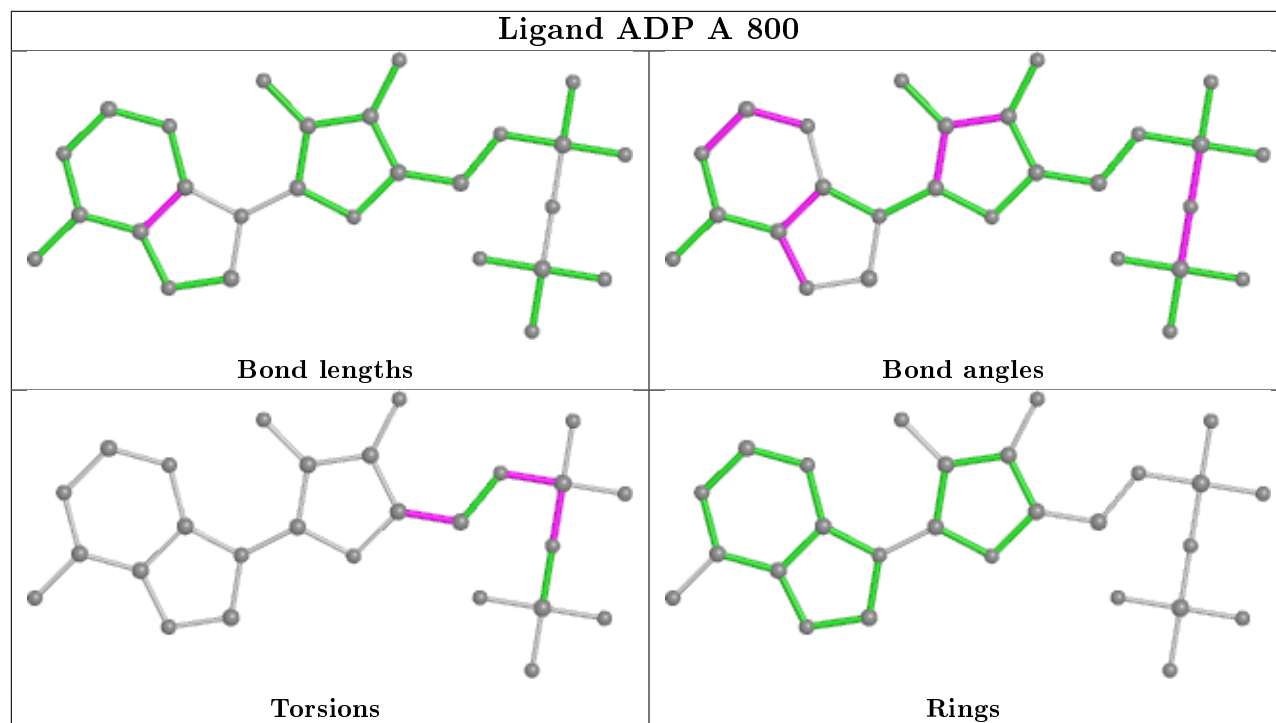
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 800 | ADP  | 2       | 0            |
| 2   | C     | 800 | ADP  | 4       | 0            |
| 2   | A     | 800 | ADP  | 2       | 0            |
| 2   | G     | 800 | ADP  | 2       | 0            |
| 2   | J     | 800 | ADP  | 2       | 0            |
| 2   | E     | 800 | ADP  | 2       | 0            |
| 2   | K     | 800 | ADP  | 3       | 0            |
| 2   | I     | 800 | ADP  | 2       | 0            |
| 2   | F     | 800 | ADP  | 3       | 0            |
| 2   | D     | 800 | ADP  | 2       | 0            |
| 2   | H     | 800 | ADP  | 3       | 0            |

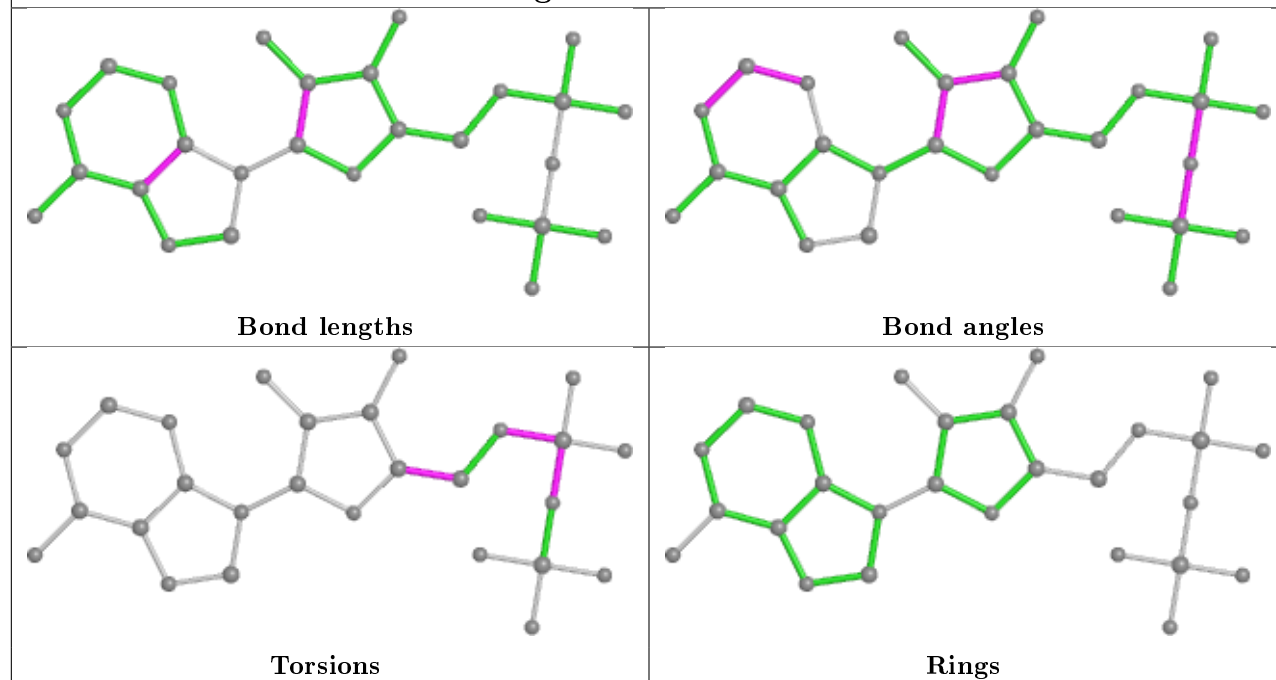
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



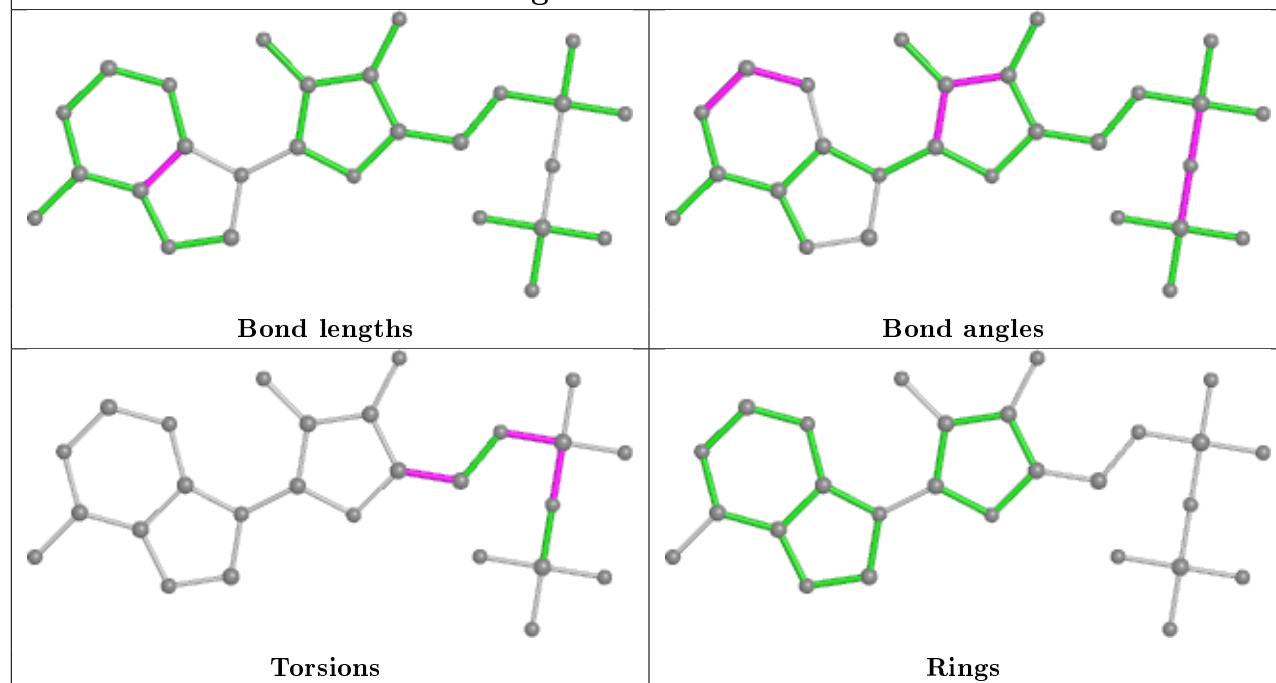




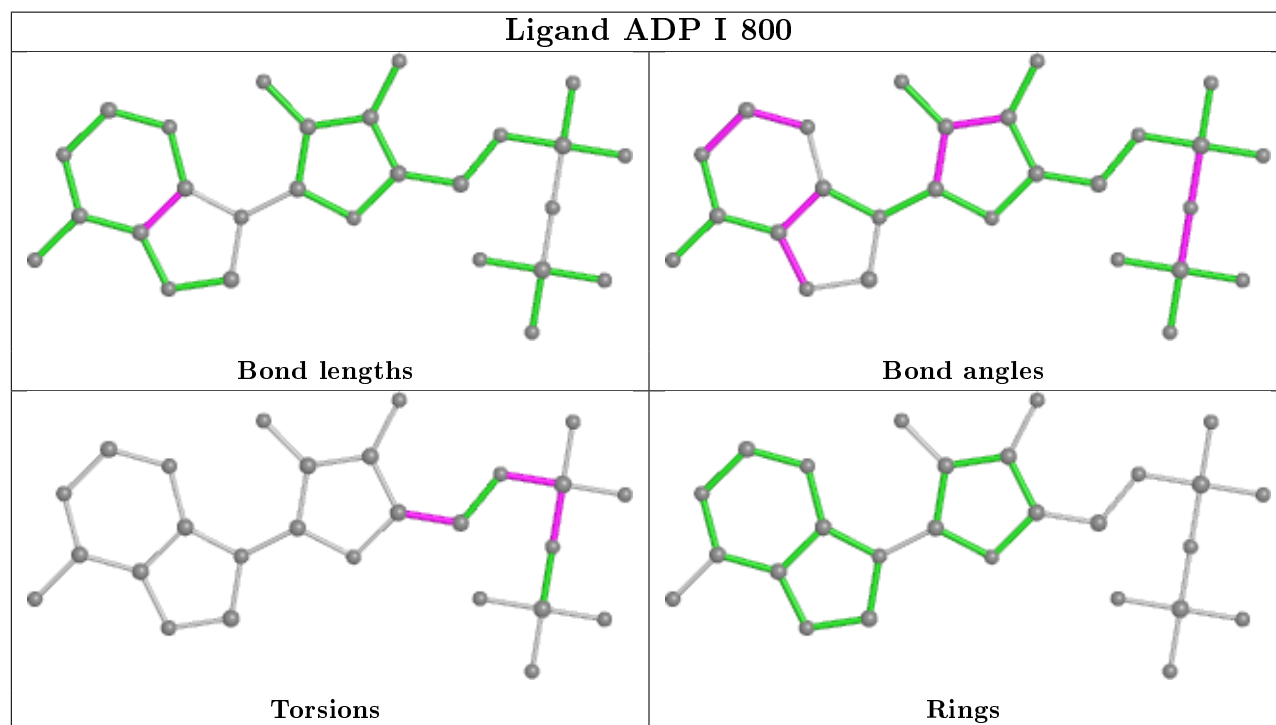
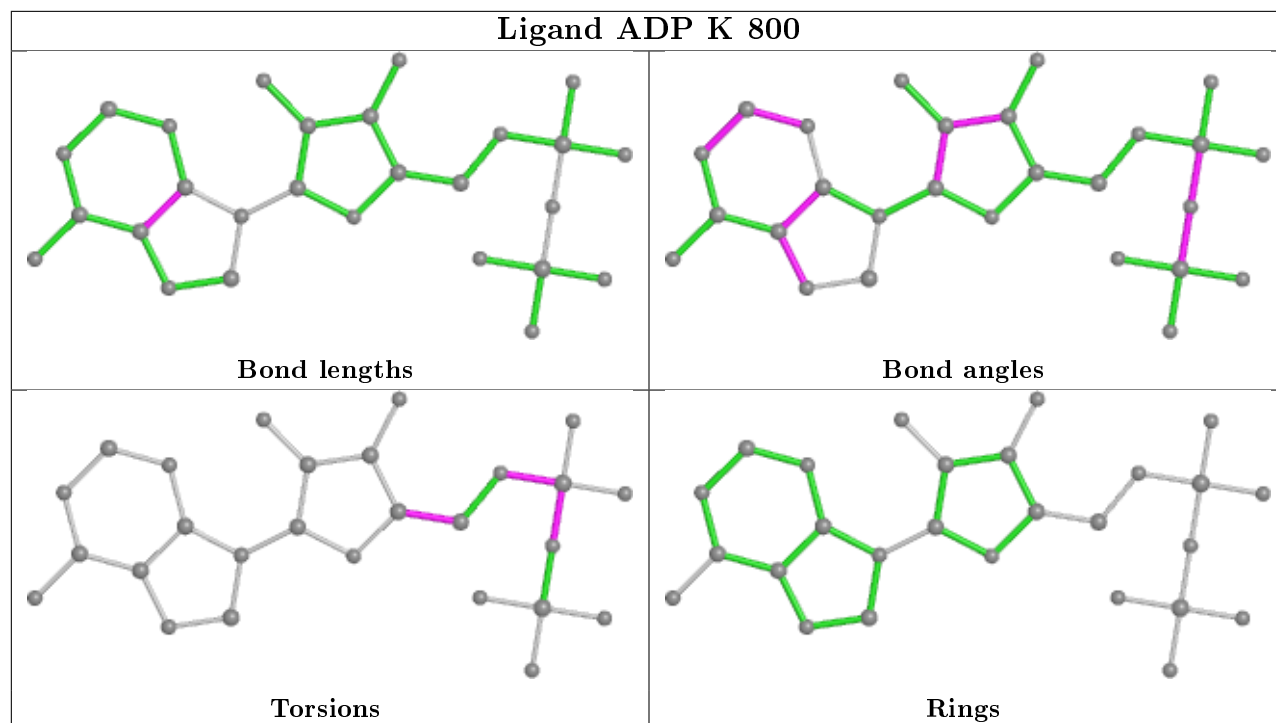
## Ligand ADP J 800

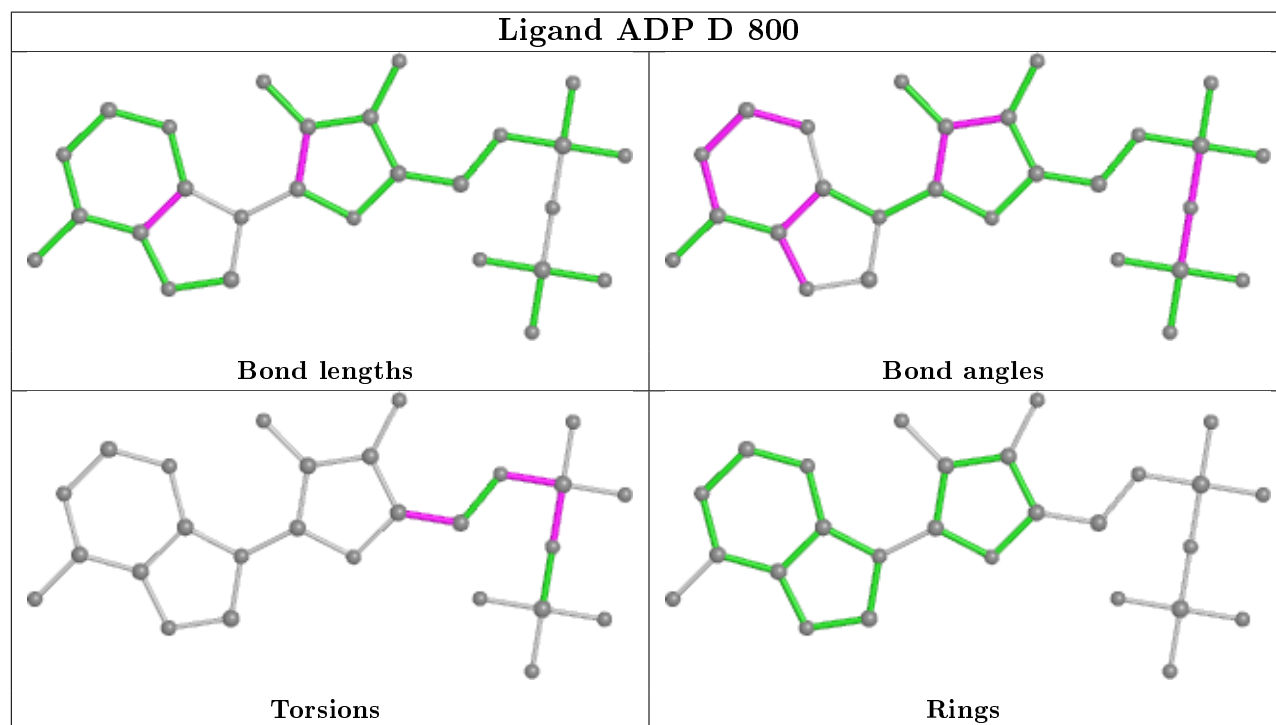
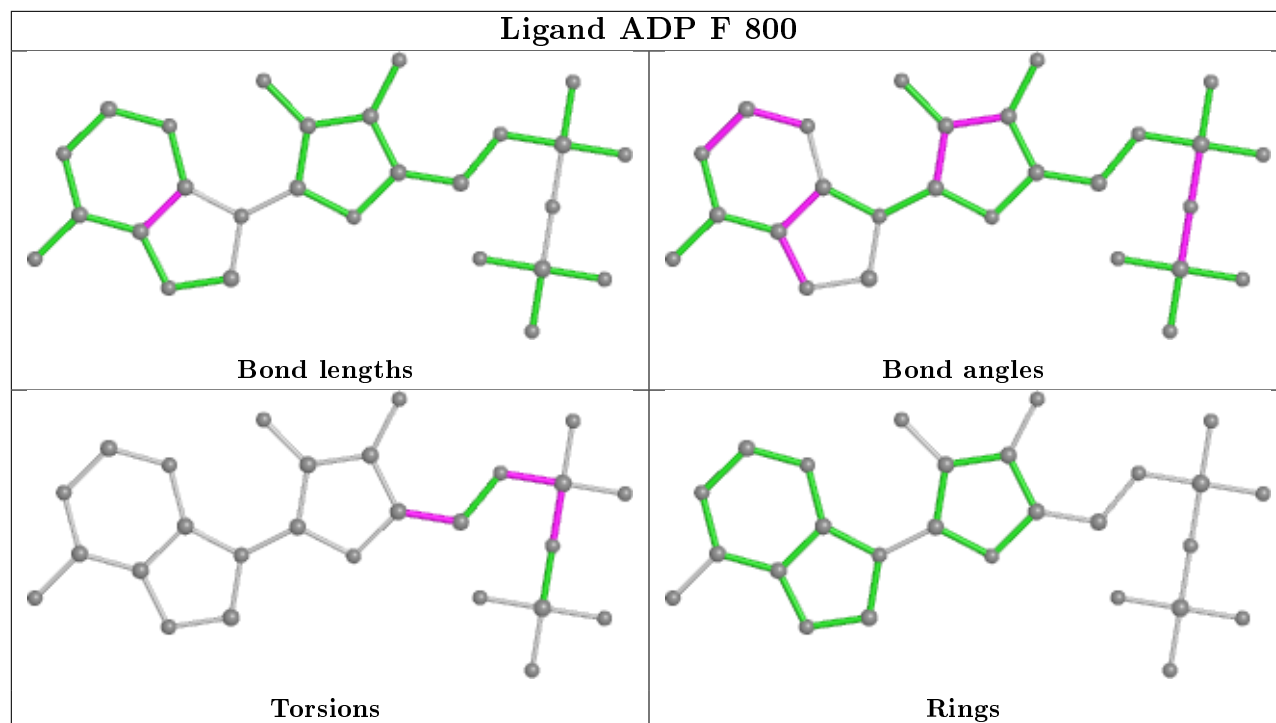


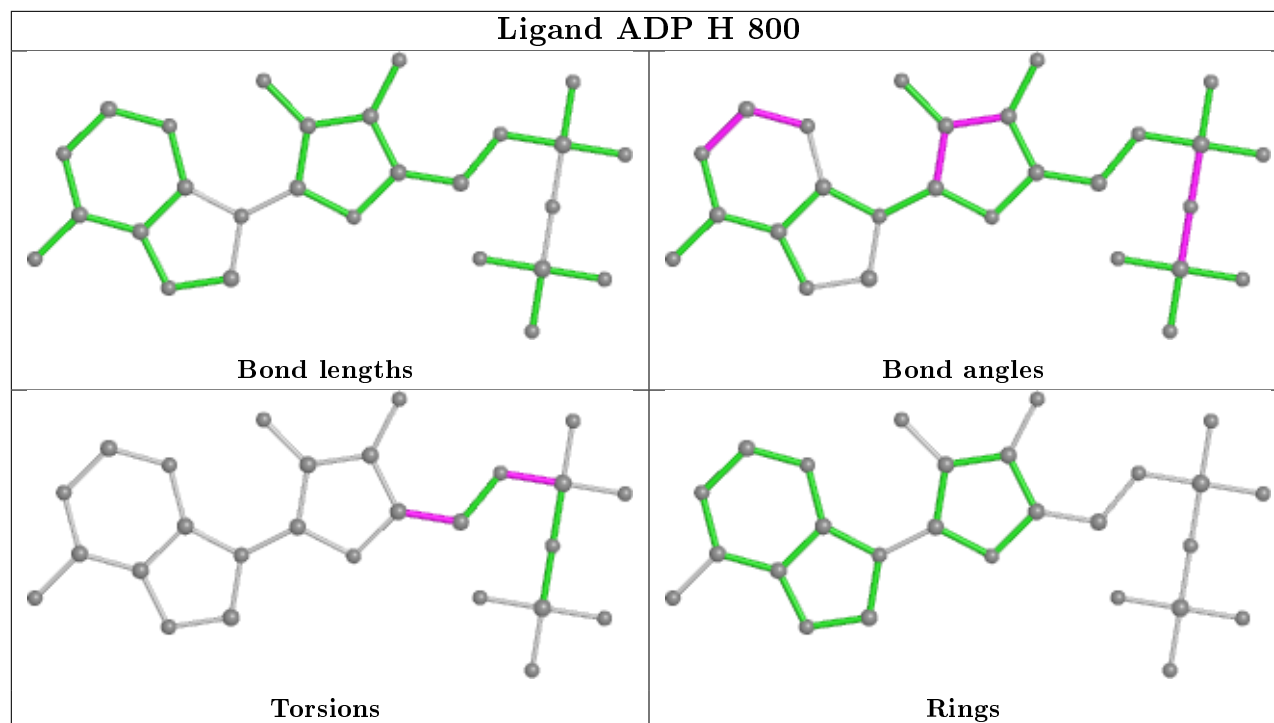
## Ligand ADP E 800











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 438/489 (89%)   | 0.29   | 34 (7%) 13 7  | 71, 120, 172, 275     | 0     |
| 1   | B     | 439/489 (89%)   | -0.03  | 20 (4%) 32 20 | 57, 92, 153, 208      | 0     |
| 1   | C     | 438/489 (89%)   | 0.19   | 31 (7%) 16 9  | 76, 120, 177, 233     | 0     |
| 1   | D     | 439/489 (89%)   | 0.24   | 35 (7%) 12 7  | 60, 115, 176, 280     | 0     |
| 1   | E     | 439/489 (89%)   | 0.52   | 57 (12%) 3 2  | 66, 132, 211, 261     | 0     |
| 1   | F     | 438/489 (89%)   | -0.01  | 17 (3%) 39 25 | 60, 95, 169, 215      | 0     |
| 1   | G     | 437/489 (89%)   | 0.24   | 31 (7%) 16 9  | 60, 111, 169, 221     | 0     |
| 1   | H     | 438/489 (89%)   | 0.06   | 20 (4%) 32 20 | 60, 105, 163, 233     | 0     |
| 1   | I     | 440/489 (89%)   | 0.24   | 32 (7%) 15 8  | 61, 122, 182, 285     | 0     |
| 1   | J     | 445/489 (91%)   | -0.01  | 16 (3%) 42 28 | 50, 93, 153, 238      | 0     |
| 1   | K     | 438/489 (89%)   | 0.82   | 87 (19%) 1 0  | 64, 142, 208, 239     | 0     |
| 1   | L     | 442/489 (90%)   | 0.40   | 46 (10%) 6 4  | 76, 139, 204, 287     | 0     |
| All | All   | 5271/5868 (89%) | 0.25   | 426 (8%) 12 6 | 50, 115, 188, 287     | 0     |

All (426) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 279 | ALA  | 9.2  |
| 1   | I     | 432 | LEU  | 8.3  |
| 1   | D     | 433 | GLU  | 7.7  |
| 1   | E     | 279 | ALA  | 7.7  |
| 1   | E     | 432 | LEU  | 7.3  |
| 1   | K     | 432 | LEU  | 7.2  |
| 1   | I     | 436 | THR  | 7.1  |
| 1   | E     | 113 | ARG  | 7.1  |
| 1   | K     | 284 | SER  | 6.8  |
| 1   | K     | 460 | ASN  | 6.3  |
| 1   | E     | 435 | GLU  | 6.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 109 | LYS  | 5.9  |
| 1   | K     | 279 | ALA  | 5.8  |
| 1   | G     | 434 | ASP  | 5.7  |
| 1   | I     | 437 | ILE  | 5.6  |
| 1   | H     | 435 | GLU  | 5.6  |
| 1   | K     | 194 | GLU  | 5.6  |
| 1   | F     | 317 | HIS  | 5.5  |
| 1   | E     | 166 | VAL  | 5.5  |
| 1   | L     | 187 | GLU  | 5.4  |
| 1   | L     | 432 | LEU  | 5.4  |
| 1   | A     | 435 | GLU  | 5.2  |
| 1   | K     | 278 | LEU  | 5.2  |
| 1   | J     | 436 | THR  | 5.2  |
| 1   | B     | 338 | ARG  | 5.1  |
| 1   | K     | 338 | ARG  | 5.0  |
| 1   | C     | 435 | GLU  | 5.0  |
| 1   | C     | 317 | HIS  | 5.0  |
| 1   | I     | 431 | ASP  | 5.0  |
| 1   | E     | 433 | GLU  | 4.9  |
| 1   | I     | 433 | GLU  | 4.9  |
| 1   | L     | 64  | ARG  | 4.9  |
| 1   | K     | 339 | ALA  | 4.9  |
| 1   | A     | 433 | GLU  | 4.8  |
| 1   | K     | 64  | ARG  | 4.8  |
| 1   | D     | 279 | ALA  | 4.8  |
| 1   | D     | 360 | PHE  | 4.7  |
| 1   | E     | 112 | LYS  | 4.7  |
| 1   | K     | 434 | ASP  | 4.7  |
| 1   | G     | 64  | ARG  | 4.7  |
| 1   | E     | 194 | GLU  | 4.7  |
| 1   | D     | 432 | LEU  | 4.7  |
| 1   | E     | 461 | PRO  | 4.7  |
| 1   | L     | 172 | PRO  | 4.7  |
| 1   | H     | 75  | ASP  | 4.7  |
| 1   | C     | 193 | ASP  | 4.6  |
| 1   | G     | 435 | GLU  | 4.6  |
| 1   | G     | 143 | TYR  | 4.6  |
| 1   | L     | 173 | TYR  | 4.6  |
| 1   | K     | 349 | ARG  | 4.5  |
| 1   | F     | 319 | GLU  | 4.5  |
| 1   | K     | 317 | HIS  | 4.5  |
| 1   | K     | 352 | SER  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 337 | GLN  | 4.5  |
| 1   | G     | 337 | GLN  | 4.4  |
| 1   | K     | 280 | GLY  | 4.4  |
| 1   | E     | 109 | LYS  | 4.4  |
| 1   | K     | 436 | THR  | 4.4  |
| 1   | K     | 340 | HIS  | 4.4  |
| 1   | I     | 279 | ALA  | 4.3  |
| 1   | K     | 277 | LYS  | 4.3  |
| 1   | L     | 53  | ARG  | 4.3  |
| 1   | B     | 53  | ARG  | 4.3  |
| 1   | G     | 338 | ARG  | 4.3  |
| 1   | K     | 173 | TYR  | 4.3  |
| 1   | I     | 428 | ASP  | 4.2  |
| 1   | J     | 434 | ASP  | 4.2  |
| 1   | L     | 63  | LYS  | 4.2  |
| 1   | D     | 434 | ASP  | 4.2  |
| 1   | J     | 433 | GLU  | 4.2  |
| 1   | B     | 337 | GLN  | 4.2  |
| 1   | K     | 350 | PRO  | 4.2  |
| 1   | F     | 337 | GLN  | 4.2  |
| 1   | L     | 21  | ASN  | 4.1  |
| 1   | J     | 239 | ARG  | 4.1  |
| 1   | K     | 112 | LYS  | 4.1  |
| 1   | L     | 244 | TYR  | 4.1  |
| 1   | J     | 461 | PRO  | 4.0  |
| 1   | A     | 345 | ALA  | 4.0  |
| 1   | A     | 338 | ARG  | 4.0  |
| 1   | E     | 108 | VAL  | 4.0  |
| 1   | K     | 286 | LEU  | 4.0  |
| 1   | L     | 101 | SER  | 3.9  |
| 1   | L     | 429 | LEU  | 3.9  |
| 1   | A     | 113 | ARG  | 3.9  |
| 1   | K     | 193 | ASP  | 3.9  |
| 1   | E     | 317 | HIS  | 3.9  |
| 1   | D     | 50  | GLN  | 3.9  |
| 1   | E     | 193 | ASP  | 3.9  |
| 1   | I     | 109 | LYS  | 3.9  |
| 1   | H     | 459 | SER  | 3.8  |
| 1   | G     | 63  | LYS  | 3.8  |
| 1   | K     | 63  | LYS  | 3.8  |
| 1   | E     | 280 | GLY  | 3.8  |
| 1   | A     | 76  | THR  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 108 | VAL  | 3.8  |
| 1   | K     | 140 | LEU  | 3.8  |
| 1   | L     | 181 | VAL  | 3.8  |
| 1   | K     | 128 | GLY  | 3.8  |
| 1   | A     | 75  | ASP  | 3.8  |
| 1   | I     | 349 | ARG  | 3.8  |
| 1   | E     | 75  | ASP  | 3.7  |
| 1   | C     | 141 | GLU  | 3.7  |
| 1   | K     | 141 | GLU  | 3.7  |
| 1   | K     | 163 | PHE  | 3.7  |
| 1   | I     | 34  | GLU  | 3.7  |
| 1   | J     | 317 | HIS  | 3.7  |
| 1   | A     | 344 | MET  | 3.6  |
| 1   | I     | 52  | PHE  | 3.6  |
| 1   | I     | 194 | GLU  | 3.6  |
| 1   | I     | 434 | ASP  | 3.6  |
| 1   | G     | 440 | GLU  | 3.6  |
| 1   | C     | 338 | ARG  | 3.6  |
| 1   | A     | 434 | ASP  | 3.5  |
| 1   | K     | 185 | GLU  | 3.5  |
| 1   | G     | 34  | GLU  | 3.5  |
| 1   | E     | 107 | ASP  | 3.5  |
| 1   | C     | 128 | GLY  | 3.5  |
| 1   | D     | 22  | ARG  | 3.5  |
| 1   | D     | 143 | TYR  | 3.5  |
| 1   | E     | 34  | GLU  | 3.5  |
| 1   | C     | 434 | ASP  | 3.5  |
| 1   | G     | 109 | LYS  | 3.4  |
| 1   | F     | 279 | ALA  | 3.4  |
| 1   | I     | 338 | ARG  | 3.4  |
| 1   | K     | 320 | VAL  | 3.4  |
| 1   | A     | 194 | GLU  | 3.4  |
| 1   | H     | 350 | PRO  | 3.4  |
| 1   | H     | 279 | ALA  | 3.4  |
| 1   | C     | 401 | ASN  | 3.4  |
| 1   | E     | 314 | GLU  | 3.4  |
| 1   | K     | 360 | PHE  | 3.4  |
| 1   | D     | 64  | ARG  | 3.4  |
| 1   | D     | 278 | LEU  | 3.4  |
| 1   | L     | 278 | LEU  | 3.4  |
| 1   | E     | 62  | LYS  | 3.4  |
| 1   | A     | 358 | ARG  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 64  | ARG  | 3.3  |
| 1   | I     | 187 | GLU  | 3.3  |
| 1   | A     | 437 | ILE  | 3.3  |
| 1   | L     | 194 | GLU  | 3.3  |
| 1   | K     | 191 | ARG  | 3.3  |
| 1   | K     | 244 | TYR  | 3.3  |
| 1   | H     | 63  | LYS  | 3.3  |
| 1   | C     | 319 | GLU  | 3.3  |
| 1   | K     | 342 | ILE  | 3.3  |
| 1   | L     | 338 | ARG  | 3.3  |
| 1   | F     | 435 | GLU  | 3.3  |
| 1   | B     | 434 | ASP  | 3.3  |
| 1   | K     | 333 | ASP  | 3.3  |
| 1   | K     | 117 | LEU  | 3.3  |
| 1   | A     | 337 | GLN  | 3.3  |
| 1   | J     | 462 | SER  | 3.3  |
| 1   | L     | 404 | HIS  | 3.3  |
| 1   | E     | 136 | LYS  | 3.3  |
| 1   | I     | 459 | SER  | 3.2  |
| 1   | K     | 267 | PHE  | 3.2  |
| 1   | G     | 155 | HIS  | 3.2  |
| 1   | I     | 318 | GLY  | 3.2  |
| 1   | B     | 109 | LYS  | 3.2  |
| 1   | K     | 62  | LYS  | 3.2  |
| 1   | H     | 337 | GLN  | 3.2  |
| 1   | K     | 190 | LYS  | 3.2  |
| 1   | D     | 317 | HIS  | 3.2  |
| 1   | K     | 179 | ASP  | 3.2  |
| 1   | A     | 234 | GLY  | 3.1  |
| 1   | B     | 435 | GLU  | 3.1  |
| 1   | D     | 140 | LEU  | 3.1  |
| 1   | K     | 345 | ALA  | 3.1  |
| 1   | K     | 355 | PRO  | 3.1  |
| 1   | G     | 52  | PHE  | 3.1  |
| 1   | D     | 128 | GLY  | 3.1  |
| 1   | E     | 189 | ILE  | 3.1  |
| 1   | L     | 193 | ASP  | 3.1  |
| 1   | G     | 186 | GLY  | 3.1  |
| 1   | I     | 32  | ILE  | 3.1  |
| 1   | A     | 343 | VAL  | 3.0  |
| 1   | E     | 103 | GLN  | 3.0  |
| 1   | E     | 190 | LYS  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 172 | PRO  | 3.0  |
| 1   | G     | 232 | ALA  | 3.0  |
| 1   | E     | 110 | TYR  | 3.0  |
| 1   | A     | 34  | GLU  | 3.0  |
| 1   | K     | 268 | LEU  | 3.0  |
| 1   | E     | 63  | LYS  | 3.0  |
| 1   | G     | 187 | GLU  | 3.0  |
| 1   | J     | 63  | LYS  | 3.0  |
| 1   | L     | 435 | GLU  | 3.0  |
| 1   | B     | 72  | LEU  | 2.9  |
| 1   | K     | 298 | PRO  | 2.9  |
| 1   | A     | 294 | GLU  | 2.9  |
| 1   | L     | 185 | GLU  | 2.9  |
| 1   | K     | 313 | ARG  | 2.9  |
| 1   | L     | 317 | HIS  | 2.9  |
| 1   | K     | 76  | THR  | 2.9  |
| 1   | K     | 107 | ASP  | 2.9  |
| 1   | K     | 143 | TYR  | 2.9  |
| 1   | C     | 231 | LYS  | 2.9  |
| 1   | D     | 280 | GLY  | 2.9  |
| 1   | D     | 436 | THR  | 2.9  |
| 1   | F     | 128 | GLY  | 2.9  |
| 1   | L     | 183 | HIS  | 2.9  |
| 1   | K     | 33  | ASN  | 2.9  |
| 1   | E     | 179 | ASP  | 2.9  |
| 1   | F     | 436 | THR  | 2.9  |
| 1   | D     | 343 | VAL  | 2.8  |
| 1   | A     | 62  | LYS  | 2.8  |
| 1   | I     | 141 | GLU  | 2.8  |
| 1   | K     | 113 | ARG  | 2.8  |
| 1   | F     | 336 | LYS  | 2.8  |
| 1   | L     | 62  | LYS  | 2.8  |
| 1   | F     | 404 | HIS  | 2.8  |
| 1   | H     | 280 | GLY  | 2.8  |
| 1   | C     | 63  | LYS  | 2.8  |
| 1   | L     | 113 | ARG  | 2.8  |
| 1   | D     | 63  | LYS  | 2.8  |
| 1   | B     | 350 | PRO  | 2.8  |
| 1   | K     | 295 | LYS  | 2.8  |
| 1   | L     | 20  | LYS  | 2.8  |
| 1   | C     | 433 | GLU  | 2.8  |
| 1   | K     | 358 | ARG  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 143 | TYR  | 2.8  |
| 1   | B     | 21  | ASN  | 2.7  |
| 1   | K     | 428 | ASP  | 2.7  |
| 1   | C     | 404 | HIS  | 2.7  |
| 1   | A     | 239 | ARG  | 2.7  |
| 1   | I     | 64  | ARG  | 2.7  |
| 1   | K     | 187 | GLU  | 2.7  |
| 1   | K     | 287 | ARG  | 2.7  |
| 1   | K     | 75  | ASP  | 2.7  |
| 1   | D     | 281 | GLU  | 2.7  |
| 1   | K     | 186 | GLY  | 2.7  |
| 1   | K     | 151 | ILE  | 2.7  |
| 1   | F     | 63  | LYS  | 2.7  |
| 1   | A     | 106 | PRO  | 2.7  |
| 1   | L     | 188 | PRO  | 2.7  |
| 1   | B     | 404 | HIS  | 2.7  |
| 1   | L     | 125 | GLY  | 2.7  |
| 1   | C     | 169 | ASP  | 2.7  |
| 1   | K     | 106 | PRO  | 2.7  |
| 1   | D     | 34  | GLU  | 2.7  |
| 1   | K     | 32  | ILE  | 2.7  |
| 1   | A     | 60  | LYS  | 2.6  |
| 1   | E     | 129 | ASN  | 2.6  |
| 1   | E     | 244 | TYR  | 2.6  |
| 1   | J     | 432 | LEU  | 2.6  |
| 1   | G     | 392 | ASP  | 2.6  |
| 1   | H     | 434 | ASP  | 2.6  |
| 1   | B     | 433 | GLU  | 2.6  |
| 1   | G     | 33  | ASN  | 2.6  |
| 1   | E     | 127 | THR  | 2.6  |
| 1   | F     | 294 | GLU  | 2.6  |
| 1   | K     | 152 | PHE  | 2.6  |
| 1   | H     | 317 | HIS  | 2.6  |
| 1   | H     | 338 | ARG  | 2.6  |
| 1   | L     | 19  | GLN  | 2.6  |
| 1   | L     | 199 | ASN  | 2.6  |
| 1   | B     | 349 | ARG  | 2.6  |
| 1   | E     | 32  | ILE  | 2.6  |
| 1   | I     | 140 | LEU  | 2.6  |
| 1   | L     | 427 | MET  | 2.6  |
| 1   | H     | 427 | MET  | 2.5  |
| 1   | E     | 173 | TYR  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 274 | ILE  | 2.5  |
| 1   | E     | 349 | ARG  | 2.5  |
| 1   | E     | 195 | GLU  | 2.5  |
| 1   | E     | 128 | GLY  | 2.5  |
| 1   | E     | 436 | THR  | 2.5  |
| 1   | K     | 328 | LEU  | 2.5  |
| 1   | K     | 319 | GLU  | 2.5  |
| 1   | A     | 404 | HIS  | 2.5  |
| 1   | E     | 140 | LEU  | 2.5  |
| 1   | G     | 32  | ILE  | 2.5  |
| 1   | D     | 338 | ARG  | 2.5  |
| 1   | E     | 80  | GLU  | 2.5  |
| 1   | K     | 110 | TYR  | 2.5  |
| 1   | D     | 52  | PHE  | 2.4  |
| 1   | I     | 193 | ASP  | 2.4  |
| 1   | C     | 127 | THR  | 2.4  |
| 1   | C     | 244 | TYR  | 2.4  |
| 1   | L     | 140 | LEU  | 2.4  |
| 1   | K     | 282 | SER  | 2.4  |
| 1   | E     | 181 | VAL  | 2.4  |
| 1   | E     | 312 | LYS  | 2.4  |
| 1   | L     | 186 | GLY  | 2.4  |
| 1   | A     | 278 | LEU  | 2.4  |
| 1   | C     | 278 | LEU  | 2.4  |
| 1   | D     | 106 | PRO  | 2.4  |
| 1   | E     | 350 | PRO  | 2.4  |
| 1   | I     | 360 | PHE  | 2.4  |
| 1   | H     | 109 | LYS  | 2.4  |
| 1   | H     | 172 | PRO  | 2.4  |
| 1   | D     | 336 | LYS  | 2.4  |
| 1   | A     | 459 | SER  | 2.4  |
| 1   | K     | 326 | SER  | 2.4  |
| 1   | K     | 150 | ASP  | 2.4  |
| 1   | G     | 140 | LEU  | 2.4  |
| 1   | C     | 239 | ARG  | 2.4  |
| 1   | F     | 338 | ARG  | 2.4  |
| 1   | K     | 330 | THR  | 2.4  |
| 1   | A     | 438 | ASP  | 2.4  |
| 1   | L     | 428 | ASP  | 2.4  |
| 1   | E     | 278 | LEU  | 2.4  |
| 1   | D     | 319 | GLU  | 2.4  |
| 1   | L     | 117 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 231 | LYS  | 2.3  |
| 1   | K     | 359 | ARG  | 2.3  |
| 1   | D     | 155 | HIS  | 2.3  |
| 1   | B     | 173 | TYR  | 2.3  |
| 1   | E     | 247 | PRO  | 2.3  |
| 1   | D     | 349 | ARG  | 2.3  |
| 1   | I     | 169 | ASP  | 2.3  |
| 1   | I     | 239 | ARG  | 2.3  |
| 1   | C     | 72  | LEU  | 2.3  |
| 1   | D     | 194 | GLU  | 2.3  |
| 1   | C     | 210 | ARG  | 2.3  |
| 1   | E     | 117 | LEU  | 2.3  |
| 1   | F     | 34  | GLU  | 2.3  |
| 1   | D     | 239 | ARG  | 2.3  |
| 1   | J     | 338 | ARG  | 2.3  |
| 1   | B     | 23  | PRO  | 2.3  |
| 1   | E     | 141 | GLU  | 2.3  |
| 1   | I     | 317 | HIS  | 2.3  |
| 1   | E     | 172 | PRO  | 2.3  |
| 1   | H     | 345 | ALA  | 2.3  |
| 1   | I     | 190 | LYS  | 2.3  |
| 1   | L     | 436 | THR  | 2.3  |
| 1   | L     | 155 | HIS  | 2.3  |
| 1   | E     | 169 | ASP  | 2.3  |
| 1   | G     | 193 | ASP  | 2.3  |
| 1   | L     | 150 | ASP  | 2.3  |
| 1   | C     | 279 | ALA  | 2.3  |
| 1   | G     | 128 | GLY  | 2.3  |
| 1   | K     | 361 | GLY  | 2.3  |
| 1   | E     | 192 | GLU  | 2.3  |
| 1   | K     | 192 | GLU  | 2.3  |
| 1   | L     | 196 | GLU  | 2.3  |
| 1   | H     | 179 | ASP  | 2.3  |
| 1   | F     | 323 | ARG  | 2.3  |
| 1   | L     | 46  | MET  | 2.3  |
| 1   | A     | 185 | GLU  | 2.3  |
| 1   | A     | 436 | THR  | 2.3  |
| 1   | K     | 285 | ASN  | 2.3  |
| 1   | K     | 351 | ASN  | 2.3  |
| 1   | B     | 140 | LEU  | 2.3  |
| 1   | L     | 431 | ASP  | 2.2  |
| 1   | G     | 53  | ARG  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 231 | LYS  | 2.2  |
| 1   | K     | 306 | LEU  | 2.2  |
| 1   | L     | 108 | VAL  | 2.2  |
| 1   | L     | 52  | PHE  | 2.2  |
| 1   | E     | 438 | ASP  | 2.2  |
| 1   | J     | 437 | ILE  | 2.2  |
| 1   | E     | 64  | ARG  | 2.2  |
| 1   | K     | 34  | GLU  | 2.2  |
| 1   | H     | 22  | ARG  | 2.2  |
| 1   | K     | 52  | PHE  | 2.2  |
| 1   | C     | 33  | ASN  | 2.2  |
| 1   | C     | 336 | LYS  | 2.2  |
| 1   | E     | 316 | THR  | 2.2  |
| 1   | I     | 244 | TYR  | 2.2  |
| 1   | G     | 231 | LYS  | 2.2  |
| 1   | D     | 345 | ALA  | 2.2  |
| 1   | I     | 172 | PRO  | 2.2  |
| 1   | E     | 313 | ARG  | 2.2  |
| 1   | B     | 432 | LEU  | 2.2  |
| 1   | H     | 278 | LEU  | 2.2  |
| 1   | K     | 327 | GLN  | 2.2  |
| 1   | C     | 343 | VAL  | 2.1  |
| 1   | C     | 428 | ASP  | 2.1  |
| 1   | C     | 460 | ASN  | 2.1  |
| 1   | K     | 291 | GLU  | 2.1  |
| 1   | L     | 366 | GLU  | 2.1  |
| 1   | H     | 315 | LYS  | 2.1  |
| 1   | K     | 72  | LEU  | 2.1  |
| 1   | G     | 124 | GLU  | 2.1  |
| 1   | G     | 405 | GLY  | 2.1  |
| 1   | D     | 53  | ARG  | 2.1  |
| 1   | D     | 342 | ILE  | 2.1  |
| 1   | G     | 141 | GLU  | 2.1  |
| 1   | J     | 141 | GLU  | 2.1  |
| 1   | A     | 140 | LEU  | 2.1  |
| 1   | C     | 167 | GLU  | 2.1  |
| 1   | E     | 434 | ASP  | 2.1  |
| 1   | K     | 281 | GLU  | 2.1  |
| 1   | C     | 312 | LYS  | 2.1  |
| 1   | J     | 404 | HIS  | 2.1  |
| 1   | A     | 52  | PHE  | 2.1  |
| 1   | K     | 431 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 160 | ALA  | 2.1  |
| 1   | A     | 280 | GLY  | 2.1  |
| 1   | G     | 443 | ASN  | 2.1  |
| 1   | K     | 344 | MET  | 2.1  |
| 1   | D     | 113 | ARG  | 2.1  |
| 1   | G     | 239 | ARG  | 2.1  |
| 1   | I     | 429 | LEU  | 2.1  |
| 1   | C     | 75  | ASP  | 2.1  |
| 1   | J     | 231 | LYS  | 2.1  |
| 1   | A     | 33  | ASN  | 2.1  |
| 1   | L     | 33  | ASN  | 2.1  |
| 1   | J     | 360 | PHE  | 2.1  |
| 1   | A     | 193 | ASP  | 2.1  |
| 1   | F     | 428 | ASP  | 2.1  |
| 1   | I     | 179 | ASP  | 2.1  |
| 1   | D     | 344 | MET  | 2.1  |
| 1   | B     | 52  | PHE  | 2.1  |
| 1   | E     | 239 | ARG  | 2.0  |
| 1   | F     | 432 | LEU  | 2.0  |
| 1   | E     | 155 | HIS  | 2.0  |
| 1   | B     | 75  | ASP  | 2.0  |
| 1   | C     | 431 | ASP  | 2.0  |
| 1   | L     | 239 | ARG  | 2.0  |
| 1   | A     | 346 | ALA  | 2.0  |
| 1   | D     | 429 | LEU  | 2.0  |
| 1   | E     | 24  | ASN  | 2.0  |
| 1   | L     | 104 | PRO  | 2.0  |
| 1   | B     | 64  | ARG  | 2.0  |
| 1   | L     | 22  | ARG  | 2.0  |
| 1   | D     | 179 | ASP  | 2.0  |
| 1   | G     | 69  | CYS  | 2.0  |
| 1   | I     | 117 | LEU  | 2.0  |
| 1   | G     | 346 | ALA  | 2.0  |
| 1   | K     | 297 | ALA  | 2.0  |
| 1   | A     | 53  | ARG  | 2.0  |
| 1   | F     | 64  | ARG  | 2.0  |
| 1   | B     | 278 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

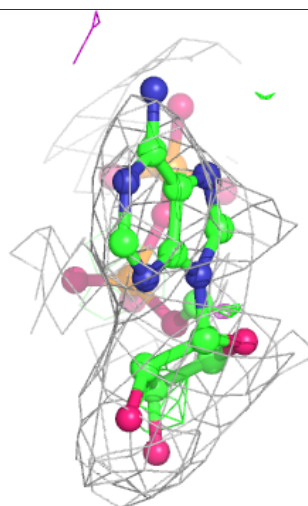
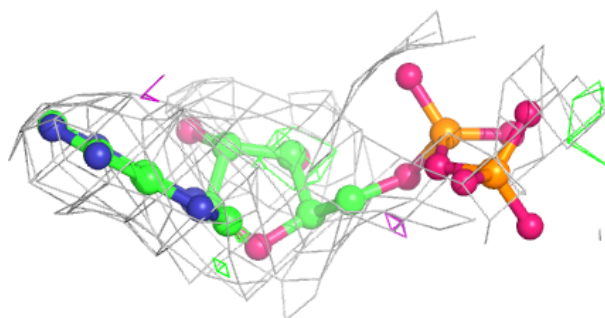
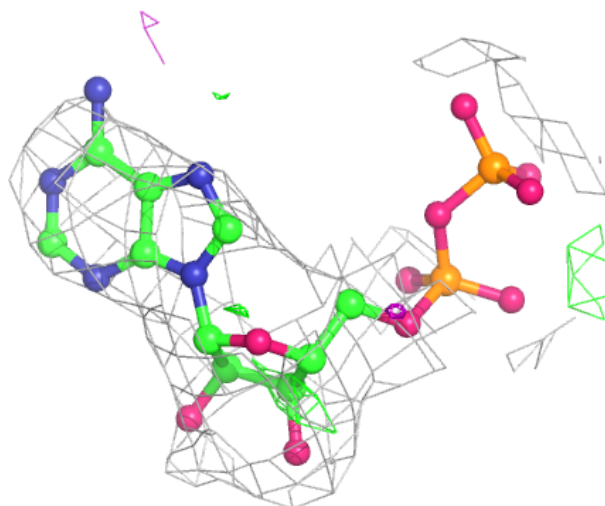
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ADP  | K     | 800 | 27/27 | 0.94 | 0.18 | 95,102,110,112             | 0     |
| 2   | ADP  | L     | 800 | 27/27 | 0.95 | 0.16 | 87,90,104,111              | 0     |
| 2   | ADP  | I     | 800 | 27/27 | 0.95 | 0.17 | 78,82,88,90                | 0     |
| 2   | ADP  | G     | 800 | 27/27 | 0.96 | 0.16 | 79,86,95,96                | 0     |
| 2   | ADP  | E     | 800 | 27/27 | 0.96 | 0.13 | 75,83,94,97                | 0     |
| 2   | ADP  | B     | 800 | 27/27 | 0.96 | 0.16 | 71,74,79,84                | 0     |
| 2   | ADP  | A     | 800 | 27/27 | 0.96 | 0.15 | 75,81,95,99                | 0     |
| 2   | ADP  | D     | 800 | 27/27 | 0.96 | 0.15 | 73,76,82,84                | 0     |
| 2   | ADP  | F     | 800 | 27/27 | 0.97 | 0.14 | 76,78,82,83                | 0     |
| 2   | ADP  | C     | 800 | 27/27 | 0.97 | 0.14 | 87,91,101,105              | 0     |
| 2   | ADP  | H     | 800 | 27/27 | 0.97 | 0.14 | 74,77,88,97                | 0     |
| 2   | ADP  | J     | 800 | 27/27 | 0.98 | 0.12 | 59,64,73,73                | 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 K 800:**

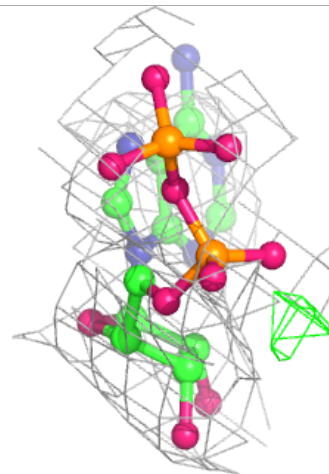
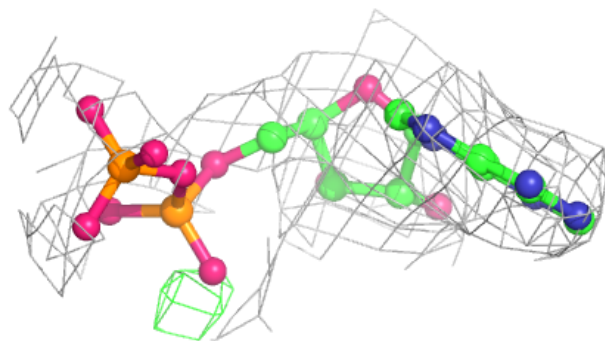
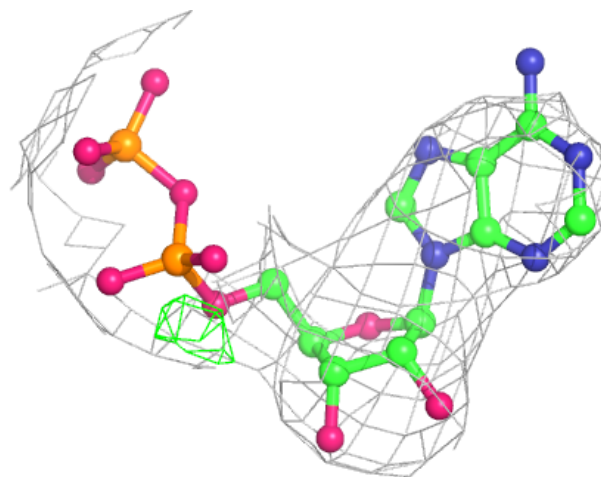
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





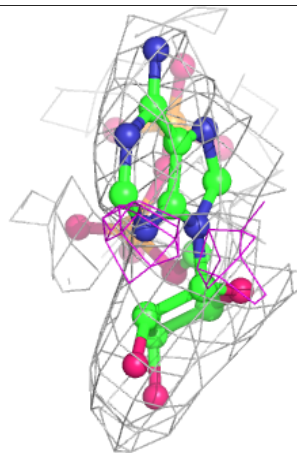
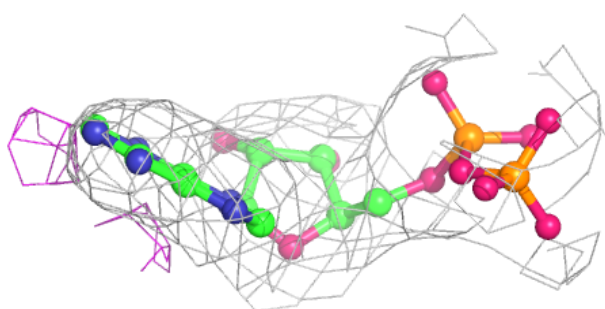
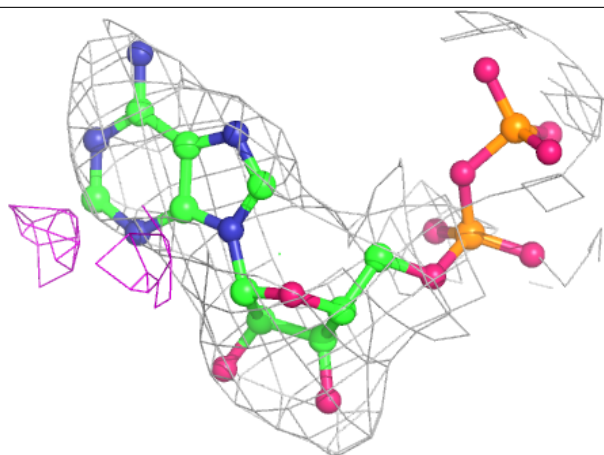
**Electron density around ADP L 800:**

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



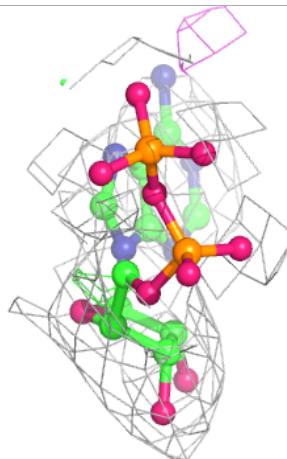
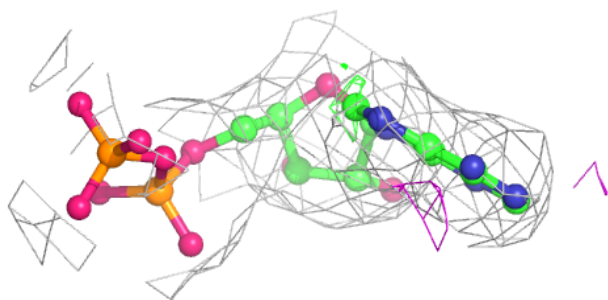
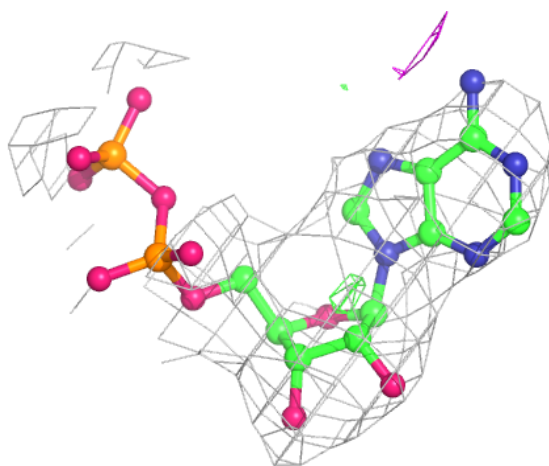
**Electron density around ADP I 800:**

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



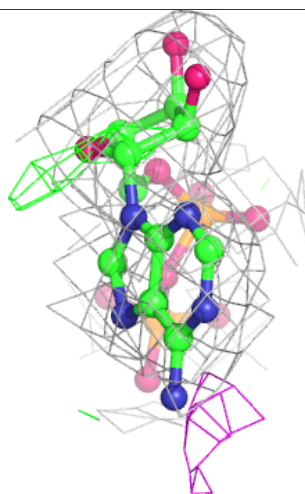
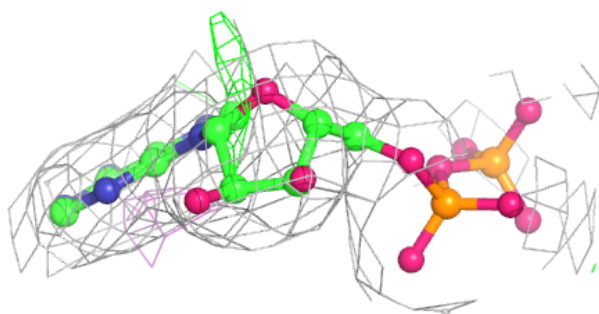
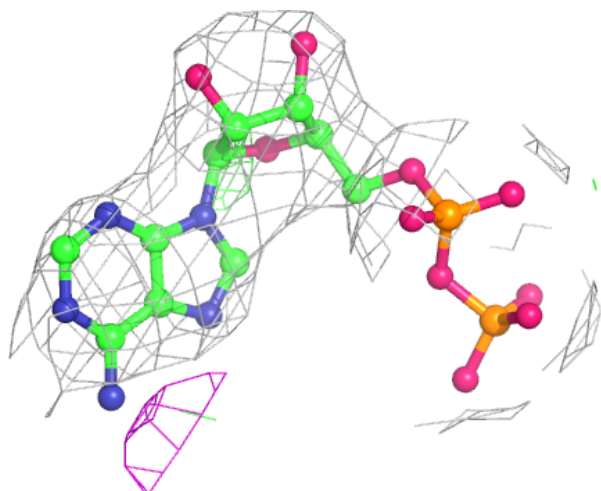
**Electron density around ADP G 800:**

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



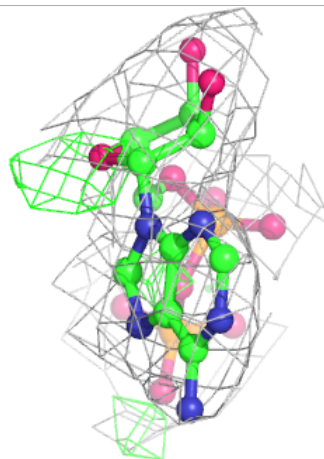
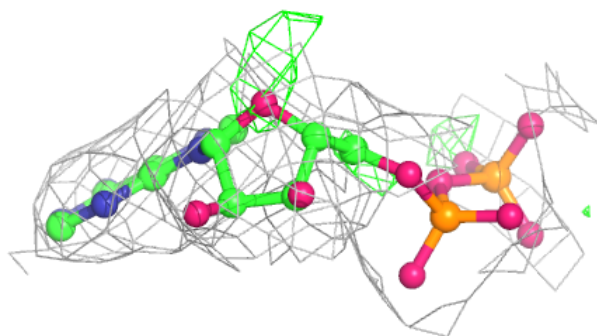
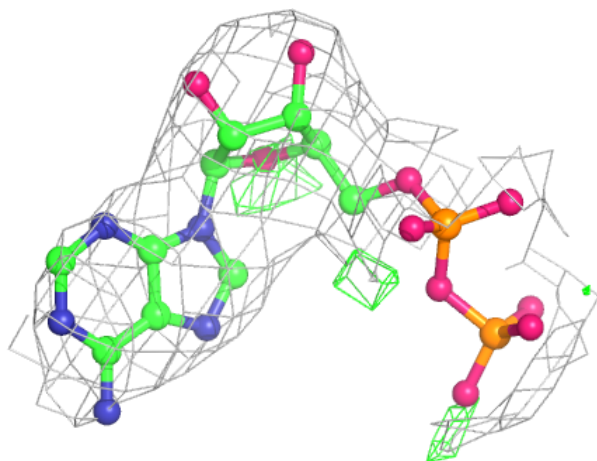
**Electron density around ADP E 800:**

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



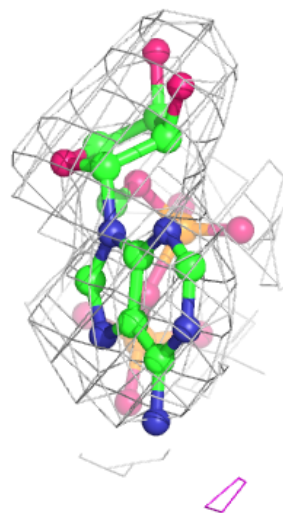
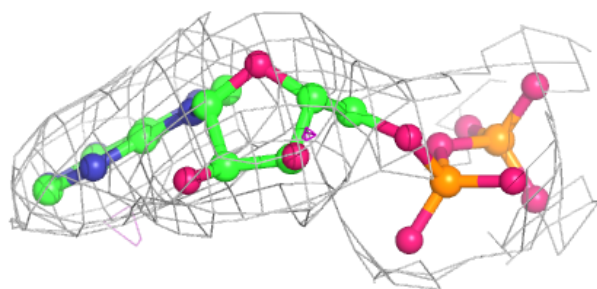
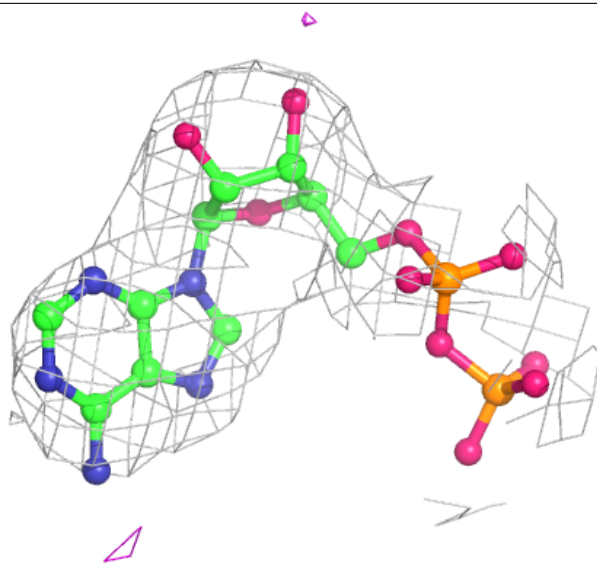
**Electron density around ADP B 800:**

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



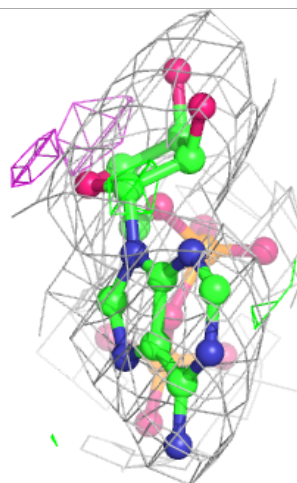
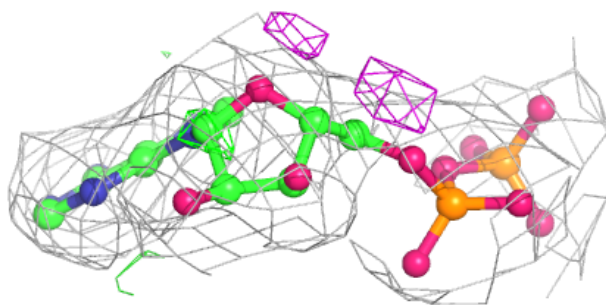
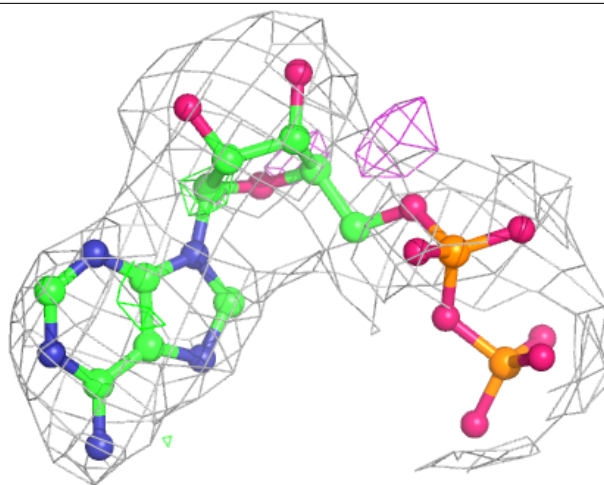
**Electron density around ADP A 800:**

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



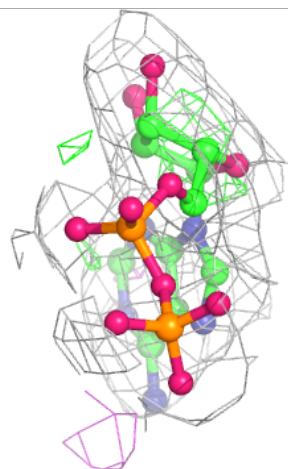
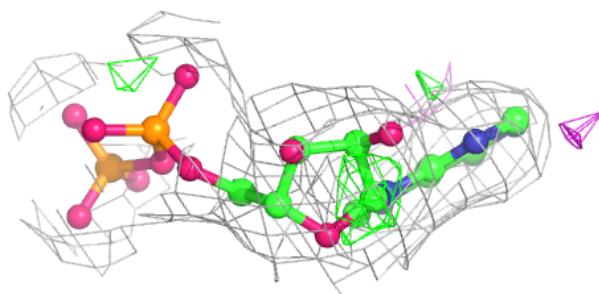
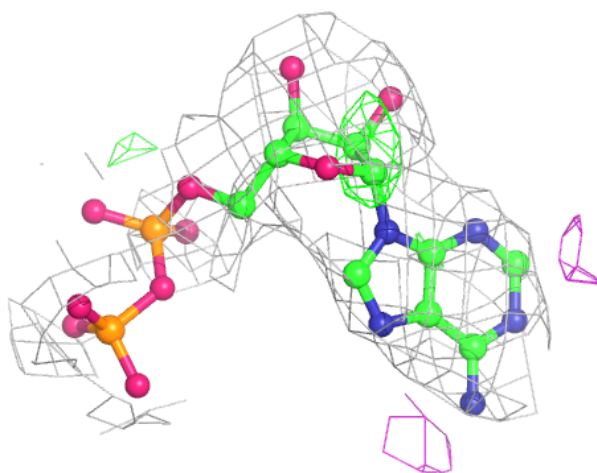
**Electron density around ADP D 800:**

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



**Electron density around ADP F 800:**

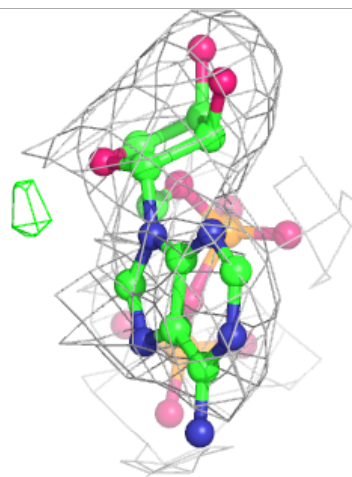
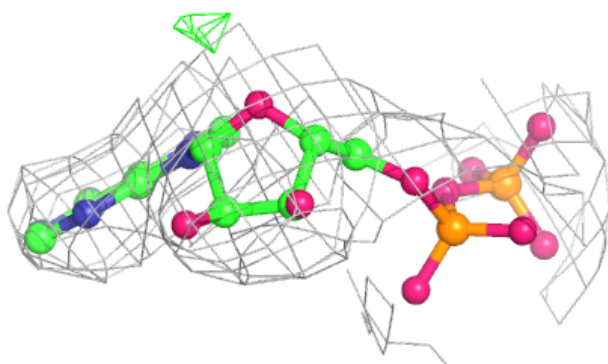
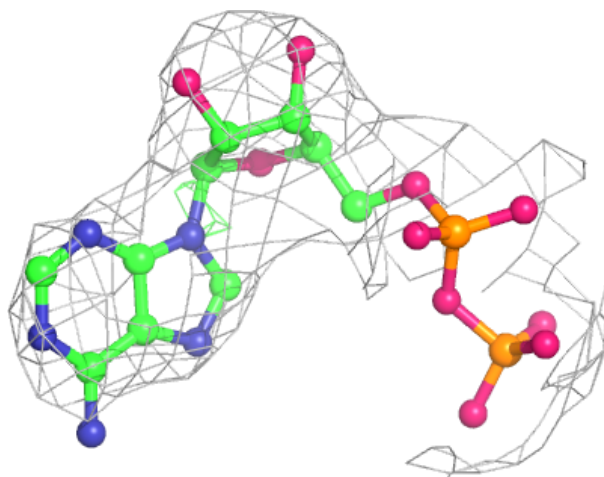
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





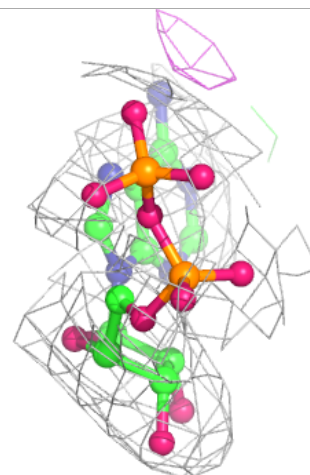
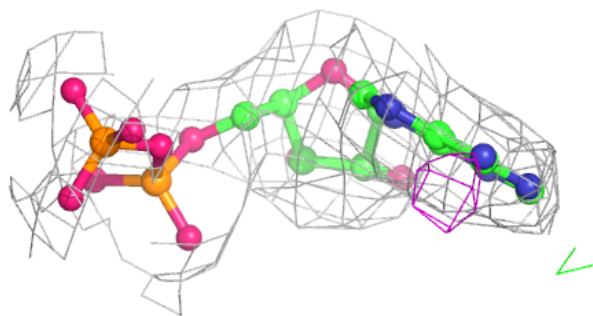
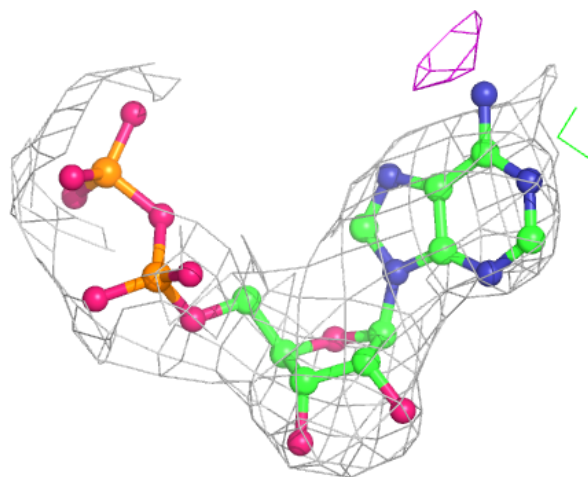
**Electron density around ADP C 800:**

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



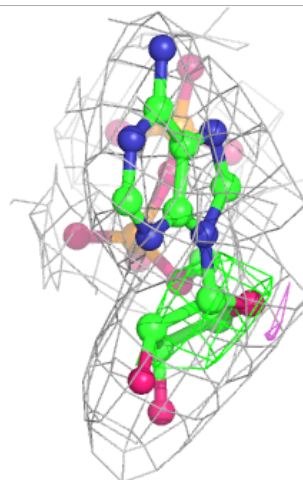
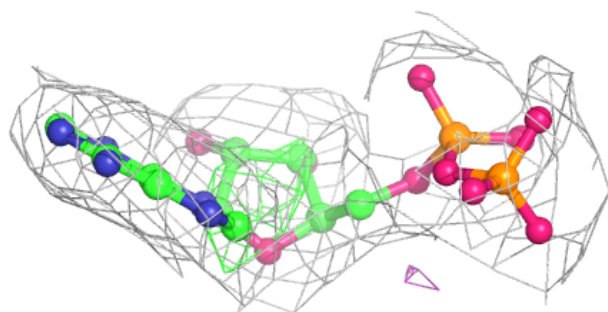
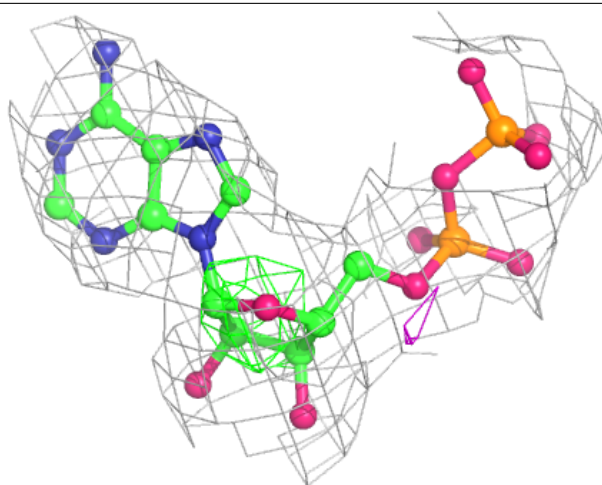
**Electron density around ADP H 800:**

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



**Electron density around ADP J 800:**

$2mF_o-DF_c$  (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.