



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:29 am BST

PDB ID : 3OEH  
Title : Structure of four mutant forms of yeast F1 ATPase: beta-V279F  
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.  
Deposited on : 2010-08-12  
Resolution : 3.00 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

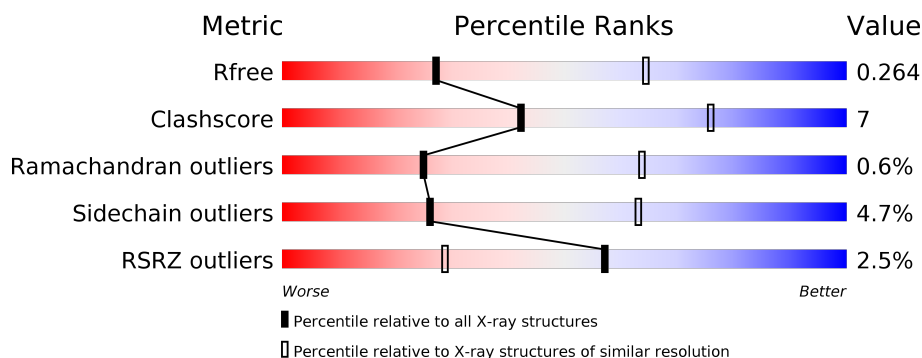
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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                      | 2092 (3.00-3.00)                                      |
| Clashscore            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (3.00-3.00)                                      |
| RSRZ outliers         | 127900                      | 1990 (3.00-3.00)                                      |

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     | 510    | <br>78% 15% • 5% |
| 1   | B     | 510    | <br>75% 18% • 5% |
| 1   | C     | 510    | <br>80% 14% • 5% |
| 1   | J     | 510    | <br>79% 15% 6%   |
| 1   | K     | 510    | <br>74% 21% • 5% |
| 1   | L     | 510    | <br>74% 19% • 5% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | S     | 510    |                  |
| 1   | T     | 510    |                  |
| 1   | U     | 510    |                  |
| 2   | D     | 484    |                  |
| 2   | E     | 484    |                  |
| 2   | F     | 484    |                  |
| 2   | M     | 484    |                  |
| 2   | N     | 484    |                  |
| 2   | O     | 484    |                  |
| 2   | V     | 484    |                  |
| 2   | W     | 484    |                  |
| 2   | X     | 484    |                  |
| 3   | G     | 278    |                  |
| 3   | P     | 278    |                  |
| 3   | Y     | 278    |                  |
| 4   | H     | 138    |                  |
| 4   | Q     | 138    |                  |
| 4   | Z     | 138    |                  |
| 5   | 1     | 61     |                  |
| 5   | I     | 61     |                  |
| 5   | R     | 61     |                  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 72707 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 ATP synthase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 482      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3664  | 2314 | 648 | 699 | 3 |         |         |       |
| 1   | B     | 483      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3669  | 2317 | 649 | 700 | 3 |         |         |       |
| 1   | C     | 484      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3680  | 2325 | 650 | 702 | 3 |         |         |       |
| 1   | J     | 481      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3655  | 2309 | 646 | 697 | 3 |         |         |       |
| 1   | K     | 486      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3688  | 2327 | 652 | 706 | 3 |         |         |       |
| 1   | L     | 482      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3664  | 2314 | 648 | 699 | 3 |         |         |       |
| 1   | S     | 478      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3635  | 2297 | 643 | 692 | 3 |         |         |       |
| 1   | T     | 479      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3642  | 2302 | 644 | 693 | 3 |         |         |       |
| 1   | U     | 481      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3655  | 2308 | 646 | 698 | 3 |         |         |       |

- Molecule 2 is a protein called ATP synthase subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | D     | 470      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3549  | 2252 | 603 | 688 | 6 |         |         |       |
| 2   | E     | 468      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3508  | 2227 | 598 | 677 | 6 |         |         |       |
| 2   | F     | 469      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3531  | 2242 | 602 | 681 | 6 |         |         |       |
| 2   | M     | 470      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3543  | 2249 | 600 | 688 | 6 |         |         |       |
| 2   | N     | 470      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3545  | 2249 | 602 | 688 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | O     | 468      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3538  | 2246 | 602 | 684 | 6 |         |         |       |
| 2   | V     | 470      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3550  | 2251 | 604 | 689 | 6 |         |         |       |
| 2   | W     | 467      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3535  | 2244 | 601 | 684 | 6 |         |         |       |
| 2   | X     | 469      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3547  | 2251 | 603 | 687 | 6 |         |         |       |

There are 81 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| D     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| E     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| E     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| F     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| F     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| M     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| M     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| M     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| N     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| N     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| O     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| O     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| V     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| V     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| W     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| W     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |
| X     | -5      | ALA      | -      | EXPRESSION TAG      | UNP P00830 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| X     | -4      | SER      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | -3      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | -2      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | -1      | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | 0       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | 1       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | 2       | HIS      | -      | EXPRESSION TAG      | UNP P00830 |
| X     | 279     | PHE      | VAL    | ENGINEERED MUTATION | UNP P00830 |

- Molecule 3 is a protein called ATP synthase subunit gamma.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | G     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2059  | 1293 | 359 | 397 | 10 |         |         |       |
| 3   | P     | 246      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1872  | 1175 | 327 | 361 | 9  |         |         |       |
| 3   | Y     | 201      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1523  | 947  | 274 | 293 | 9  |         |         |       |

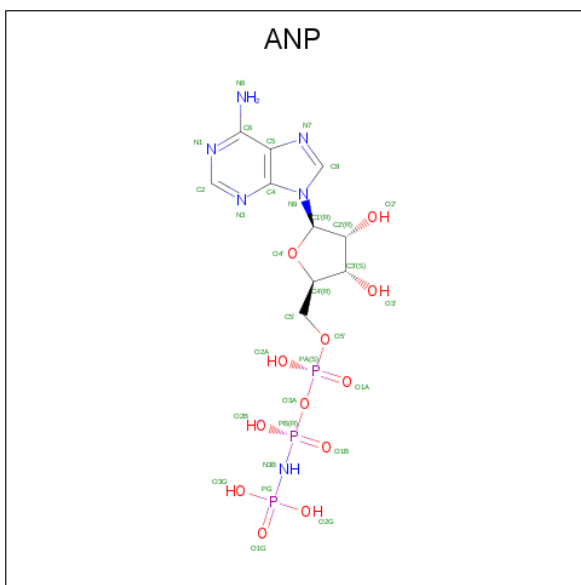
- Molecule 4 is a protein called ATP synthase subunit delta.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | H     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 477 | 132 | 152 | 2 |         |         |       |
| 4   | Q     | 84       | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 454   | 277 | 89  | 88  |   |         |         |       |
| 4   | Z     | 17       | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 85    | 51  | 17  | 17  |   |         |         |       |

- Molecule 5 is a protein called ATP synthase subunit epsilon.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 5   | I     | 49       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 339   | 212 | 57 | 70 |  |         |         |       |
| 5   | R     | 34       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 189   | 116 | 34 | 39 |  |         |         |       |
| 5   | 1     | 27       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 145   | 86  | 31 | 28 |  |         |         |       |

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 6   | A     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | B     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | C     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | D     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | F     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | J     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | K     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | L     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | M     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | O     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | S     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | T     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | U     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 6   | V     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 6   | X     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |

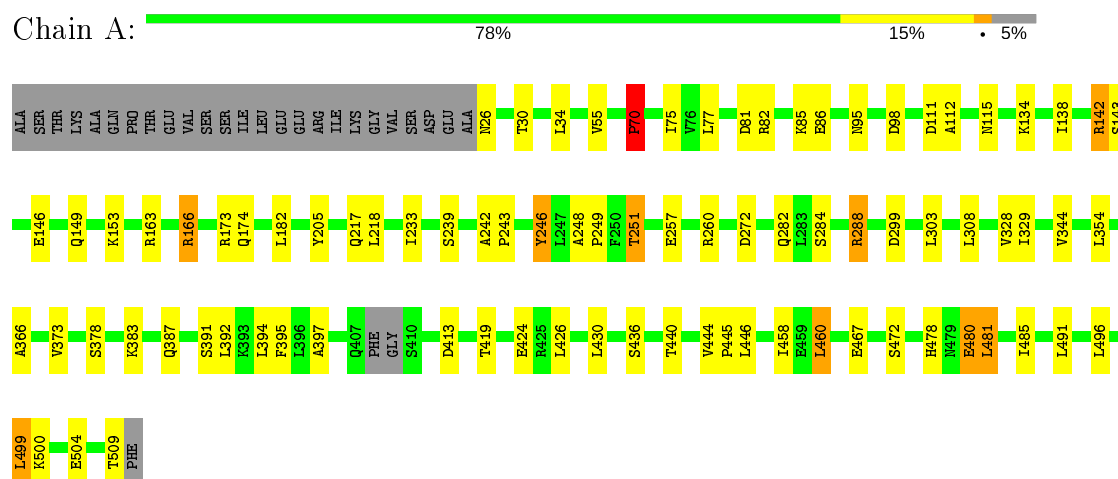
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | V     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | T     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | U     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | X     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | O     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | L     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | S     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | M     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

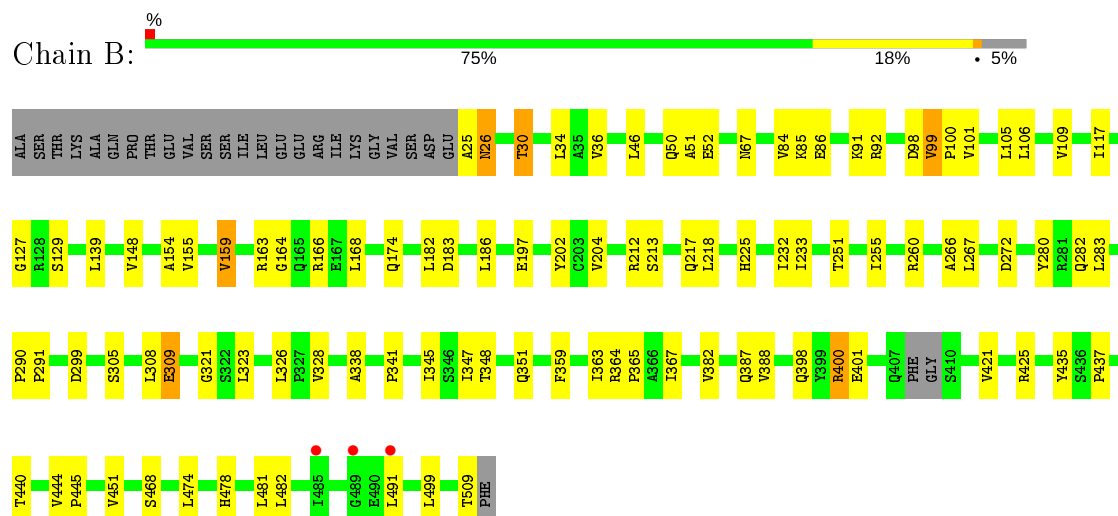
### 3 Residue-property plots

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: ATP synthase subunit alpha



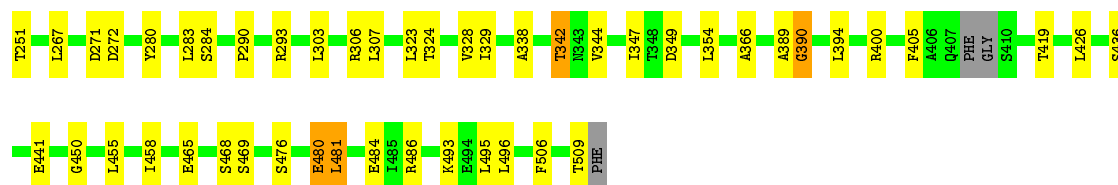
#### • Molecule 1: ATP synthase subunit alpha



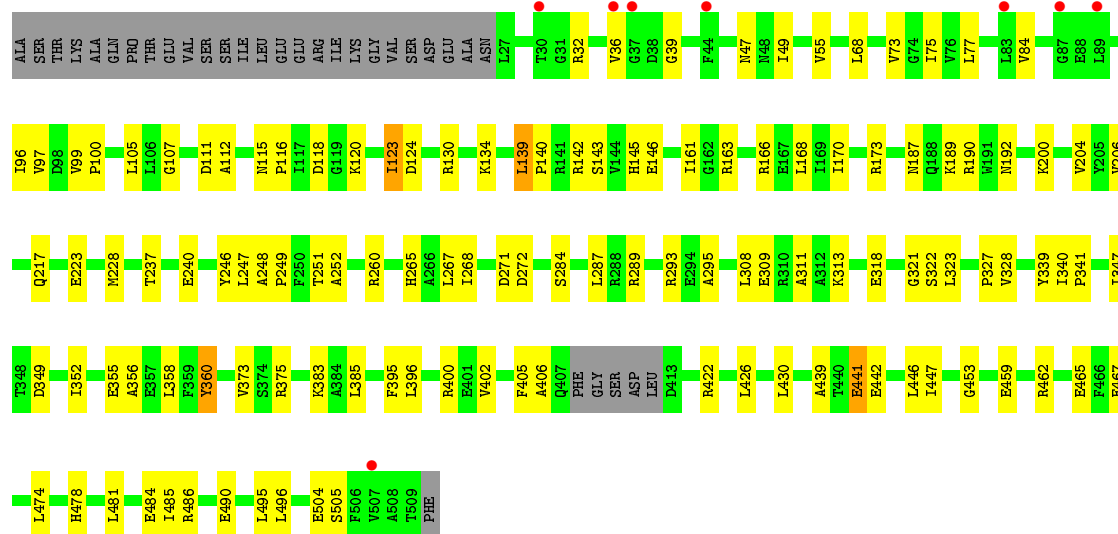
#### • Molecule 1: ATP synthase subunit alpha



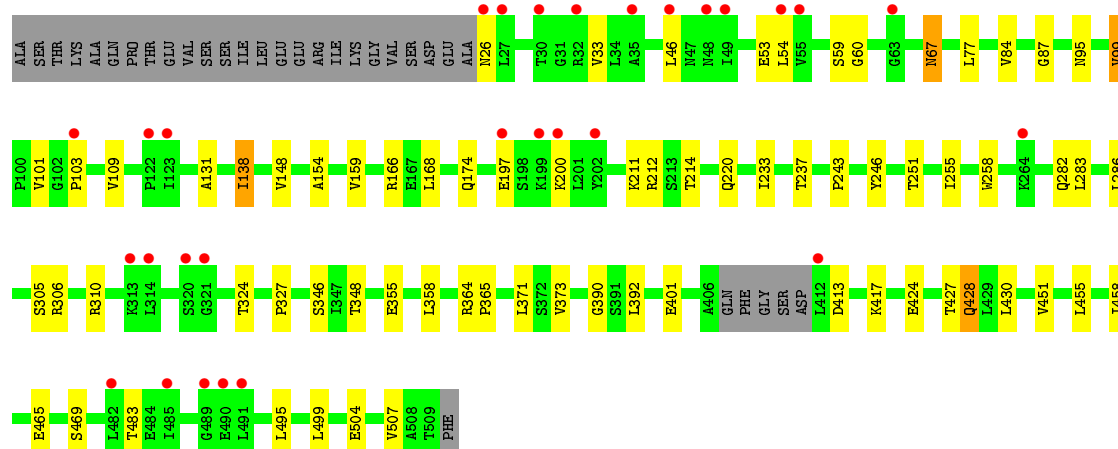
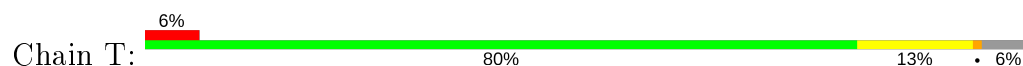




• Molecule 1: ATP synthase subunit alpha

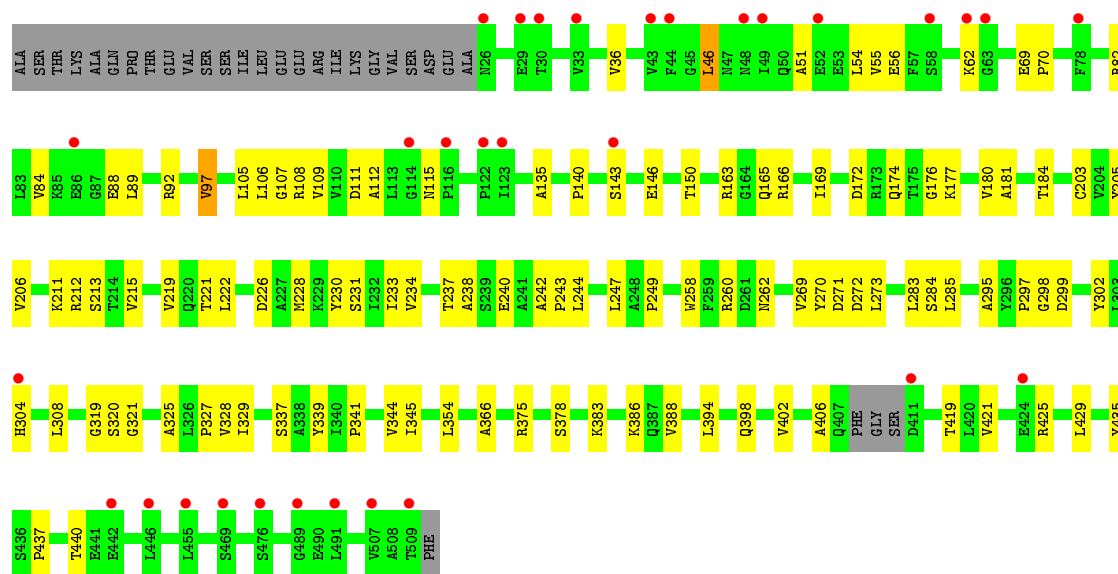


• Molecule 1: ATP synthase subunit alpha

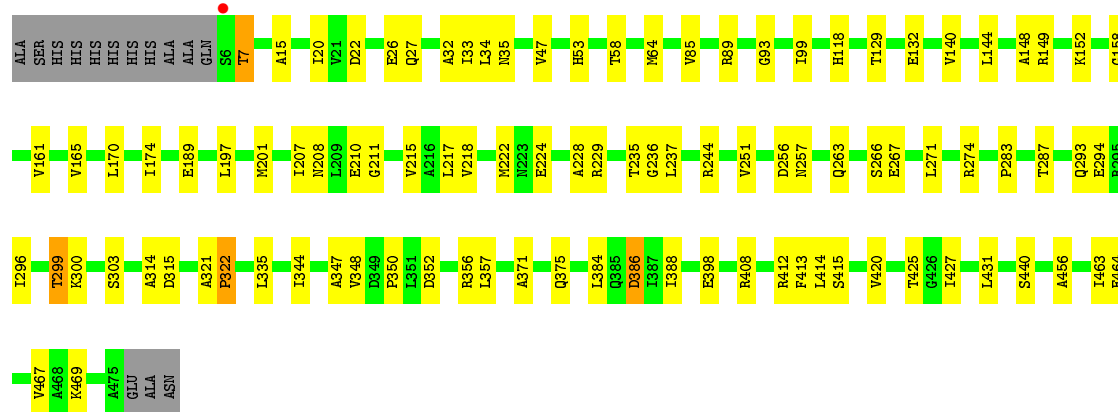


• Molecule 1: ATP synthase subunit alpha

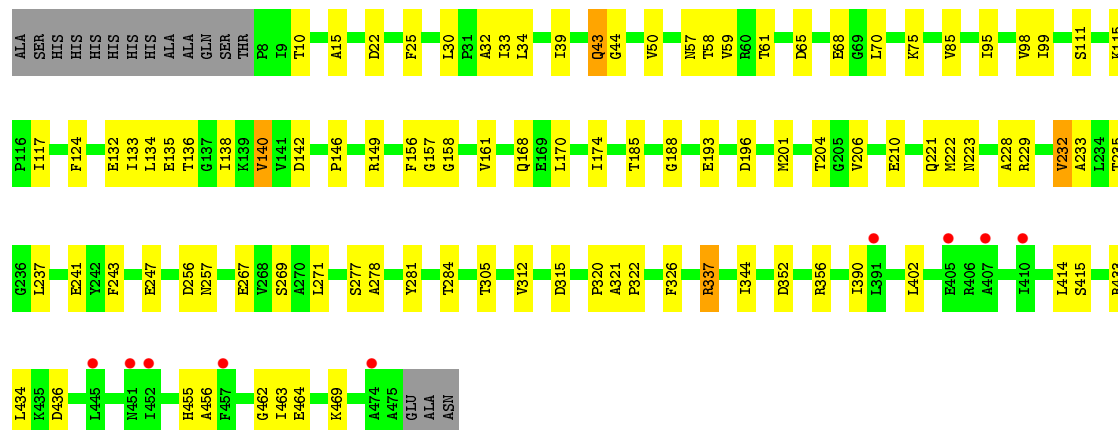
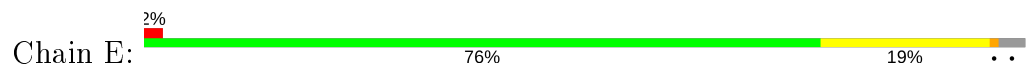




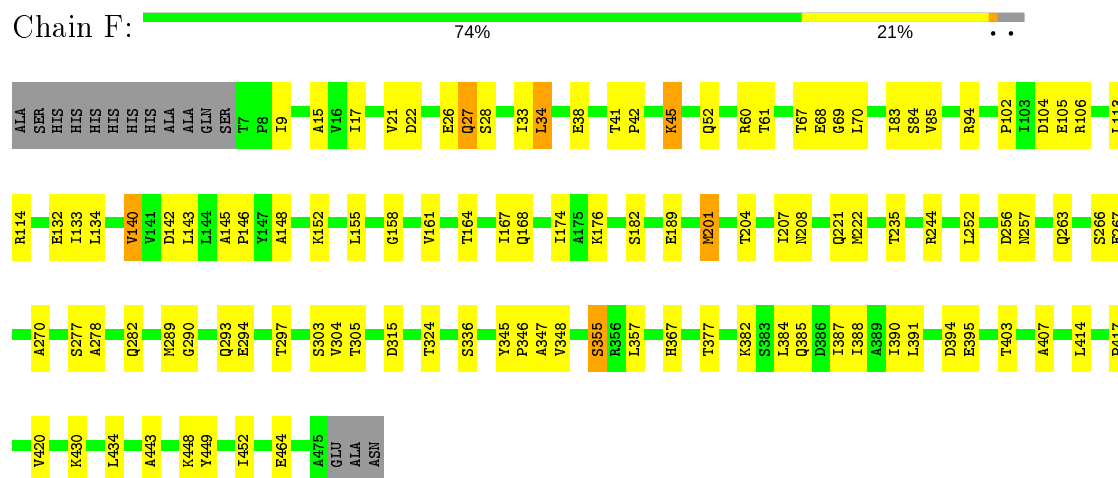
- Molecule 2: ATP synthase subunit beta



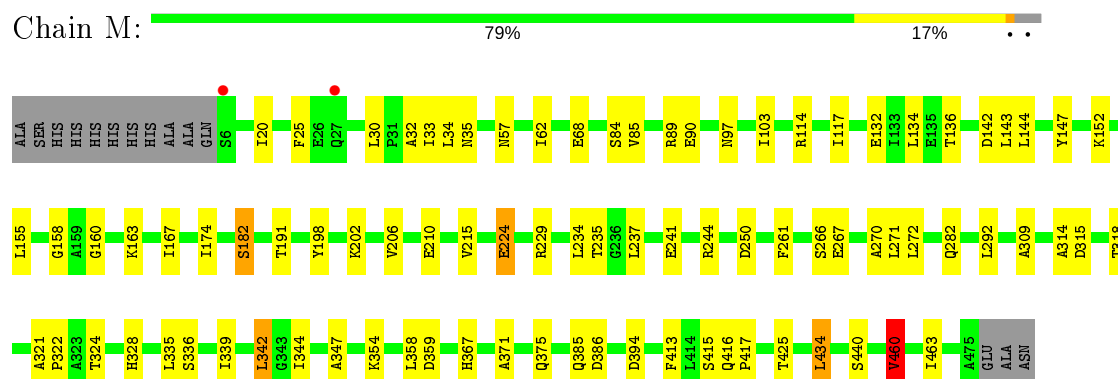
- Molecule 2: ATP synthase subunit beta



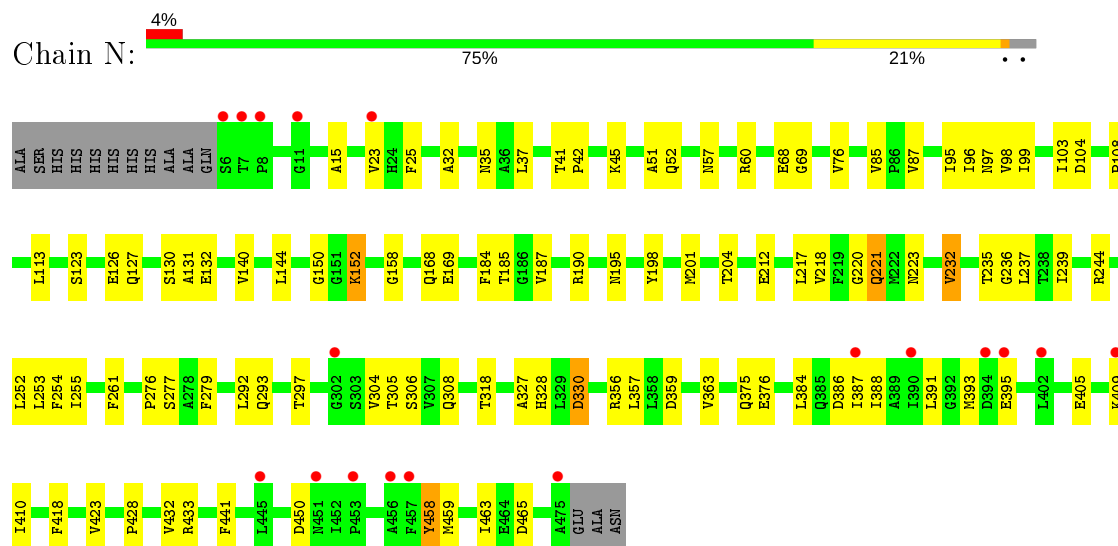
- Molecule 2: ATP synthase subunit beta




- Molecule 2: ATP synthase subunit beta

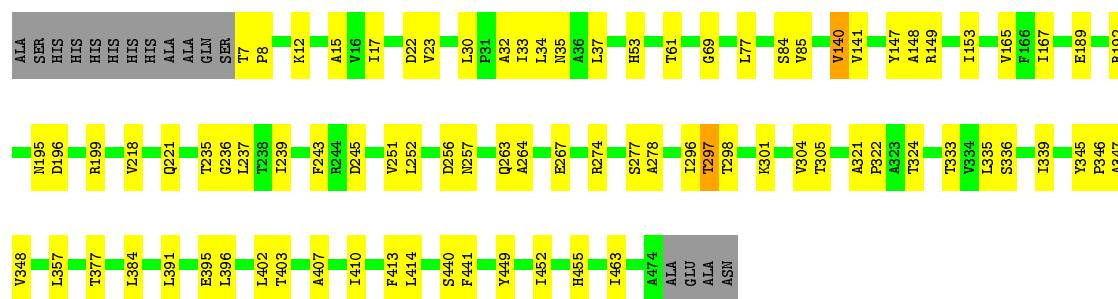


- Molecule 2: ATP synthase subunit beta



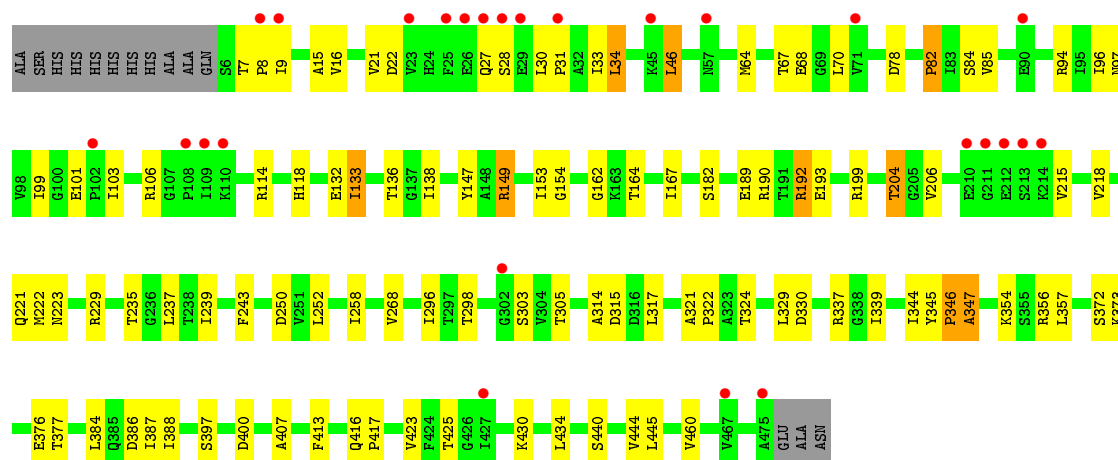
- Molecule 2: ATP synthase subunit beta

Chain O:  79% 17%




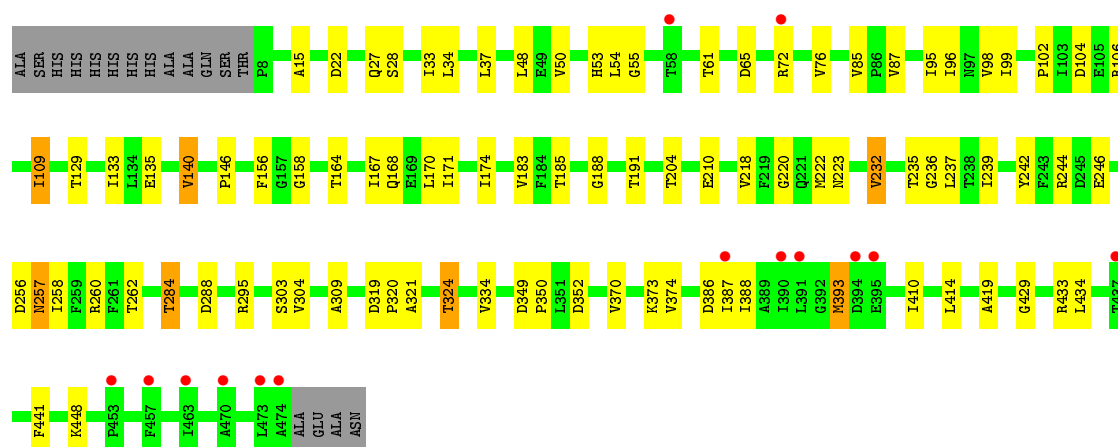
• Molecule 2: ATP synthase subunit beta

Chain V:  5% 75% 20%




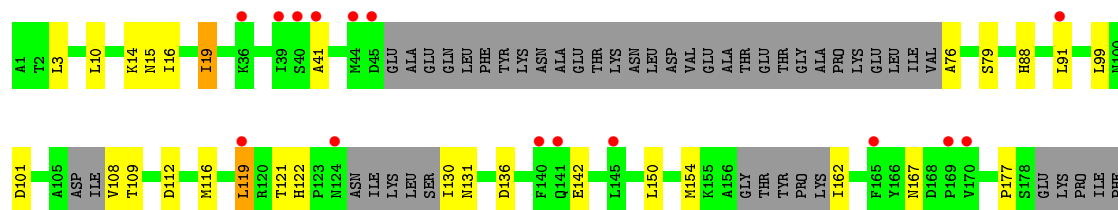
• Molecule 2: ATP synthase subunit beta

Chain W:  3% 78% 17%

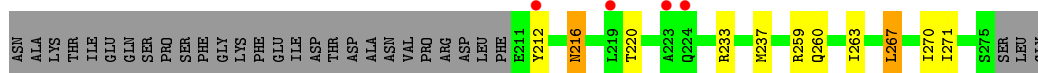


• Molecule 2: ATP synthase subunit beta

Chain X:  4% 83% 14%



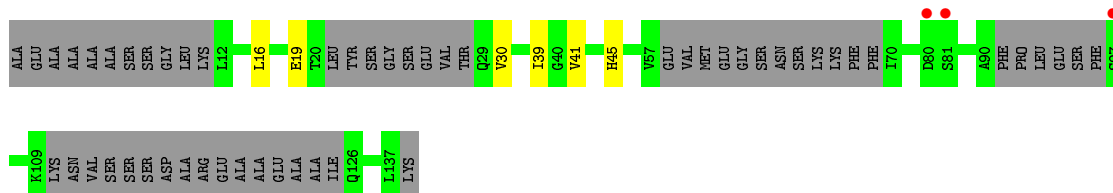




- Molecule 4: ATP synthase subunit delta



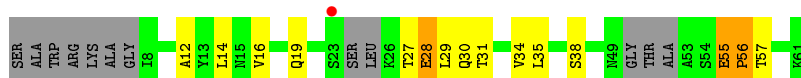
- Molecule 4: ATP synthase subunit delta



- Molecule 4: ATP synthase subunit delta

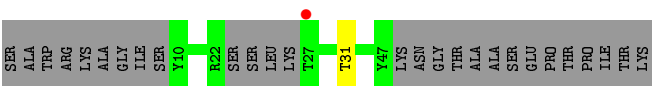


- Molecule 5: ATP synthase subunit epsilon

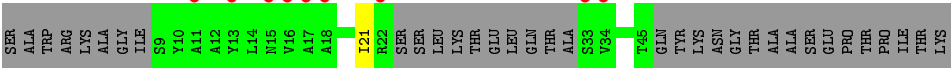


- Molecule 5: ATP synthase subunit epsilon





● Molecule 5: ATP synthase subunit epsilon



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 110.93Å 291.90Å 188.76Å<br>90.00° 101.91° 90.00°            | Depositor        |
| Resolution (Å)  | 20.00 – 3.00<br>49.39 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.8 (20.00-3.00)<br>88.6 (49.39-3.00)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.05  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.29 (at 3.01Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0102   | Depositor        |
| R, $R_{free}$   | 0.209 , 0.270<br>0.207 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4161 reflections (2.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 82.8  | Xtriage          |
| Anisotropy  | 0.128   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 55.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 72707   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 110.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.46         | 0/3718      | 0.65        | 0/5032         |
| 1   | B     | 0.39         | 0/3723      | 0.59        | 0/5039         |
| 1   | C     | 0.42         | 0/3736      | 0.62        | 1/5057 (0.0%)  |
| 1   | J     | 0.36         | 0/3709      | 0.56        | 0/5020         |
| 1   | K     | 0.35         | 0/3742      | 0.54        | 0/5065         |
| 1   | L     | 0.43         | 0/3718      | 0.61        | 1/5032 (0.0%)  |
| 1   | S     | 0.37         | 0/3689      | 0.54        | 0/4992         |
| 1   | T     | 0.34         | 0/3696      | 0.50        | 0/5002         |
| 1   | U     | 0.35         | 0/3709      | 0.54        | 0/5021         |
| 2   | D     | 0.47         | 0/3606      | 0.61        | 0/4890         |
| 2   | E     | 0.42         | 0/3565      | 0.58        | 0/4840         |
| 2   | F     | 0.40         | 0/3588      | 0.58        | 0/4868         |
| 2   | M     | 0.39         | 0/3600      | 0.58        | 0/4883         |
| 2   | N     | 0.37         | 0/3602      | 0.53        | 1/4886 (0.0%)  |
| 2   | O     | 0.37         | 0/3595      | 0.56        | 0/4875         |
| 2   | V     | 0.37         | 0/3607      | 0.53        | 0/4891         |
| 2   | W     | 0.36         | 0/3592      | 0.52        | 0/4869         |
| 2   | X     | 0.36         | 0/3604      | 0.53        | 0/4887         |
| 3   | G     | 0.39         | 0/2084      | 0.53        | 0/2803         |
| 3   | P     | 0.36         | 0/1889      | 0.53        | 0/2537         |
| 3   | Y     | 0.34         | 0/1533      | 0.51        | 0/2056         |
| 4   | H     | 0.39         | 0/772       | 0.59        | 0/1058         |
| 4   | Q     | 0.36         | 0/453       | 0.51        | 0/621          |
| 4   | Z     | 0.35         | 0/84        | 0.45        | 0/116          |
| 5   | 1     | 0.30         | 0/143       | 0.42        | 0/195          |
| 5   | I     | 0.42         | 0/343       | 0.59        | 0/470          |
| 5   | R     | 0.39         | 0/189       | 0.50        | 0/261          |
| All | All   | 0.39         | 0/73289     | 0.56        | 3/99266 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | L     | 283 | LEU  | CA-CB-CG | 5.70 | 128.40      | 115.30   |
| 2   | N     | 37  | LEU  | CA-CB-CG | 5.34 | 127.57      | 115.30   |
| 1   | C     | 283 | LEU  | CA-CB-CG | 5.04 | 126.88      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 3664  | 0        | 3747     | 59      | 0            |
| 1   | B     | 3669  | 0        | 3752     | 59      | 0            |
| 1   | C     | 3680  | 0        | 3763     | 40      | 0            |
| 1   | J     | 3655  | 0        | 3739     | 43      | 0            |
| 1   | K     | 3688  | 0        | 3763     | 63      | 0            |
| 1   | L     | 3664  | 0        | 3747     | 54      | 0            |
| 1   | S     | 3635  | 0        | 3724     | 70      | 0            |
| 1   | T     | 3642  | 0        | 3733     | 36      | 0            |
| 1   | U     | 3655  | 0        | 3734     | 62      | 0            |
| 2   | D     | 3549  | 0        | 3614     | 59      | 0            |
| 2   | E     | 3508  | 0        | 3550     | 51      | 0            |
| 2   | F     | 3531  | 0        | 3592     | 58      | 0            |
| 2   | M     | 3543  | 0        | 3603     | 49      | 0            |
| 2   | N     | 3545  | 0        | 3604     | 63      | 0            |
| 2   | O     | 3538  | 0        | 3606     | 47      | 0            |
| 2   | V     | 3550  | 0        | 3611     | 64      | 0            |
| 2   | W     | 3535  | 0        | 3605     | 47      | 0            |
| 2   | X     | 3547  | 0        | 3615     | 39      | 0            |
| 3   | G     | 2059  | 0        | 2127     | 43      | 0            |
| 3   | P     | 1872  | 0        | 1917     | 34      | 0            |
| 3   | Y     | 1523  | 0        | 1569     | 16      | 0            |
| 4   | H     | 763   | 0        | 653      | 21      | 0            |
| 4   | Q     | 454   | 0        | 259      | 2       | 0            |
| 4   | Z     | 85    | 0        | 45       | 0       | 0            |
| 5   | 1     | 145   | 0        | 87       | 0       | 0            |
| 5   | I     | 339   | 0        | 280      | 8       | 0            |
| 5   | R     | 189   | 0        | 114      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | A     | 31    | 0        | 13       | 1       | 0            |
| 6   | B     | 31    | 0        | 13       | 4       | 0            |
| 6   | C     | 31    | 0        | 13       | 0       | 0            |
| 6   | D     | 31    | 0        | 13       | 0       | 0            |
| 6   | F     | 31    | 0        | 13       | 1       | 0            |
| 6   | J     | 31    | 0        | 13       | 1       | 0            |
| 6   | K     | 31    | 0        | 13       | 3       | 0            |
| 6   | L     | 31    | 0        | 13       | 1       | 0            |
| 6   | M     | 31    | 0        | 13       | 4       | 0            |
| 6   | O     | 31    | 0        | 13       | 3       | 0            |
| 6   | S     | 31    | 0        | 13       | 0       | 0            |
| 6   | T     | 31    | 0        | 13       | 1       | 0            |
| 6   | U     | 31    | 0        | 13       | 1       | 0            |
| 6   | V     | 31    | 0        | 13       | 1       | 0            |
| 6   | X     | 31    | 0        | 13       | 4       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | C     | 1     | 0        | 0        | 0       | 0            |
| 7   | D     | 1     | 0        | 0        | 0       | 0            |
| 7   | F     | 1     | 0        | 0        | 0       | 0            |
| 7   | J     | 1     | 0        | 0        | 0       | 0            |
| 7   | K     | 1     | 0        | 0        | 0       | 0            |
| 7   | L     | 1     | 0        | 0        | 0       | 0            |
| 7   | M     | 1     | 0        | 0        | 0       | 0            |
| 7   | O     | 1     | 0        | 0        | 0       | 0            |
| 7   | S     | 1     | 0        | 0        | 0       | 0            |
| 7   | T     | 1     | 0        | 0        | 0       | 0            |
| 7   | U     | 1     | 0        | 0        | 0       | 0            |
| 7   | V     | 1     | 0        | 0        | 0       | 0            |
| 7   | X     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 72707 | 0        | 73348    | 1008    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1008) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 2:M:85:VAL:HG11 | 2:M:235:THR:HG23 | 1.30                     | 1.12              |
| 2:D:85:VAL:HG11 | 2:D:235:THR:HG23 | 1.15                     | 1.09              |
| 1:A:395:PHE:HZ  | 1:A:419:THR:HA   | 1.15                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:85:VAL:HG11  | 2:E:235:THR:HG23 | 1.38                     | 1.01              |
| 1:B:174:GLN:HA   | 6:B:600:ANP:HNB1 | 1.28                     | 0.97              |
| 1:A:395:PHE:CZ   | 1:A:419:THR:HA   | 2.00                     | 0.96              |
| 1:A:77:LEU:HD12  | 1:A:81:ASP:HB3   | 1.49                     | 0.95              |
| 3:P:205:VAL:H    | 3:P:206:PRO:HD2  | 1.30                     | 0.94              |
| 2:M:160:GLY:H    | 6:M:600:ANP:HNB1 | 1.03                     | 0.93              |
| 1:A:182:LEU:HD13 | 1:A:218:LEU:HD11 | 1.50                     | 0.92              |
| 1:S:293:ARG:HD3  | 1:S:339:TYR:HD1  | 1.36                     | 0.91              |
| 2:O:85:VAL:HG11  | 2:O:235:THR:HG23 | 1.51                     | 0.91              |
| 1:K:67:ASN:HB3   | 2:O:17:ILE:HD13  | 1.55                     | 0.89              |
| 1:L:182:LEU:HD13 | 1:L:218:LEU:HD11 | 1.55                     | 0.87              |
| 2:M:142:ASP:HB3  | 2:M:434:LEU:HD12 | 1.55                     | 0.86              |
| 5:I:55:GLU:CB    | 5:I:56:PRO:HD3   | 2.06                     | 0.86              |
| 2:V:85:VAL:HG11  | 2:V:235:THR:HG23 | 1.56                     | 0.86              |
| 2:D:85:VAL:CG1   | 2:D:235:THR:HG23 | 2.04                     | 0.85              |
| 1:S:293:ARG:HD3  | 1:S:339:TYR:CD1  | 2.11                     | 0.84              |
| 3:P:122:HIS:N    | 3:P:123:PRO:HD3  | 1.93                     | 0.84              |
| 1:S:146:GLU:OE1  | 1:S:313:LYS:HE2  | 1.77                     | 0.83              |
| 2:N:85:VAL:HG11  | 2:N:235:THR:HG23 | 1.60                     | 0.82              |
| 1:T:99:VAL:HG11  | 1:T:251:THR:HB   | 1.62                     | 0.82              |
| 2:M:182:SER:HB2  | 2:M:215:VAL:HG23 | 1.61                     | 0.81              |
| 2:W:85:VAL:HG11  | 2:W:235:THR:HG23 | 1.61                     | 0.81              |
| 3:P:205:VAL:N    | 3:P:206:PRO:HD2  | 1.97                     | 0.80              |
| 1:C:192:ASN:HA   | 1:C:200:LYS:HG2  | 1.65                     | 0.79              |
| 2:F:85:VAL:HG11  | 2:F:235:THR:HG23 | 1.64                     | 0.78              |
| 3:G:23:MET:HG3   | 3:G:237:MET:HG3  | 1.66                     | 0.78              |
| 1:S:112:ALA:O    | 1:S:251:THR:HG21 | 1.85                     | 0.77              |
| 1:K:444:VAL:HG23 | 1:K:445:PRO:HD3  | 1.67                     | 0.77              |
| 2:V:7:THR:HB     | 2:V:8:PRO:HD2    | 1.66                     | 0.77              |
| 1:B:174:GLN:HA   | 6:B:600:ANP:N3B  | 2.00                     | 0.76              |
| 2:D:371:ALA:O    | 2:D:375:GLN:HG3  | 1.86                     | 0.75              |
| 1:U:166:ARG:HD3  | 1:U:308:LEU:O    | 1.87                     | 0.75              |
| 1:J:469:SER:HB3  | 1:J:506:PHE:HZ   | 1.51                     | 0.74              |
| 2:N:391:LEU:HB3  | 2:N:395:GLU:HG3  | 1.68                     | 0.73              |
| 3:P:107:ILE:HG13 | 3:P:126:ILE:HA   | 1.71                     | 0.73              |
| 1:T:346:SER:HA   | 6:X:600:ANP:O1G  | 1.89                     | 0.73              |
| 3:G:89:SER:HA    | 3:G:117:GLN:HE21 | 1.53                     | 0.73              |
| 1:K:364:ARG:HD3  | 6:K:600:ANP:C2   | 2.18                     | 0.73              |
| 1:K:375:ARG:NH1  | 6:O:600:ANP:O2A  | 2.23                     | 0.71              |
| 1:S:116:PRO:HB3  | 1:S:123:ILE:HD11 | 1.71                     | 0.71              |
| 3:P:205:VAL:H    | 3:P:206:PRO:CD   | 2.03                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:ALA:HA   | 1:C:240:GLU:OE2  | 1.91                     | 0.70              |
| 2:E:140:VAL:HG13 | 2:E:414:LEU:HB3  | 1.73                     | 0.70              |
| 3:G:14:LYS:HA    | 3:G:248:ILE:HD11 | 1.73                     | 0.70              |
| 3:P:155:LYS:HG2  | 3:P:155:LYS:O    | 1.89                     | 0.70              |
| 2:V:154:GLY:HA3  | 2:V:329:LEU:HD13 | 1.71                     | 0.70              |
| 1:C:343:ASN:O    | 1:C:346:SER:HB2  | 1.91                     | 0.70              |
| 1:S:441:GLU:HG2  | 1:S:486:ARG:HB2  | 1.74                     | 0.70              |
| 1:U:146:GLU:HB3  | 1:U:163:ARG:HD2  | 1.74                     | 0.69              |
| 1:L:40:ILE:CD1   | 1:L:76:VAL:HG12  | 2.23                     | 0.69              |
| 2:W:244:ARG:HD3  | 2:W:304:VAL:HG23 | 1.75                     | 0.69              |
| 3:P:212:TYR:O    | 3:P:216:ASN:HB2  | 1.93                     | 0.69              |
| 2:E:168:GLN:HE21 | 2:E:201:MET:HG3  | 1.58                     | 0.69              |
| 1:L:52:GLU:OE1   | 2:M:68:GLU:HB3   | 1.92                     | 0.69              |
| 2:V:440:SER:O    | 2:V:444:VAL:HG23 | 1.93                     | 0.69              |
| 1:J:139:LEU:HD13 | 2:N:104:ASP:HA   | 1.75                     | 0.68              |
| 2:O:391:LEU:HB3  | 2:O:395:GLU:HG3  | 1.74                     | 0.68              |
| 1:A:149:GLN:OE1  | 1:A:440:THR:OG1  | 2.10                     | 0.68              |
| 1:B:398:GLN:HA   | 1:B:401:GLU:HG2  | 1.75                     | 0.68              |
| 3:G:23:MET:HA    | 3:G:26:VAL:HB    | 1.75                     | 0.68              |
| 1:A:174:GLN:HA   | 6:A:600:ANP:HNB1 | 1.59                     | 0.68              |
| 3:G:89:SER:HA    | 3:G:117:GLN:NE2  | 2.08                     | 0.68              |
| 2:N:237:LEU:HD22 | 2:N:292:LEU:HD12 | 1.74                     | 0.68              |
| 2:N:41:THR:HB    | 2:N:42:PRO:HD2   | 1.76                     | 0.68              |
| 3:G:77:ILE:HG21  | 3:G:222:MET:HG2  | 1.75                     | 0.68              |
| 2:X:163:LYS:N    | 6:X:600:ANP:O1B  | 2.27                     | 0.68              |
| 2:D:7:THR:HG23   | 2:D:7:THR:O      | 1.94                     | 0.67              |
| 2:N:279:PHE:HE1  | 3:P:263:ILE:HD12 | 1.59                     | 0.67              |
| 2:O:377:THR:HG22 | 2:O:407:ALA:HB2  | 1.76                     | 0.67              |
| 1:B:272:ASP:HB2  | 1:B:328:VAL:O    | 1.95                     | 0.67              |
| 2:E:133:ILE:HD12 | 2:E:146:PRO:HB2  | 1.76                     | 0.67              |
| 2:N:279:PHE:CE1  | 3:P:263:ILE:HD12 | 2.30                     | 0.67              |
| 2:F:346:PRO:HB2  | 2:F:348:VAL:HG23 | 1.77                     | 0.67              |
| 2:V:97:ASN:HD21  | 2:V:101:GLU:HB2  | 1.60                     | 0.67              |
| 1:B:36:VAL:HG11  | 1:B:84:VAL:O     | 1.94                     | 0.67              |
| 1:T:33:VAL:HB    | 1:T:87:GLY:H     | 1.60                     | 0.66              |
| 2:X:128:SER:HB2  | 2:X:300:LYS:HG3  | 1.78                     | 0.66              |
| 1:U:135:ALA:HB3  | 2:V:223:ASN:HD22 | 1.60                     | 0.66              |
| 2:D:26:GLU:OE2   | 2:D:26:GLU:HA    | 1.96                     | 0.65              |
| 1:J:192:ASN:HA   | 1:J:200:LYS:HG2  | 1.77                     | 0.65              |
| 1:S:73:VAL:HG22  | 2:W:72:ARG:HH12  | 1.60                     | 0.65              |
| 1:B:109:VAL:HG22 | 1:B:233:ILE:HB   | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:358:LEU:HB2  | 1:K:366:ALA:HB1  | 1.79                     | 0.65              |
| 1:K:99:VAL:HG11  | 1:K:251:THR:HB   | 1.79                     | 0.65              |
| 1:S:349:ASP:O    | 1:S:375:ARG:HB2  | 1.96                     | 0.65              |
| 1:B:166:ARG:HD3  | 1:B:308:LEU:O    | 1.96                     | 0.65              |
| 1:S:107:GLY:HA2  | 1:S:228:MET:O    | 1.96                     | 0.65              |
| 1:A:112:ALA:O    | 1:A:251:THR:HG21 | 1.97                     | 0.64              |
| 1:C:168:LEU:HB2  | 1:C:348:THR:HG21 | 1.79                     | 0.64              |
| 1:A:173:ARG:NH2  | 2:D:352:ASP:OD1  | 2.30                     | 0.64              |
| 1:J:70:PRO:HD3   | 2:N:15:ALA:HB2   | 1.78                     | 0.64              |
| 1:L:164:GLY:HA2  | 1:L:323:LEU:O    | 1.96                     | 0.64              |
| 2:O:264:ALA:HA   | 2:O:267:GLU:HG3  | 1.79                     | 0.64              |
| 1:T:101:VAL:HG12 | 1:T:255:ILE:HA   | 1.79                     | 0.64              |
| 2:E:98:VAL:HB    | 2:E:232:VAL:HG13 | 1.79                     | 0.64              |
| 2:N:405:GLU:HG2  | 2:N:409:LYS:HE2  | 1.80                     | 0.64              |
| 2:E:158:GLY:O    | 2:E:161:VAL:HG22 | 1.98                     | 0.64              |
| 1:A:329:ILE:HD11 | 1:A:344:VAL:HG21 | 1.80                     | 0.64              |
| 3:G:15:ASN:O     | 3:G:19:ILE:HG12  | 1.98                     | 0.64              |
| 1:L:290:PRO:HB2  | 2:M:270:ALA:HB1  | 1.79                     | 0.64              |
| 1:U:111:ASP:OD1  | 1:U:115:ASN:HB2  | 1.98                     | 0.64              |
| 2:F:41:THR:HB    | 2:F:42:PRO:HD2   | 1.79                     | 0.63              |
| 2:O:252:LEU:HD23 | 2:O:305:THR:HB   | 1.80                     | 0.63              |
| 2:F:15:ALA:HB3   | 2:F:22:ASP:HB2   | 1.81                     | 0.63              |
| 1:J:375:ARG:HH22 | 2:N:190:ARG:NE   | 1.97                     | 0.63              |
| 1:L:99:VAL:HG11  | 1:L:251:THR:HB   | 1.81                     | 0.63              |
| 2:F:33:ILE:O     | 2:F:34:LEU:HB2   | 1.99                     | 0.63              |
| 2:E:157:GLY:HA2  | 2:E:337:ARG:HH22 | 1.64                     | 0.63              |
| 1:J:223:GLU:HG3  | 1:J:228:MET:HG3  | 1.79                     | 0.63              |
| 3:P:42:LYS:HD3   | 3:P:42:LYS:O     | 1.99                     | 0.63              |
| 1:T:504:GLU:HA   | 1:T:507:VAL:HB   | 1.81                     | 0.63              |
| 1:U:176:GLY:O    | 1:U:180:VAL:HG23 | 1.98                     | 0.63              |
| 2:V:84:SER:HB3   | 2:V:114:ARG:HE   | 1.62                     | 0.63              |
| 2:V:189:GLU:O    | 2:V:222:MET:HG2  | 1.99                     | 0.62              |
| 2:M:224:GLU:O    | 2:M:229:ARG:HD3  | 1.99                     | 0.62              |
| 1:S:223:GLU:HG3  | 1:S:228:MET:HG3  | 1.81                     | 0.62              |
| 3:P:122:HIS:N    | 3:P:123:PRO:CD   | 2.63                     | 0.62              |
| 4:H:35:LYS:HD3   | 4:H:35:LYS:H     | 1.64                     | 0.62              |
| 2:W:133:ILE:HD12 | 2:W:146:PRO:HB2  | 1.82                     | 0.62              |
| 1:T:392:LEU:HD13 | 1:T:451:VAL:HG22 | 1.82                     | 0.62              |
| 2:E:15:ALA:HB3   | 2:E:22:ASP:HB2   | 1.82                     | 0.61              |
| 2:M:160:GLY:N    | 6:M:600:ANP:HNB1 | 1.87                     | 0.61              |
| 1:U:212:ARG:HG2  | 1:U:237:THR:HG21 | 1.80                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:345:TYR:HA   | 2:F:346:PRO:C    | 2.18                     | 0.61              |
| 2:F:148:ALA:HB2  | 2:F:357:LEU:HD11 | 1.82                     | 0.61              |
| 1:J:302:TYR:O    | 1:J:306:ARG:HB2  | 2.00                     | 0.61              |
| 2:N:244:ARG:HD3  | 2:N:304:VAL:HG23 | 1.81                     | 0.61              |
| 2:X:160:GLY:H    | 6:X:600:ANP:HNB1 | 1.46                     | 0.61              |
| 1:B:99:VAL:HG11  | 1:B:251:THR:HB   | 1.81                     | 0.61              |
| 2:D:197:LEU:O    | 2:D:201:MET:HG2  | 2.01                     | 0.61              |
| 1:J:469:SER:HB3  | 1:J:506:PHE:CZ   | 2.35                     | 0.61              |
| 2:E:39:ILE:HD13  | 2:E:70:LEU:HD21  | 1.83                     | 0.61              |
| 2:E:43:GLN:HG2   | 2:E:44:GLY:N     | 2.15                     | 0.61              |
| 1:B:148:VAL:HG23 | 1:B:163:ARG:HG2  | 1.83                     | 0.61              |
| 1:B:387:GLN:OE1  | 1:B:491:LEU:HB2  | 2.01                     | 0.61              |
| 1:K:173:ARG:HH12 | 2:N:327:ALA:HA   | 1.66                     | 0.61              |
| 2:N:458:TYR:HD2  | 2:N:459:MET:HG2  | 1.66                     | 0.61              |
| 1:J:306:ARG:HA   | 2:N:223:ASN:HB2  | 1.83                     | 0.60              |
| 2:V:252:LEU:HD23 | 2:V:305:THR:HB   | 1.83                     | 0.60              |
| 2:X:386:ASP:O    | 2:X:390:ILE:HG12 | 2.01                     | 0.60              |
| 2:W:15:ALA:HB3   | 2:W:22:ASP:HB2   | 1.83                     | 0.60              |
| 6:F:600:ANP:O5'  | 6:F:600:ANP:H8   | 2.01                     | 0.60              |
| 1:K:211:LYS:HD2  | 2:N:328:HIS:HA   | 1.83                     | 0.60              |
| 1:U:97:VAL:HG11  | 1:U:247:LEU:HD11 | 1.83                     | 0.60              |
| 3:G:115:LYS:O    | 3:G:119:LEU:HB2  | 2.01                     | 0.60              |
| 2:N:255:ILE:HB   | 2:N:308:GLN:HG2  | 1.81                     | 0.60              |
| 2:V:204:THR:HB   | 2:V:206:VAL:HG23 | 1.84                     | 0.60              |
| 1:S:145:HIS:H    | 1:S:313:LYS:HZ3  | 1.50                     | 0.60              |
| 1:L:116:PRO:HG3  | 1:L:123:ILE:HG12 | 1.84                     | 0.60              |
| 3:G:49:GLN:HE21  | 3:G:217:GLN:NE2  | 1.99                     | 0.60              |
| 3:G:205:VAL:O    | 3:G:209:LEU:HB2  | 2.02                     | 0.59              |
| 1:K:346:SER:HA   | 6:O:600:ANP:O3G  | 2.02                     | 0.59              |
| 1:T:220:GLN:HB2  | 2:W:129:THR:HB   | 1.84                     | 0.59              |
| 3:P:81:LYS:HE3   | 3:P:135:LYS:HD2  | 1.84                     | 0.59              |
| 1:J:173:ARG:HD2  | 1:J:174:GLN:HE21 | 1.66                     | 0.59              |
| 1:C:116:PRO:HG3  | 1:C:123:ILE:HG12 | 1.85                     | 0.59              |
| 1:L:248:ALA:HB3  | 1:L:249:PRO:HD3  | 1.85                     | 0.59              |
| 2:N:23:VAL:HG11  | 2:N:76:VAL:HG21  | 1.84                     | 0.59              |
| 1:A:77:LEU:CD1   | 1:A:81:ASP:HB3   | 2.29                     | 0.59              |
| 2:D:208:ASN:ND2  | 2:D:211:GLY:HA3  | 2.18                     | 0.59              |
| 2:M:234:LEU:CD2  | 2:M:292:LEU:HD13 | 2.33                     | 0.59              |
| 2:V:94:ARG:NH2   | 2:V:106:ARG:HB2  | 2.18                     | 0.59              |
| 2:M:371:ALA:O    | 2:M:375:GLN:HG3  | 2.03                     | 0.59              |
| 2:D:344:ILE:HG23 | 2:D:415:SER:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:34:LEU:HD21  | 1:K:44:PHE:HB2   | 1.85                     | 0.58              |
| 1:L:493:LYS:HA   | 1:L:496:LEU:HD12 | 1.85                     | 0.58              |
| 3:P:168:ASP:HB2  | 3:P:178:SER:OG   | 2.03                     | 0.58              |
| 2:V:64:MET:CE    | 2:V:99:ILE:HG22  | 2.33                     | 0.58              |
| 5:I:12:ALA:O     | 5:I:16:VAL:HG23  | 2.03                     | 0.58              |
| 1:A:239:SER:HB3  | 2:D:294:GLU:HG3  | 1.86                     | 0.58              |
| 2:F:146:PRO:O    | 2:F:355:SER:OG   | 2.21                     | 0.58              |
| 1:S:309:GLU:HG3  | 2:W:223:ASN:HB3  | 1.86                     | 0.58              |
| 1:U:206:VAL:HG13 | 1:U:234:VAL:HB   | 1.84                     | 0.58              |
| 2:X:384:LEU:O    | 2:X:388:ILE:HG12 | 2.04                     | 0.58              |
| 2:V:164:THR:O    | 2:V:167:ILE:HG22 | 2.04                     | 0.58              |
| 1:B:98:ASP:HB2   | 1:B:129:SER:O    | 2.04                     | 0.58              |
| 1:K:260:ARG:O    | 1:K:321:GLY:HA3  | 2.04                     | 0.58              |
| 1:K:364:ARG:HA   | 1:K:365:PRO:C    | 2.24                     | 0.58              |
| 1:L:148:VAL:HG21 | 1:L:324:THR:HG21 | 1.85                     | 0.58              |
| 2:O:449:TYR:HB3  | 2:O:452:ILE:HD12 | 1.86                     | 0.58              |
| 3:P:169:PRO:HG3  | 3:P:227:ALA:HB3  | 1.84                     | 0.58              |
| 3:Y:16:ILE:HA    | 3:Y:19:ILE:HG22  | 1.86                     | 0.58              |
| 2:V:182:SER:O    | 2:V:215:VAL:HA   | 2.04                     | 0.57              |
| 1:K:186:LEU:O    | 1:K:189:LYS:HE3  | 2.03                     | 0.57              |
| 2:X:178:HIS:HE2  | 2:X:250:ASP:HB3  | 1.69                     | 0.57              |
| 1:S:439:ALA:HB3  | 1:S:442:GLU:HG3  | 1.85                     | 0.57              |
| 1:T:67:ASN:HB3   | 2:X:17:ILE:HG23  | 1.86                     | 0.57              |
| 1:S:217:GLN:HG2  | 2:V:356:ARG:HH21 | 1.68                     | 0.57              |
| 1:A:146:GLU:HB2  | 1:A:163:ARG:HG3  | 1.87                     | 0.57              |
| 1:B:26:ASN:O     | 1:B:30:THR:HB    | 2.05                     | 0.57              |
| 2:D:15:ALA:HB3   | 2:D:22:ASP:HB2   | 1.87                     | 0.57              |
| 2:D:263:GLN:O    | 2:D:266:SER:HB3  | 2.05                     | 0.57              |
| 1:S:166:ARG:HD3  | 1:S:308:LEU:O    | 2.05                     | 0.57              |
| 1:U:243:PRO:HA   | 1:U:283:LEU:HD11 | 1.87                     | 0.57              |
| 2:V:339:ILE:HG22 | 2:V:344:ILE:HB   | 1.86                     | 0.57              |
| 2:F:189:GLU:O    | 2:F:221:GLN:HB3  | 2.04                     | 0.57              |
| 2:F:26:GLU:OE1   | 2:F:26:GLU:HA    | 2.04                     | 0.57              |
| 1:A:182:LEU:CD1  | 1:A:218:LEU:HD11 | 2.31                     | 0.56              |
| 2:V:345:TYR:HA   | 2:V:346:PRO:C    | 2.25                     | 0.56              |
| 2:V:162:GLY:HA2  | 6:V:600:ANP:H8   | 1.86                     | 0.56              |
| 2:O:345:TYR:HA   | 2:O:346:PRO:C    | 2.24                     | 0.56              |
| 2:X:85:VAL:HG11  | 2:X:235:THR:HG23 | 1.86                     | 0.56              |
| 1:A:383:LYS:O    | 1:A:387:GLN:HG3  | 2.06                     | 0.56              |
| 2:E:277:SER:OG   | 2:E:278:ALA:N    | 2.38                     | 0.56              |
| 2:O:237:LEU:HD13 | 2:O:296:ILE:HG12 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:W:319:ASP:HA   | 3:Y:260:GLN:HE22 | 1.69                     | 0.56              |
| 4:H:14:PHE:CB    | 4:H:22:TYR:HB2   | 2.35                     | 0.56              |
| 2:N:96:ILE:HB    | 2:N:218:VAL:HG22 | 1.87                     | 0.56              |
| 1:S:192:ASN:HA   | 1:S:200:LYS:HG2  | 1.88                     | 0.56              |
| 1:S:284:SER:O    | 1:S:289:ARG:HB2  | 2.06                     | 0.56              |
| 1:S:163:ARG:O    | 1:S:313:LYS:HE3  | 2.06                     | 0.56              |
| 1:S:265:HIS:ND1  | 1:S:322:SER:HB2  | 2.21                     | 0.56              |
| 4:H:14:PHE:CZ    | 4:H:70:ILE:HD11  | 2.40                     | 0.56              |
| 2:M:229:ARG:NH2  | 2:M:267:GLU:OE1  | 2.37                     | 0.56              |
| 1:A:55:VAL:HG21  | 1:A:75:ILE:HD13  | 1.87                     | 0.56              |
| 1:J:364:ARG:HA   | 1:J:365:PRO:C    | 2.26                     | 0.56              |
| 2:V:346:PRO:O    | 2:V:347:ALA:HB3  | 2.04                     | 0.56              |
| 5:I:55:GLU:CB    | 5:I:56:PRO:CD    | 2.83                     | 0.56              |
| 1:K:444:VAL:CG2  | 1:K:445:PRO:HD3  | 2.36                     | 0.56              |
| 2:N:51:ALA:O     | 2:N:52:GLN:HG3   | 2.06                     | 0.56              |
| 2:O:140:VAL:HG13 | 2:O:414:LEU:HB3  | 1.88                     | 0.56              |
| 1:U:378:SER:HB3  | 1:U:386:LYS:HE2  | 1.88                     | 0.56              |
| 1:C:450:GLY:HA2  | 1:C:455:LEU:HD12 | 1.87                     | 0.55              |
| 4:H:14:PHE:HB3   | 4:H:22:TYR:HB2   | 1.88                     | 0.55              |
| 1:K:488:LYS:HE3  | 1:K:490:GLU:HB2  | 1.88                     | 0.55              |
| 1:U:237:THR:H    | 1:U:240:GLU:HG3  | 1.71                     | 0.55              |
| 2:V:46:LEU:HD22  | 2:V:70:LEU:HD21  | 1.88                     | 0.55              |
| 3:Y:108:VAL:HG12 | 3:Y:130:ILE:HG13 | 1.88                     | 0.55              |
| 3:G:46:GLU:O     | 3:G:50:LEU:HB2   | 2.05                     | 0.55              |
| 1:S:36:VAL:HG21  | 1:S:84:VAL:HB    | 1.88                     | 0.55              |
| 1:S:484:GLU:HG2  | 1:S:495:LEU:HD11 | 1.87                     | 0.55              |
| 1:B:260:ARG:O    | 1:B:321:GLY:HA3  | 2.06                     | 0.55              |
| 1:U:169:ILE:HB   | 1:U:328:VAL:HG22 | 1.88                     | 0.55              |
| 1:B:105:LEU:O    | 1:B:232:ILE:HG12 | 2.07                     | 0.55              |
| 3:G:247:MET:HG3  | 3:G:250:ARG:HH21 | 1.71                     | 0.55              |
| 1:L:344:VAL:HA   | 1:L:347:ILE:HD12 | 1.89                     | 0.55              |
| 2:O:377:THR:HG23 | 2:O:403:THR:HG23 | 1.88                     | 0.55              |
| 2:V:192:ARG:NH1  | 2:V:193:GLU:HG2  | 2.22                     | 0.55              |
| 2:V:9:ILE:HB     | 2:V:78:ASP:HB3   | 1.89                     | 0.55              |
| 2:D:144:LEU:HD22 | 2:D:375:GLN:HE21 | 1.72                     | 0.55              |
| 1:L:306:ARG:HG2  | 1:L:307:LEU:N    | 2.21                     | 0.55              |
| 2:N:220:GLY:HA3  | 2:N:232:VAL:HG11 | 1.89                     | 0.55              |
| 3:P:111:GLY:HA2  | 3:P:133:ILE:HD11 | 1.88                     | 0.55              |
| 1:A:500:LYS:O    | 1:A:504:GLU:HG3  | 2.06                     | 0.55              |
| 4:H:72:GLY:O     | 4:H:87:ALA:HA    | 2.07                     | 0.55              |
| 2:V:15:ALA:HB3   | 2:V:22:ASP:HB2   | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:52:GLN:HG2   | 2:F:60:ARG:HB3   | 1.89                     | 0.55              |
| 2:O:324:THR:O    | 2:O:324:THR:HG22 | 2.07                     | 0.55              |
| 1:T:67:ASN:HB2   | 2:X:17:ILE:HG12  | 1.89                     | 0.55              |
| 1:B:444:VAL:HG22 | 1:B:445:PRO:HD3  | 1.88                     | 0.54              |
| 1:C:503:THR:O    | 1:C:507:VAL:HG23 | 2.07                     | 0.54              |
| 2:X:167:ILE:HD12 | 2:X:309:ALA:HB2  | 1.89                     | 0.54              |
| 2:M:440:SER:OG   | 2:M:463:ILE:HG12 | 2.07                     | 0.54              |
| 2:V:346:PRO:O    | 2:V:347:ALA:CB   | 2.55                     | 0.54              |
| 2:X:258:ILE:HD13 | 2:X:308:GLN:OE1  | 2.07                     | 0.54              |
| 1:L:222:LEU:HD12 | 1:L:228:MET:HE2  | 1.90                     | 0.54              |
| 1:B:359:PHE:HZ   | 6:B:600:ANP:O4'  | 1.90                     | 0.54              |
| 1:S:311:ALA:HA   | 1:S:323:LEU:HB3  | 1.90                     | 0.54              |
| 1:S:55:VAL:HG21  | 1:S:75:ILE:HD13  | 1.89                     | 0.54              |
| 1:T:282:GLN:O    | 1:T:286:LEU:HG   | 2.08                     | 0.54              |
| 2:E:321:ALA:HB3  | 2:E:322:PRO:CD   | 2.37                     | 0.54              |
| 1:L:196:ASP:OD1  | 1:L:198:SER:OG   | 2.23                     | 0.54              |
| 1:L:174:GLN:HA   | 6:L:600:ANP:HNB1 | 1.73                     | 0.54              |
| 2:N:169:GLU:HG2  | 2:N:418:PHE:CD1  | 2.42                     | 0.54              |
| 3:P:205:VAL:N    | 3:P:206:PRO:CD   | 2.66                     | 0.54              |
| 3:P:229:GLU:HG3  | 3:P:230:ILE:N    | 2.23                     | 0.54              |
| 2:D:299:THR:OG1  | 2:D:300:LYS:N    | 2.41                     | 0.54              |
| 3:G:118:LEU:HB3  | 3:G:126:ILE:HD11 | 1.90                     | 0.54              |
| 5:I:19:GLN:HE22  | 5:I:38:SER:HB3   | 1.73                     | 0.54              |
| 1:J:332:GLN:HB3  | 2:M:318:THR:HB   | 1.89                     | 0.54              |
| 1:U:165:GLN:HG2  | 1:U:166:ARG:H    | 1.73                     | 0.54              |
| 2:D:237:LEU:HD13 | 2:D:296:ILE:HG12 | 1.90                     | 0.54              |
| 1:U:56:GLU:HG2   | 1:U:62:LYS:HG2   | 1.90                     | 0.54              |
| 3:Y:91:LEU:HD12  | 3:Y:177:PRO:HB3  | 1.89                     | 0.54              |
| 1:A:111:ASP:OD2  | 1:A:115:ASN:HB2  | 2.08                     | 0.54              |
| 1:C:429:LEU:HD11 | 1:C:446:LEU:HB3  | 1.90                     | 0.54              |
| 2:W:388:ILE:HD12 | 2:W:393:MET:HG2  | 1.90                     | 0.54              |
| 3:P:86:SER:HB2   | 3:P:90:GLN:HG3   | 1.90                     | 0.53              |
| 1:S:462:ARG:HH11 | 1:S:465:GLU:HG3  | 1.73                     | 0.53              |
| 2:X:237:LEU:HD13 | 2:X:296:ILE:HG12 | 1.89                     | 0.53              |
| 2:E:344:ILE:HG23 | 2:E:415:SER:HB3  | 1.89                     | 0.53              |
| 2:M:321:ALA:HB3  | 2:M:322:PRO:CD   | 2.38                     | 0.53              |
| 1:S:402:VAL:HA   | 1:S:405:PHE:HD1  | 1.73                     | 0.53              |
| 2:X:345:TYR:HA   | 2:X:346:PRO:C    | 2.29                     | 0.53              |
| 1:T:305:SER:HB2  | 2:X:222:MET:HB2  | 1.90                     | 0.53              |
| 1:K:217:GLN:NE2  | 2:N:131:ALA:HB2  | 2.24                     | 0.53              |
| 2:N:131:ALA:HB1  | 2:N:357:LEU:HD11 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:87:ILE:HG23  | 3:G:167:ASN:ND2  | 2.24                     | 0.53              |
| 2:V:237:LEU:HD13 | 2:V:296:ILE:HG12 | 1.91                     | 0.53              |
| 2:D:33:ILE:O     | 2:D:34:LEU:HB2   | 2.08                     | 0.53              |
| 1:J:253:ALA:O    | 1:J:257:GLU:HG3  | 2.08                     | 0.53              |
| 2:O:15:ALA:HB3   | 2:O:22:ASP:HB2   | 1.91                     | 0.53              |
| 1:S:187:ASN:O    | 1:S:190:ARG:HG3  | 2.08                     | 0.53              |
| 1:U:249:PRO:HB3  | 1:U:270:TYR:HD1  | 1.73                     | 0.53              |
| 2:V:346:PRO:HD3  | 2:V:416:GLN:H    | 1.74                     | 0.53              |
| 2:W:170:LEU:O    | 2:W:174:ILE:HG12 | 2.09                     | 0.53              |
| 3:G:77:ILE:HD13  | 3:G:110:ILE:HD12 | 1.90                     | 0.53              |
| 2:V:321:ALA:HB3  | 2:V:322:PRO:CD   | 2.39                     | 0.53              |
| 4:H:57:VAL:CG2   | 4:H:70:ILE:HD12  | 2.38                     | 0.53              |
| 2:E:228:ALA:O    | 2:E:232:VAL:HG22 | 2.09                     | 0.53              |
| 2:M:425:THR:CG2  | 6:M:600:ANP:H2   | 2.39                     | 0.53              |
| 1:K:301:PHE:CB   | 2:O:263:GLN:HE22 | 2.21                     | 0.53              |
| 1:A:257:GLU:HG2  | 1:A:260:ARG:CZ   | 2.39                     | 0.52              |
| 2:V:189:GLU:O    | 2:V:221:GLN:HB3  | 2.09                     | 0.52              |
| 1:J:108:ARG:NH2  | 1:J:121:GLY:O    | 2.37                     | 0.52              |
| 1:U:354:LEU:HA   | 1:U:366:ALA:O    | 2.08                     | 0.52              |
| 1:K:148:VAL:HB   | 1:K:161:ILE:HB   | 1.91                     | 0.52              |
| 3:P:133:ILE:O    | 3:P:135:LYS:N    | 2.35                     | 0.52              |
| 1:S:118:ASP:OD1  | 1:S:120:LYS:HD2  | 2.09                     | 0.52              |
| 1:U:54:LEU:HD21  | 1:U:97:VAL:HG13  | 1.90                     | 0.52              |
| 1:L:54:LEU:O     | 1:L:93:THR:HB    | 2.10                     | 0.52              |
| 2:M:336:SER:HB3  | 2:M:339:ILE:HG13 | 1.91                     | 0.52              |
| 3:Y:79:SER:HB3   | 3:Y:88:HIS:HE1   | 1.73                     | 0.52              |
| 2:N:384:LEU:O    | 2:N:388:ILE:HG12 | 2.08                     | 0.52              |
| 2:V:192:ARG:HH11 | 2:V:193:GLU:HG2  | 1.74                     | 0.52              |
| 1:C:43:VAL:HG21  | 1:C:75:ILE:HD12  | 1.90                     | 0.52              |
| 2:D:158:GLY:O    | 2:D:161:VAL:HG22 | 2.09                     | 0.52              |
| 2:O:221:GLN:OE1  | 2:O:221:GLN:HA   | 2.10                     | 0.52              |
| 1:A:478:HIS:HB3  | 1:A:481:LEU:HD21 | 1.91                     | 0.52              |
| 1:C:189:LYS:HE3  | 1:C:226:ASP:HB3  | 1.91                     | 0.52              |
| 2:D:244:ARG:HD2  | 2:D:299:THR:HG22 | 1.91                     | 0.52              |
| 3:G:49:GLN:HE21  | 3:G:217:GLN:HE22 | 1.57                     | 0.52              |
| 2:N:152:LYS:HE2  | 2:N:293:GLN:O    | 2.10                     | 0.52              |
| 2:N:184:PHE:HB3  | 2:N:217:LEU:HD23 | 1.90                     | 0.52              |
| 2:N:98:VAL:HG13  | 2:N:99:ILE:HG23  | 1.90                     | 0.52              |
| 1:S:311:ALA:HB1  | 1:S:323:LEU:O    | 2.10                     | 0.52              |
| 1:C:103:PRO:HD3  | 1:C:258:TRP:CH2  | 2.45                     | 0.51              |
| 2:E:136:THR:HG23 | 2:E:138:ILE:H    | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:421:VAL:O    | 1:J:425:ARG:HD2  | 2.10                     | 0.51              |
| 3:P:168:ASP:N    | 3:P:176:GLU:O    | 2.40                     | 0.51              |
| 1:U:249:PRO:HB3  | 1:U:270:TYR:CD1  | 2.45                     | 0.51              |
| 1:L:481:LEU:HD13 | 1:L:495:LEU:HD22 | 1.91                     | 0.51              |
| 1:J:135:ALA:HB3  | 2:N:223:ASN:ND2  | 2.25                     | 0.51              |
| 1:T:77:LEU:O     | 1:T:243:PRO:HG2  | 2.11                     | 0.51              |
| 1:U:150:THR:HA   | 1:U:184:THR:HG23 | 1.91                     | 0.51              |
| 1:U:211:LYS:HE3  | 1:U:213:SER:HB2  | 1.92                     | 0.51              |
| 2:W:370:VAL:O    | 2:W:374:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:77:LEU:HD12  | 1:A:81:ASP:CB    | 2.33                     | 0.51              |
| 1:K:269:VAL:HG22 | 1:K:326:LEU:HB2  | 1.91                     | 0.51              |
| 1:L:187:ASN:O    | 1:L:190:ARG:HG3  | 2.09                     | 0.51              |
| 2:F:176:LYS:HE2  | 2:F:204:THR:HB   | 1.93                     | 0.51              |
| 4:H:33:PRO:HB3   | 4:H:38:ARG:NH1   | 2.26                     | 0.51              |
| 1:J:174:GLN:HA   | 6:J:600:ANP:HNB1 | 1.74                     | 0.51              |
| 1:K:354:LEU:HA   | 1:K:366:ALA:O    | 2.11                     | 0.51              |
| 1:K:66:LEU:HD21  | 1:K:289:ARG:HH22 | 1.75                     | 0.51              |
| 1:L:222:LEU:HD12 | 1:L:228:MET:CE   | 2.40                     | 0.51              |
| 1:U:258:TRP:O    | 1:U:262:ASN:ND2  | 2.44                     | 0.51              |
| 2:V:133:ILE:HD11 | 2:V:434:LEU:HD13 | 1.92                     | 0.51              |
| 2:E:50:VAL:HA    | 2:E:61:THR:HG22  | 1.91                     | 0.51              |
| 2:O:37:LEU:HD12  | 2:O:61:THR:HG21  | 1.91                     | 0.51              |
| 1:S:99:VAL:HG21  | 1:S:251:THR:HG23 | 1.92                     | 0.51              |
| 1:S:422:ARG:HH21 | 1:S:453:GLY:HA3  | 1.75                     | 0.51              |
| 1:A:142:ARG:HD3  | 1:A:143:SER:O    | 2.11                     | 0.51              |
| 1:A:153:LYS:NZ   | 1:A:467:GLU:OE1  | 2.42                     | 0.51              |
| 1:A:391:SER:O    | 1:A:394:LEU:HB2  | 2.10                     | 0.51              |
| 1:C:159:VAL:HG21 | 1:C:352:ILE:HG12 | 1.92                     | 0.51              |
| 2:D:7:THR:CG2    | 2:D:7:THR:O      | 2.59                     | 0.51              |
| 3:G:110:ILE:HA   | 3:G:130:ILE:HB   | 1.93                     | 0.51              |
| 1:J:243:PRO:HD3  | 1:J:283:LEU:HD21 | 1.93                     | 0.51              |
| 2:M:62:ILE:HD11  | 2:M:272:LEU:HD11 | 1.93                     | 0.51              |
| 2:M:425:THR:HG23 | 6:M:600:ANP:H2   | 1.93                     | 0.51              |
| 1:S:422:ARG:HE   | 1:S:453:GLY:HA2  | 1.76                     | 0.51              |
| 3:G:165:PHE:CE2  | 3:G:179:GLU:HB2  | 2.46                     | 0.51              |
| 2:W:220:GLY:HA3  | 2:W:232:VAL:HG11 | 1.92                     | 0.51              |
| 2:D:64:MET:CE    | 2:D:228:ALA:HA   | 2.41                     | 0.50              |
| 1:J:50:GLN:HB3   | 2:N:69:GLY:HA2   | 1.92                     | 0.50              |
| 2:D:408:ARG:O    | 2:D:412:ARG:HD2  | 2.11                     | 0.50              |
| 1:J:375:ARG:HH22 | 2:N:190:ARG:CZ   | 2.25                     | 0.50              |
| 1:K:421:VAL:O    | 1:K:425:ARG:HG2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:168:GLN:HE21 | 2:N:201:MET:HG2  | 1.77                     | 0.50              |
| 2:V:298:THR:HG23 | 2:V:303:SER:HA   | 1.93                     | 0.50              |
| 2:V:82:PRO:HB3   | 2:V:118:HIS:HD2  | 1.76                     | 0.50              |
| 2:W:140:VAL:HG22 | 2:W:414:LEU:O    | 2.12                     | 0.50              |
| 1:A:444:VAL:HG22 | 1:A:445:PRO:HD3  | 1.92                     | 0.50              |
| 1:K:174:GLN:HA   | 6:K:600:ANP:N3B  | 2.27                     | 0.50              |
| 1:K:32:ARG:HD2   | 1:K:87:GLY:O     | 2.11                     | 0.50              |
| 2:D:20:ILE:HG13  | 2:D:271:LEU:HB3  | 1.93                     | 0.50              |
| 2:D:148:ALA:HA   | 2:D:357:LEU:HD11 | 1.93                     | 0.50              |
| 1:S:481:LEU:O    | 1:S:485:ILE:HG13 | 2.12                     | 0.50              |
| 2:X:321:ALA:HB3  | 2:X:322:PRO:CD   | 2.42                     | 0.50              |
| 1:B:421:VAL:O    | 1:B:425:ARG:HG2  | 2.12                     | 0.50              |
| 1:C:107:GLY:HA2  | 1:C:228:MET:O    | 2.11                     | 0.50              |
| 2:E:243:PHE:O    | 2:E:247:GLU:HB2  | 2.12                     | 0.50              |
| 4:H:57:VAL:HG21  | 4:H:70:ILE:HD12  | 1.93                     | 0.50              |
| 3:G:205:VAL:HB   | 3:G:206:PRO:HD3  | 1.93                     | 0.50              |
| 2:M:20:ILE:HG13  | 2:M:271:LEU:HB3  | 1.94                     | 0.50              |
| 1:A:282:GLN:HG3  | 2:D:283:PRO:O    | 2.11                     | 0.50              |
| 1:S:248:ALA:HB3  | 1:S:249:PRO:HD3  | 1.92                     | 0.50              |
| 2:W:242:TYR:CE1  | 2:W:246:GLU:HG3  | 2.47                     | 0.50              |
| 2:W:284:THR:HB   | 2:W:288:ASP:OD1  | 2.12                     | 0.50              |
| 1:C:219:VAL:HB   | 1:C:228:MET:HE3  | 1.94                     | 0.49              |
| 3:P:162:ILE:HB   | 3:P:182:ILE:HB   | 1.94                     | 0.49              |
| 1:S:287:LEU:HB2  | 1:S:289:ARG:HD2  | 1.94                     | 0.49              |
| 3:Y:150:LEU:HA   | 3:Y:154:MET:HB2  | 1.93                     | 0.49              |
| 1:B:168:LEU:HB2  | 1:B:348:THR:HG21 | 1.94                     | 0.49              |
| 2:D:218:VAL:HG21 | 2:D:236:GLY:HA2  | 1.94                     | 0.49              |
| 4:H:14:PHE:HZ    | 4:H:70:ILE:HD11  | 1.76                     | 0.49              |
| 2:V:33:ILE:O     | 2:V:34:LEU:HB2   | 2.12                     | 0.49              |
| 3:Y:263:ILE:O    | 3:Y:267:LEU:HB3  | 2.13                     | 0.49              |
| 1:L:197:GLU:HA   | 1:L:200:LYS:HD2  | 1.95                     | 0.49              |
| 2:W:419:ALA:HA   | 2:W:429:GLY:HA3  | 1.92                     | 0.49              |
| 3:G:118:LEU:HA   | 3:G:121:THR:HG22 | 1.94                     | 0.49              |
| 1:K:109:VAL:HG22 | 1:K:233:ILE:HB   | 1.93                     | 0.49              |
| 1:K:273:LEU:HD22 | 1:K:276:GLN:OE1  | 2.13                     | 0.49              |
| 2:N:253:LEU:O    | 2:N:306:SER:HA   | 2.13                     | 0.49              |
| 2:D:201:MET:HE2  | 2:D:217:LEU:HD21 | 1.93                     | 0.49              |
| 1:T:138:ILE:HD13 | 2:X:95:ILE:HG21  | 1.93                     | 0.49              |
| 2:N:359:ASP:O    | 2:N:363:VAL:HG22 | 2.12                     | 0.49              |
| 2:X:178:HIS:NE2  | 2:X:250:ASP:HB3  | 2.27                     | 0.49              |
| 2:D:201:MET:HE1  | 2:D:215:VAL:HG11 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:117:ILE:HD12 | 2:E:124:PHE:HB3  | 1.95                     | 0.49              |
| 2:F:140:VAL:HG12 | 2:F:414:LEU:HD22 | 1.94                     | 0.49              |
| 1:L:166:ARG:HH21 | 1:L:349:ASP:CG   | 2.16                     | 0.49              |
| 2:N:410:ILE:HG23 | 2:N:441:PHE:HE2  | 1.77                     | 0.49              |
| 1:L:338:ALA:O    | 1:L:342:THR:OG1  | 2.31                     | 0.49              |
| 2:M:152:LYS:HD3  | 2:M:328:HIS:O    | 2.12                     | 0.49              |
| 2:N:220:GLY:CA   | 2:N:232:VAL:HG11 | 2.42                     | 0.49              |
| 1:J:428:GLN:HA   | 1:J:431:LYS:HD2  | 1.94                     | 0.49              |
| 1:L:441:GLU:OE2  | 1:L:486:ARG:HD3  | 2.13                     | 0.49              |
| 1:L:484:GLU:HB3  | 1:L:495:LEU:HD11 | 1.95                     | 0.49              |
| 3:P:150:LEU:HA   | 3:P:154:MET:HB2  | 1.95                     | 0.49              |
| 1:T:103:PRO:HD3  | 1:T:258:TRP:CZ2  | 2.48                     | 0.49              |
| 2:W:33:ILE:O     | 2:W:34:LEU:HB2   | 2.12                     | 0.49              |
| 2:E:33:ILE:O     | 2:E:34:LEU:HB2   | 2.13                     | 0.48              |
| 5:I:28:GLU:O     | 5:I:30:GLN:N     | 2.42                     | 0.48              |
| 1:U:242:ALA:HB3  | 1:U:243:PRO:HD3  | 1.95                     | 0.48              |
| 1:U:285:LEU:HD11 | 1:U:295:ALA:HB1  | 1.95                     | 0.48              |
| 2:F:84:SER:HB2   | 2:F:114:ARG:HH11 | 1.78                     | 0.48              |
| 1:S:441:GLU:CG   | 1:S:486:ARG:HB2  | 2.41                     | 0.48              |
| 1:S:39:GLY:HA2   | 1:S:77:LEU:HD12  | 1.94                     | 0.48              |
| 1:B:445:PRO:HB3  | 1:B:499:LEU:HD11 | 1.95                     | 0.48              |
| 3:G:75:VAL:HB    | 3:G:164:ILE:HD13 | 1.95                     | 0.48              |
| 1:J:173:ARG:HH11 | 1:J:174:GLN:HE21 | 1.60                     | 0.48              |
| 1:L:161:ILE:HA   | 1:L:165:GLN:OE1  | 2.13                     | 0.48              |
| 2:M:234:LEU:HD22 | 2:M:292:LEU:HD13 | 1.96                     | 0.48              |
| 1:U:166:ARG:HG2  | 1:U:325:ALA:HB3  | 1.95                     | 0.48              |
| 2:D:34:LEU:HD22  | 2:D:118:HIS:CE1  | 2.49                     | 0.48              |
| 2:F:9:ILE:HG23   | 2:F:27:GLN:NE2   | 2.28                     | 0.48              |
| 2:O:346:PRO:HB2  | 2:O:348:VAL:HG23 | 1.95                     | 0.48              |
| 1:S:340:ILE:HB   | 1:S:341:PRO:HD3  | 1.95                     | 0.48              |
| 2:D:384:LEU:O    | 2:D:388:ILE:HG12 | 2.13                     | 0.48              |
| 2:E:456:ALA:HA   | 2:E:469:LYS:HD3  | 1.96                     | 0.48              |
| 3:G:17:GLU:O     | 3:G:21:LYS:HB2   | 2.14                     | 0.48              |
| 3:G:267:LEU:O    | 3:G:271:ILE:HG12 | 2.14                     | 0.48              |
| 2:M:335:LEU:HA   | 2:M:347:ALA:O    | 2.13                     | 0.48              |
| 1:A:394:LEU:O    | 1:A:397:ALA:HB3  | 2.13                     | 0.48              |
| 1:C:88:GLU:HG3   | 1:C:89:LEU:N     | 2.28                     | 0.48              |
| 1:K:51:ALA:O     | 1:K:52:GLU:HB2   | 2.13                     | 0.48              |
| 2:O:165:VAL:HG23 | 6:O:600:ANP:O1A  | 2.13                     | 0.48              |
| 1:C:481:LEU:HD21 | 1:C:498:SER:HB3  | 1.95                     | 0.48              |
| 2:D:386:ASP:OD1  | 2:D:386:ASP:N    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:10:THR:HG21  | 2:E:75:LYS:HE2   | 1.96                     | 0.48              |
| 1:K:478:HIS:HB3  | 1:K:481:LEU:HG   | 1.96                     | 0.48              |
| 2:N:252:LEU:HA   | 2:N:305:THR:O    | 2.14                     | 0.48              |
| 2:X:85:VAL:CG1   | 2:X:235:THR:HG23 | 2.44                     | 0.48              |
| 1:A:134:LYS:HE2  | 2:E:65:ASP:OD1   | 2.13                     | 0.48              |
| 4:H:88:ILE:HD11  | 5:I:14:LEU:HB3   | 1.95                     | 0.48              |
| 1:K:152:LEU:HD22 | 1:K:365:PRO:HG3  | 1.96                     | 0.48              |
| 2:V:190:ARG:HB2  | 2:V:193:GLU:HG3  | 1.96                     | 0.48              |
| 1:B:345:ILE:HG12 | 1:B:351:GLN:HG2  | 1.94                     | 0.48              |
| 1:L:172:ASP:O    | 1:L:177:LYS:NZ   | 2.47                     | 0.48              |
| 2:M:143:LEU:O    | 2:M:367:HIS:HE1  | 1.97                     | 0.48              |
| 1:S:47:ASN:HA    | 2:W:72:ARG:HH21  | 1.79                     | 0.48              |
| 2:D:47:VAL:HG21  | 2:D:99:ILE:HG21  | 1.95                     | 0.48              |
| 2:E:221:GLN:HB2  | 2:E:223:ASN:OD1  | 2.14                     | 0.48              |
| 2:N:330:ASP:O    | 2:N:356:ARG:HD3  | 2.14                     | 0.48              |
| 1:S:395:PHE:HE1  | 1:S:422:ARG:HH11 | 1.61                     | 0.48              |
| 1:A:395:PHE:HZ   | 1:A:419:THR:CA   | 2.06                     | 0.47              |
| 1:B:291:PRO:HG2  | 3:G:268:VAL:HG22 | 1.96                     | 0.47              |
| 4:H:88:ILE:CD1   | 5:I:14:LEU:HB3   | 2.44                     | 0.47              |
| 2:X:190:ARG:NH1  | 6:X:600:ANP:O3G  | 2.45                     | 0.47              |
| 1:A:272:ASP:HB2  | 1:A:328:VAL:O    | 2.14                     | 0.47              |
| 1:K:428:GLN:O    | 1:K:431:LYS:HB2  | 2.14                     | 0.47              |
| 1:B:46:LEU:HD22  | 1:B:92:ARG:HG3   | 1.96                     | 0.47              |
| 2:F:67:THR:HB    | 2:F:70:LEU:HD12  | 1.96                     | 0.47              |
| 1:L:108:ARG:NH2  | 1:L:120:LYS:HB2  | 2.28                     | 0.47              |
| 1:S:260:ARG:O    | 1:S:321:GLY:HA3  | 2.13                     | 0.47              |
| 1:T:355:GLU:HB3  | 1:T:358:LEU:HD12 | 1.97                     | 0.47              |
| 1:B:26:ASN:ND2   | 1:B:26:ASN:H     | 2.13                     | 0.47              |
| 1:J:100:PRO:HD3  | 1:J:128:ARG:NH1  | 2.30                     | 0.47              |
| 1:L:55:VAL:HG21  | 1:L:75:ILE:HD13  | 1.96                     | 0.47              |
| 2:M:167:ILE:HD12 | 2:M:309:ALA:HB2  | 1.96                     | 0.47              |
| 2:N:184:PHE:HA   | 2:N:254:PHE:HB2  | 1.96                     | 0.47              |
| 1:T:413:ASP:O    | 1:T:417:LYS:HB2  | 2.15                     | 0.47              |
| 2:V:397:SER:HB3  | 2:V:400:ASP:HB2  | 1.95                     | 0.47              |
| 1:C:80:SER:OG    | 1:C:82:ARG:HG2   | 2.13                     | 0.47              |
| 2:F:263:GLN:O    | 2:F:267:GLU:HG3  | 2.15                     | 0.47              |
| 1:L:506:PHE:O    | 1:L:509:THR:HA   | 2.15                     | 0.47              |
| 1:S:142:ARG:HG2  | 1:S:143:SER:N    | 2.29                     | 0.47              |
| 1:B:213:SER:O    | 1:B:217:GLN:HG3  | 2.15                     | 0.47              |
| 1:J:388:VAL:HG21 | 1:J:444:VAL:HB   | 1.96                     | 0.47              |
| 2:N:127:GLN:HE22 | 2:N:297:THR:HG21 | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:136:ASP:N    | 3:P:136:ASP:OD2  | 2.48                     | 0.47              |
| 1:K:271:ASP:HA   | 1:K:272:ASP:HA   | 1.62                     | 0.47              |
| 2:M:416:GLN:HA   | 2:M:417:PRO:HD2  | 1.78                     | 0.47              |
| 1:C:364:ARG:HA   | 1:C:365:PRO:C    | 2.34                     | 0.47              |
| 5:I:31:THR:HG22  | 5:I:34:VAL:HG23  | 1.97                     | 0.47              |
| 1:L:280:TYR:CD2  | 1:L:303:LEU:HD22 | 2.50                     | 0.47              |
| 1:S:309:GLU:OE1  | 2:W:191:THR:OG1  | 2.26                     | 0.47              |
| 2:V:330:ASP:O    | 2:V:356:ARG:HG2  | 2.14                     | 0.47              |
| 2:W:220:GLY:CA   | 2:W:232:VAL:HG11 | 2.45                     | 0.47              |
| 3:Y:116:MET:HA   | 3:Y:119:LEU:HB2  | 1.95                     | 0.47              |
| 1:A:354:LEU:HA   | 1:A:366:ALA:O    | 2.15                     | 0.47              |
| 2:F:346:PRO:C    | 2:F:348:VAL:H    | 2.18                     | 0.47              |
| 1:J:205:TYR:HB3  | 1:J:233:ILE:HD13 | 1.97                     | 0.47              |
| 1:U:46:LEU:HD22  | 1:U:92:ARG:HG3   | 1.97                     | 0.47              |
| 2:W:98:VAL:HG13  | 2:W:99:ILE:HG23  | 1.95                     | 0.47              |
| 1:A:82:ARG:O     | 1:A:82:ARG:HG2   | 2.14                     | 0.47              |
| 1:B:202:TYR:O    | 1:B:266:ALA:HA   | 2.15                     | 0.47              |
| 1:C:187:ASN:O    | 1:C:190:ARG:HG3  | 2.14                     | 0.47              |
| 2:D:189:GLU:O    | 2:D:222:MET:HG2  | 2.14                     | 0.47              |
| 2:F:164:THR:O    | 2:F:168:GLN:HG3  | 2.15                     | 0.47              |
| 3:G:81:LYS:HD2   | 3:G:134:GLY:O    | 2.14                     | 0.47              |
| 2:M:158:GLY:O    | 2:M:163:LYS:NZ   | 2.48                     | 0.47              |
| 1:S:168:LEU:HD12 | 1:S:327:PRO:O    | 2.15                     | 0.47              |
| 2:F:289:MET:SD   | 2:F:324:THR:HG22 | 2.55                     | 0.46              |
| 2:F:394:ASP:HB3  | 3:G:85:GLY:O     | 2.15                     | 0.46              |
| 1:S:168:LEU:HD21 | 1:S:170:ILE:HD12 | 1.96                     | 0.46              |
| 2:V:136:THR:HG21 | 2:V:147:TYR:CD2  | 2.49                     | 0.46              |
| 2:V:315:ASP:OD2  | 2:V:337:ARG:NE   | 2.33                     | 0.46              |
| 2:V:373:LYS:HG2  | 2:V:445:LEU:HD22 | 1.97                     | 0.46              |
| 1:C:42:ARG:HE    | 1:C:72:GLN:HE22  | 1.61                     | 0.46              |
| 2:E:136:THR:HG22 | 2:E:142:ASP:CG   | 2.36                     | 0.46              |
| 2:E:188:GLY:O    | 2:E:222:MET:HG3  | 2.16                     | 0.46              |
| 3:G:56:GLU:O     | 3:G:58:LYS:HD3   | 2.15                     | 0.46              |
| 1:J:164:GLY:HA2  | 1:J:323:LEU:O    | 2.15                     | 0.46              |
| 1:J:459:GLU:HG3  | 1:J:462:ARG:HG3  | 1.97                     | 0.46              |
| 1:B:51:ALA:O     | 1:B:52:GLU:HB2   | 2.16                     | 0.46              |
| 3:G:180:LYS:HZ1  | 3:G:220:THR:HB   | 1.80                     | 0.46              |
| 1:J:270:TYR:O    | 1:J:272:ASP:HA   | 2.15                     | 0.46              |
| 1:S:272:ASP:HB2  | 1:S:328:VAL:O    | 2.15                     | 0.46              |
| 1:A:445:PRO:HB3  | 1:A:499:LEU:HD11 | 1.98                     | 0.46              |
| 1:C:349:ASP:O    | 1:C:375:ARG:HB2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:338:ALA:HB3  | 1:K:341:PRO:HG2  | 1.98                     | 0.46              |
| 2:O:245:ASP:OD1  | 2:O:301:LYS:HD3  | 2.15                     | 0.46              |
| 1:S:206:VAL:HG22 | 1:S:252:ALA:CB   | 2.46                     | 0.46              |
| 2:V:96:ILE:HB    | 2:V:218:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:391:SER:O    | 1:A:394:LEU:N    | 2.49                     | 0.46              |
| 2:D:256:ASP:OD1  | 2:D:257:ASN:HB2  | 2.15                     | 0.46              |
| 1:A:70:PRO:HD3   | 2:E:15:ALA:HB2   | 1.97                     | 0.46              |
| 4:H:56:VAL:HA    | 4:H:68:PHE:O     | 2.15                     | 0.46              |
| 2:N:52:GLN:HB2   | 2:N:60:ARG:HB3   | 1.97                     | 0.46              |
| 1:T:166:ARG:HH22 | 2:X:190:ARG:CD   | 2.28                     | 0.46              |
| 1:U:106:LEU:HD22 | 1:U:230:TYR:HA   | 1.96                     | 0.46              |
| 1:B:364:ARG:HA   | 1:B:365:PRO:C    | 2.35                     | 0.46              |
| 2:M:84:SER:HB2   | 2:M:114:ARG:HH21 | 1.80                     | 0.46              |
| 2:V:222:MET:HA   | 2:V:229:ARG:HD2  | 1.97                     | 0.46              |
| 2:F:152:LYS:HZ1  | 2:F:293:GLN:HB3  | 1.81                     | 0.46              |
| 2:N:187:VAL:HG11 | 2:N:261:PHE:HB2  | 1.97                     | 0.46              |
| 2:O:336:SER:HB3  | 2:O:339:ILE:HD12 | 1.97                     | 0.46              |
| 4:Q:16:LEU:HB2   | 4:Q:19:GLU:HB2   | 1.96                     | 0.46              |
| 2:V:417:PRO:HG2  | 2:V:430:LYS:HB2  | 1.98                     | 0.46              |
| 2:F:382:LYS:HA   | 2:F:385:GLN:HG2  | 1.97                     | 0.46              |
| 3:G:13:ILE:HG22  | 3:G:248:ILE:HG13 | 1.98                     | 0.46              |
| 1:K:64:MET:HB2   | 1:K:78:PHE:CE2   | 2.51                     | 0.46              |
| 2:M:32:ALA:O     | 2:M:35:ASN:HB2   | 2.16                     | 0.46              |
| 2:V:99:ILE:HD11  | 2:V:101:GLU:CD   | 2.36                     | 0.46              |
| 2:E:30:LEU:HD11  | 2:E:57:ASN:HA    | 1.98                     | 0.45              |
| 2:N:96:ILE:HG22  | 2:N:97:ASN:N     | 2.31                     | 0.45              |
| 1:T:154:ALA:HB2  | 1:T:430:LEU:HB3  | 1.98                     | 0.45              |
| 1:U:112:ALA:HB3  | 1:U:244:LEU:HD22 | 1.97                     | 0.45              |
| 1:U:177:LYS:HG2  | 1:U:354:LEU:HD12 | 1.98                     | 0.45              |
| 1:U:421:VAL:O    | 1:U:425:ARG:HD2  | 2.16                     | 0.45              |
| 2:X:252:LEU:HD23 | 2:X:305:THR:HB   | 1.99                     | 0.45              |
| 4:H:113:SER:N    | 4:H:114:SER:HA   | 2.30                     | 0.45              |
| 1:J:30:THR:HA    | 1:J:90:VAL:O     | 2.15                     | 0.45              |
| 2:E:134:LEU:HD22 | 2:E:305:THR:HG21 | 1.97                     | 0.45              |
| 1:J:139:LEU:O    | 1:J:141:ARG:N    | 2.44                     | 0.45              |
| 1:J:141:ARG:HB2  | 2:N:195:ASN:ND2  | 2.31                     | 0.45              |
| 2:N:276:PRO:HD2  | 3:P:271:ILE:HD11 | 1.98                     | 0.45              |
| 2:O:7:THR:HA     | 2:O:8:PRO:HD3    | 1.81                     | 0.45              |
| 1:S:396:LEU:O    | 1:S:400:ARG:HG3  | 2.17                     | 0.45              |
| 1:T:424:GLU:O    | 1:T:428:GLN:HB2  | 2.16                     | 0.45              |
| 2:X:36:ALA:HB2   | 2:X:83:ILE:HG12  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:155:VAL:HA   | 1:B:159:VAL:HG23 | 1.98                     | 0.45              |
| 1:C:159:VAL:HG23 | 1:C:159:VAL:O    | 2.16                     | 0.45              |
| 2:W:53:HIS:O     | 2:W:55:GLY:N     | 2.49                     | 0.45              |
| 1:B:67:ASN:HB2   | 2:F:17:ILE:HG13  | 1.98                     | 0.45              |
| 1:K:182:LEU:HA   | 1:K:185:ILE:HD12 | 1.99                     | 0.45              |
| 2:N:23:VAL:CG1   | 2:N:76:VAL:HG21  | 2.46                     | 0.45              |
| 1:K:188:GLN:HB3  | 1:K:192:ASN:ND2  | 2.31                     | 0.45              |
| 1:L:227:ALA:HA   | 1:L:230:TYR:CE2  | 2.51                     | 0.45              |
| 1:L:455:LEU:HA   | 1:L:458:ILE:HD12 | 1.99                     | 0.45              |
| 1:L:97:VAL:HG11  | 1:L:247:LEU:HD21 | 1.98                     | 0.45              |
| 2:N:144:LEU:HD22 | 2:N:375:GLN:HG3  | 1.98                     | 0.45              |
| 2:O:384:LEU:HD22 | 2:O:396:LEU:HD21 | 1.99                     | 0.45              |
| 1:S:146:GLU:H    | 1:S:313:LYS:NZ   | 2.14                     | 0.45              |
| 1:T:77:LEU:HD21  | 1:T:84:VAL:HG21  | 1.99                     | 0.45              |
| 1:U:205:TYR:HB3  | 1:U:233:ILE:HD13 | 1.99                     | 0.45              |
| 1:U:181:ALA:HB1  | 1:U:269:VAL:HG21 | 1.97                     | 0.45              |
| 3:Y:212:TYR:O    | 3:Y:216:ASN:HB2  | 2.15                     | 0.45              |
| 1:A:446:LEU:CD2  | 1:A:467:GLU:HG3  | 2.47                     | 0.45              |
| 1:B:435:TYR:C    | 1:B:437:PRO:HD3  | 2.37                     | 0.45              |
| 1:A:217:GLN:HG2  | 2:D:356:ARG:HH21 | 1.82                     | 0.45              |
| 3:Y:76:ALA:HB1   | 3:Y:109:THR:HG22 | 1.99                     | 0.45              |
| 1:C:166:ARG:HD2  | 1:C:308:LEU:O    | 2.17                     | 0.45              |
| 2:F:143:LEU:O    | 2:F:367:HIS:HE1  | 2.00                     | 0.45              |
| 2:F:384:LEU:O    | 2:F:388:ILE:HG12 | 2.17                     | 0.45              |
| 2:F:390:ILE:HD12 | 3:G:244:ALA:HA   | 1.99                     | 0.45              |
| 4:H:71:SER:HB3   | 4:H:89:GLU:HB2   | 1.99                     | 0.45              |
| 1:L:243:PRO:O    | 1:L:247:LEU:HB2  | 2.16                     | 0.45              |
| 2:O:251:VAL:HB   | 2:O:304:VAL:HG22 | 1.99                     | 0.45              |
| 1:T:148:VAL:HG21 | 1:T:324:THR:HG21 | 1.97                     | 0.45              |
| 2:W:256:ASP:HA   | 2:W:257:ASN:HA   | 1.66                     | 0.45              |
| 2:X:284:THR:O    | 2:X:288:ASP:HB2  | 2.16                     | 0.45              |
| 1:A:424:GLU:HB3  | 1:A:460:LEU:HD21 | 1.98                     | 0.45              |
| 2:O:189:GLU:O    | 2:O:221:GLN:HB3  | 2.17                     | 0.45              |
| 1:T:243:PRO:HG3  | 1:T:283:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:446:LEU:HD22 | 1:A:467:GLU:HG3  | 1.99                     | 0.45              |
| 1:B:474:LEU:HB3  | 1:B:482:LEU:HD11 | 2.00                     | 0.45              |
| 1:C:78:PHE:HB3   | 1:C:244:LEU:HD21 | 1.98                     | 0.45              |
| 2:E:170:LEU:O    | 2:E:174:ILE:HG12 | 2.17                     | 0.45              |
| 2:M:144:LEU:O    | 2:M:358:LEU:HD22 | 2.17                     | 0.45              |
| 1:S:161:ILE:HD11 | 1:S:352:ILE:HD11 | 1.98                     | 0.45              |
| 2:D:425:THR:HB   | 2:D:427:ILE:HD12 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:21:VAL:O     | 2:F:61:THR:OG1   | 2.30                     | 0.44              |
| 2:F:277:SER:OG   | 2:F:278:ALA:N    | 2.50                     | 0.44              |
| 2:F:33:ILE:O     | 2:F:34:LEU:CB    | 2.64                     | 0.44              |
| 1:K:109:VAL:HB   | 1:K:118:ASP:HB3  | 1.98                     | 0.44              |
| 2:M:33:ILE:O     | 2:M:34:LEU:HB2   | 2.17                     | 0.44              |
| 1:J:360:TYR:OH   | 2:M:354:LYS:HE2  | 2.16                     | 0.44              |
| 2:N:96:ILE:HG22  | 2:N:97:ASN:O     | 2.18                     | 0.44              |
| 2:O:196:ASP:OD1  | 2:O:199:ARG:NH2  | 2.49                     | 0.44              |
| 2:O:277:SER:OG   | 2:O:278:ALA:N    | 2.50                     | 0.44              |
| 2:O:32:ALA:O     | 2:O:35:ASN:HB2   | 2.17                     | 0.44              |
| 1:A:205:TYR:HB3  | 1:A:233:ILE:HD13 | 1.99                     | 0.44              |
| 1:A:288:ARG:HG2  | 1:A:288:ARG:HH11 | 1.83                     | 0.44              |
| 2:D:229:ARG:NH2  | 2:D:267:GLU:OE1  | 2.48                     | 0.44              |
| 2:D:456:ALA:HA   | 2:D:469:LYS:HD3  | 1.99                     | 0.44              |
| 1:B:290:PRO:HG2  | 2:F:270:ALA:HB2  | 1.98                     | 0.44              |
| 1:U:341:PRO:O    | 1:U:345:ILE:HG13 | 2.16                     | 0.44              |
| 2:W:168:GLN:HA   | 2:W:171:ILE:HD12 | 1.99                     | 0.44              |
| 2:D:152:LYS:NZ   | 2:D:293:GLN:HB3  | 2.32                     | 0.44              |
| 2:D:321:ALA:HB3  | 2:D:322:PRO:CD   | 2.48                     | 0.44              |
| 2:E:142:ASP:HB3  | 2:E:434:LEU:HD12 | 1.99                     | 0.44              |
| 2:E:256:ASP:HA   | 2:E:257:ASN:HA   | 1.76                     | 0.44              |
| 2:E:229:ARG:NH2  | 2:E:267:GLU:OE1  | 2.49                     | 0.44              |
| 2:F:94:ARG:NH2   | 2:F:102:PRO:HB2  | 2.32                     | 0.44              |
| 2:O:33:ILE:HG22  | 2:O:34:LEU:HG    | 1.99                     | 0.44              |
| 1:S:146:GLU:H    | 1:S:313:LYS:HZ3  | 1.65                     | 0.44              |
| 1:S:385:LEU:HD11 | 1:S:447:ILE:HD12 | 1.98                     | 0.44              |
| 6:U:600:ANP:N3B  | 6:U:600:ANP:O2A  | 2.48                     | 0.44              |
| 2:W:102:PRO:HG3  | 2:W:109:ILE:HG13 | 2.00                     | 0.44              |
| 2:W:185:THR:OG1  | 2:W:236:GLY:HA3  | 2.17                     | 0.44              |
| 2:W:188:GLY:HA3  | 2:W:260:ARG:HD2  | 2.00                     | 0.44              |
| 2:W:410:ILE:HG23 | 2:W:441:PHE:HE2  | 1.82                     | 0.44              |
| 2:W:95:ILE:HB    | 2:W:104:ASP:HB3  | 1.98                     | 0.44              |
| 1:B:25:ALA:HB1   | 1:B:30:THR:HG21  | 1.99                     | 0.44              |
| 1:C:55:VAL:HG21  | 1:C:75:ILE:HD13  | 1.99                     | 0.44              |
| 1:B:50:GLN:HB3   | 2:F:69:GLY:HA2   | 1.99                     | 0.44              |
| 3:G:9:ARG:HD2    | 3:G:251:TYR:HE2  | 1.81                     | 0.44              |
| 1:L:40:ILE:HD11  | 1:L:76:VAL:HG12  | 2.00                     | 0.44              |
| 2:N:45:LYS:O     | 2:N:45:LYS:HG3   | 2.18                     | 0.44              |
| 1:T:168:LEU:HD12 | 1:T:327:PRO:O    | 2.17                     | 0.44              |
| 1:U:211:LYS:O    | 1:U:215:VAL:HG23 | 2.16                     | 0.44              |
| 1:U:219:VAL:HA   | 1:U:222:LEU:HD12 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:X:234:LEU:HD23 | 2:X:292:LEU:HD13 | 1.99                     | 0.44              |
| 2:E:117:ILE:HG22 | 2:E:235:THR:HA   | 1.99                     | 0.44              |
| 1:B:117:ILE:HD12 | 2:E:124:PHE:CB   | 2.48                     | 0.44              |
| 2:F:104:ASP:C    | 2:F:106:ARG:H    | 2.21                     | 0.44              |
| 2:F:182:SER:HA   | 2:F:252:LEU:O    | 2.17                     | 0.44              |
| 4:H:35:LYS:HE2   | 4:H:37:GLY:H     | 1.83                     | 0.44              |
| 1:L:187:ASN:OD1  | 1:L:190:ARG:NH1  | 2.47                     | 0.44              |
| 1:L:426:LEU:HD21 | 1:L:450:GLY:HA3  | 1.99                     | 0.44              |
| 2:M:314:ALA:O    | 2:M:315:ASP:HB2  | 2.18                     | 0.44              |
| 3:P:42:LYS:HA    | 3:P:45:ASP:HB2   | 1.99                     | 0.44              |
| 1:T:306:ARG:O    | 1:T:310:ARG:HD3  | 2.18                     | 0.44              |
| 1:U:89:LEU:N     | 1:U:89:LEU:HD12  | 2.33                     | 0.44              |
| 2:W:320:PRO:O    | 2:W:324:THR:OG1  | 2.28                     | 0.44              |
| 2:X:141:VAL:HG22 | 2:X:333:THR:HG21 | 1.99                     | 0.44              |
| 1:B:166:ARG:CD   | 1:B:308:LEU:O    | 2.65                     | 0.44              |
| 2:D:314:ALA:O    | 2:D:315:ASP:HB2  | 2.18                     | 0.44              |
| 1:K:112:ALA:HB2  | 1:K:236:ALA:HB2  | 1.98                     | 0.44              |
| 1:L:150:THR:HA   | 1:L:184:THR:HG23 | 2.00                     | 0.44              |
| 2:V:138:ILE:HA   | 2:V:416:GLN:OE1  | 2.18                     | 0.44              |
| 1:A:248:ALA:HB3  | 1:A:249:PRO:HD3  | 1.99                     | 0.44              |
| 2:N:150:GLY:HA2  | 2:N:304:VAL:O    | 2.18                     | 0.44              |
| 3:Y:41:ALA:HB1   | 3:Y:220:THR:HA   | 2.00                     | 0.44              |
| 1:A:426:LEU:O    | 1:A:430:LEU:HG   | 2.18                     | 0.44              |
| 1:B:182:LEU:HD13 | 1:B:218:LEU:HD11 | 2.00                     | 0.44              |
| 2:E:237:LEU:O    | 2:E:241:GLU:HG3  | 2.18                     | 0.44              |
| 2:F:158:GLY:O    | 2:F:161:VAL:HG22 | 2.18                     | 0.44              |
| 1:J:300:VAL:O    | 1:J:303:LEU:HB3  | 2.18                     | 0.44              |
| 1:L:271:ASP:HA   | 1:L:272:ASP:HA   | 1.76                     | 0.44              |
| 2:M:198:TYR:CZ   | 2:M:202:LYS:HE2  | 2.52                     | 0.44              |
| 3:P:94:ALA:C     | 3:P:96:ARG:H     | 2.21                     | 0.44              |
| 2:V:97:ASN:HD22  | 2:V:103:ILE:HG23 | 1.83                     | 0.44              |
| 1:U:375:ARG:NH1  | 2:V:190:ARG:NH2  | 2.66                     | 0.44              |
| 2:X:333:THR:HA   | 2:X:353:SER:HB3  | 2.00                     | 0.44              |
| 1:B:164:GLY:HA2  | 1:B:323:LEU:O    | 2.18                     | 0.44              |
| 1:B:34:LEU:O     | 1:B:86:GLU:HG3   | 2.18                     | 0.44              |
| 3:G:133:ILE:HD13 | 3:G:133:ILE:HA   | 1.70                     | 0.44              |
| 2:O:218:VAL:HG21 | 2:O:236:GLY:HA2  | 2.00                     | 0.44              |
| 1:B:338:ALA:HB3  | 1:B:341:PRO:HG2  | 2.01                     | 0.43              |
| 2:D:224:GLU:O    | 2:D:229:ARG:NH1  | 2.44                     | 0.43              |
| 2:F:201:MET:HB2  | 2:F:207:ILE:HD12 | 2.00                     | 0.43              |
| 1:T:131:ALA:HB2  | 1:T:251:THR:HG22 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:107:GLY:HA2  | 1:U:228:MET:HG3  | 1.98                     | 0.43              |
| 1:U:299:ASP:HB2  | 1:U:302:TYR:HB3  | 2.00                     | 0.43              |
| 1:U:329:ILE:HD11 | 1:U:344:VAL:HG21 | 2.00                     | 0.43              |
| 2:W:258:ILE:HG22 | 2:W:309:ALA:O    | 2.18                     | 0.43              |
| 2:W:37:LEU:HD13  | 2:W:76:VAL:HG11  | 2.00                     | 0.43              |
| 1:B:400:ARG:HE   | 1:B:400:ARG:HB3  | 1.46                     | 0.43              |
| 3:G:87:ILE:HG23  | 3:G:167:ASN:HD22 | 1.84                     | 0.43              |
| 1:K:173:ARG:HH22 | 2:N:327:ALA:HB2  | 1.83                     | 0.43              |
| 1:K:37:GLY:HA3   | 2:N:52:GLN:HG2   | 2.00                     | 0.43              |
| 1:K:455:LEU:HD23 | 1:K:458:ILE:HD12 | 1.99                     | 0.43              |
| 1:K:364:ARG:HD3  | 6:K:600:ANP:N1   | 2.31                     | 0.43              |
| 1:L:177:LYS:HD2  | 1:L:328:VAL:HG13 | 2.00                     | 0.43              |
| 1:L:480:GLU:H    | 1:L:480:GLU:HG3  | 1.67                     | 0.43              |
| 1:T:495:LEU:O    | 1:T:499:LEU:HD13 | 2.18                     | 0.43              |
| 1:A:480:GLU:H    | 1:A:480:GLU:HG3  | 1.38                     | 0.43              |
| 1:A:77:LEU:CD1   | 1:A:81:ASP:CB    | 2.96                     | 0.43              |
| 2:E:98:VAL:HG13  | 2:E:99:ILE:HG23  | 1.99                     | 0.43              |
| 4:H:51:GLN:HG2   | 4:H:74:PHE:CZ    | 2.53                     | 0.43              |
| 2:M:136:THR:HG21 | 2:M:147:TYR:CD2  | 2.53                     | 0.43              |
| 2:M:342:LEU:HD13 | 2:M:344:ILE:HD12 | 2.01                     | 0.43              |
| 1:A:392:LEU:HD13 | 1:A:426:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:354:LEU:HA   | 1:C:366:ALA:O    | 2.18                     | 0.43              |
| 2:E:25:PHE:O     | 2:E:57:ASN:HB3   | 2.19                     | 0.43              |
| 2:F:387:ILE:HG23 | 2:F:391:LEU:HD12 | 1.99                     | 0.43              |
| 1:L:389:ALA:O    | 1:L:390:GLY:C    | 2.55                     | 0.43              |
| 1:K:301:PHE:HB3  | 2:O:263:GLN:NE2  | 2.33                     | 0.43              |
| 1:U:271:ASP:HA   | 1:U:272:ASP:HA   | 1.68                     | 0.43              |
| 1:A:246:TYR:CE1  | 1:A:303:LEU:HD11 | 2.53                     | 0.43              |
| 1:B:100:PRO:HA   | 1:B:127:GLY:O    | 2.19                     | 0.43              |
| 1:C:46:LEU:O     | 1:C:49:ILE:HG22  | 2.18                     | 0.43              |
| 2:D:64:MET:HE3   | 2:D:228:ALA:HA   | 2.00                     | 0.43              |
| 1:L:99:VAL:CG1   | 1:L:251:THR:HB   | 2.49                     | 0.43              |
| 1:A:217:GLN:OE1  | 2:D:129:THR:HB   | 2.19                     | 0.43              |
| 1:C:238:ALA:O    | 2:F:290:GLY:HA3  | 2.18                     | 0.43              |
| 2:D:149:ARG:HG2  | 2:D:149:ARG:HH11 | 1.83                     | 0.43              |
| 2:F:38:GLU:HG2   | 2:F:45:LYS:HG2   | 2.00                     | 0.43              |
| 2:F:395:GLU:HG3  | 3:G:83:LEU:HD23  | 1.99                     | 0.43              |
| 1:J:422:ARG:HE   | 1:J:453:GLY:HA2  | 1.83                     | 0.43              |
| 1:J:55:VAL:HG21  | 1:J:75:ILE:HD13  | 2.01                     | 0.43              |
| 1:K:285:LEU:HD13 | 2:N:277:SER:HB3  | 2.00                     | 0.43              |
| 1:L:109:VAL:HG12 | 1:L:117:ILE:HD11 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:435:TYR:C    | 1:U:437:PRO:HD3  | 2.39                     | 0.43              |
| 2:E:22:ASP:HA    | 2:E:59:VAL:O     | 2.18                     | 0.43              |
| 2:E:312:VAL:HG12 | 2:E:315:ASP:HA   | 2.01                     | 0.43              |
| 1:K:444:VAL:HG21 | 1:K:485:ILE:HG21 | 2.01                     | 0.43              |
| 1:L:36:VAL:HG12  | 2:O:53:HIS:HB2   | 2.01                     | 0.43              |
| 2:O:239:ILE:HG22 | 2:O:243:PHE:HE2  | 1.83                     | 0.43              |
| 2:O:141:VAL:HG22 | 2:O:333:THR:HG21 | 2.01                     | 0.43              |
| 1:S:474:LEU:HD23 | 1:S:478:HIS:HB2  | 2.01                     | 0.43              |
| 1:U:211:LYS:HB3  | 1:U:211:LYS:HE2  | 1.77                     | 0.43              |
| 2:W:87:VAL:HG12  | 2:W:239:ILE:HA   | 2.00                     | 0.43              |
| 1:B:388:VAL:O    | 1:B:451:VAL:HG21 | 2.18                     | 0.43              |
| 1:C:146:GLU:O    | 1:C:162:GLY:HA2  | 2.19                     | 0.43              |
| 2:F:142:ASP:HB3  | 2:F:434:LEU:HD12 | 2.01                     | 0.43              |
| 3:G:151:LEU:HD23 | 3:G:156:ALA:HB3  | 2.00                     | 0.43              |
| 2:W:164:THR:HA   | 2:W:167:ILE:HB   | 2.01                     | 0.43              |
| 2:F:148:ALA:CB   | 2:F:357:LEU:HD11 | 2.49                     | 0.43              |
| 2:F:377:THR:HG22 | 2:F:407:ALA:HB2  | 2.01                     | 0.43              |
| 1:L:91:LYS:HG3   | 1:L:92:ARG:O     | 2.19                     | 0.43              |
| 1:A:85:LYS:HG2   | 2:D:53:HIS:HE1   | 1.84                     | 0.43              |
| 2:F:155:LEU:CD1  | 2:F:167:ILE:HG12 | 2.48                     | 0.43              |
| 3:G:44:MET:HE2   | 4:H:86:THR:HB    | 2.00                     | 0.43              |
| 2:M:241:GLU:HG2  | 2:M:244:ARG:NH2  | 2.33                     | 0.43              |
| 2:O:12:LYS:O     | 2:O:23:VAL:HA    | 2.19                     | 0.43              |
| 1:S:142:ARG:HG2  | 1:S:143:SER:H    | 1.84                     | 0.43              |
| 1:S:246:TYR:CD2  | 1:S:247:LEU:HG   | 2.54                     | 0.43              |
| 1:S:446:LEU:HD21 | 1:S:467:GLU:HA   | 2.01                     | 0.43              |
| 1:U:238:ALA:HB1  | 2:X:328:HIS:HE1  | 1.84                     | 0.43              |
| 2:W:135:GLU:HG3  | 2:W:434:LEU:HB2  | 2.01                     | 0.43              |
| 2:W:349:ASP:HA   | 2:W:350:PRO:HD3  | 1.86                     | 0.43              |
| 2:X:256:ASP:HA   | 2:X:257:ASN:HA   | 1.79                     | 0.43              |
| 1:S:295:ALA:HB2  | 3:Y:270:ILE:HD13 | 2.01                     | 0.43              |
| 1:A:34:LEU:O     | 1:A:86:GLU:HG3   | 2.19                     | 0.42              |
| 1:C:148:VAL:HG22 | 1:C:163:ARG:HG3  | 2.00                     | 0.42              |
| 2:E:132:GLU:OE2  | 2:E:149:ARG:NH1  | 2.52                     | 0.42              |
| 3:G:150:LEU:HD12 | 3:G:150:LEU:HA   | 1.93                     | 0.42              |
| 4:H:46:VAL:HA    | 4:H:47:PRO:HD3   | 1.94                     | 0.42              |
| 1:J:172:ASP:O    | 1:J:175:THR:OG1  | 2.34                     | 0.42              |
| 1:L:394:LEU:HD11 | 2:M:425:THR:HG22 | 2.01                     | 0.42              |
| 2:N:97:ASN:HB3   | 2:N:103:ILE:HD13 | 2.01                     | 0.42              |
| 3:P:74:ILE:HG23  | 3:P:165:PHE:HD2  | 1.84                     | 0.42              |
| 1:U:429:LEU:HG   | 1:U:429:LEU:O    | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:143:SER:OG   | 2:V:199:ARG:NH2  | 2.52                     | 0.42              |
| 2:V:30:LEU:HA    | 2:V:31:PRO:HD3   | 1.87                     | 0.42              |
| 2:X:189:GLU:O    | 2:X:221:GLN:HB3  | 2.19                     | 0.42              |
| 3:Y:99:LEU:HD23  | 3:Y:122:HIS:CE1  | 2.54                     | 0.42              |
| 1:C:139:LEU:HB3  | 1:C:140:PRO:HD3  | 2.01                     | 0.42              |
| 2:D:201:MET:H    | 2:D:201:MET:HG2  | 1.66                     | 0.42              |
| 2:N:432:VAL:HG12 | 2:N:433:ARG:H    | 1.83                     | 0.42              |
| 1:U:284:SER:HB2  | 1:U:297:PRO:HG3  | 2.00                     | 0.42              |
| 1:U:319:GLY:O    | 1:U:320:SER:HB2  | 2.19                     | 0.42              |
| 2:W:37:LEU:HD12  | 2:W:61:THR:HG21  | 2.01                     | 0.42              |
| 2:W:37:LEU:HB2   | 2:W:48:LEU:HB2   | 2.02                     | 0.42              |
| 2:W:96:ILE:O     | 2:W:218:VAL:HA   | 2.19                     | 0.42              |
| 2:X:275:ILE:O    | 2:X:283:PRO:HG3  | 2.19                     | 0.42              |
| 2:X:339:ILE:HG22 | 2:X:344:ILE:HB   | 2.00                     | 0.42              |
| 2:F:244:ARG:HD3  | 2:F:304:VAL:HG23 | 2.00                     | 0.42              |
| 2:F:145:ALA:HA   | 2:F:355:SER:HB2  | 2.01                     | 0.42              |
| 2:M:155:LEU:HD12 | 2:M:167:ILE:HG13 | 2.01                     | 0.42              |
| 2:D:256:ASP:HA   | 2:D:257:ASN:HA   | 1.88                     | 0.42              |
| 4:H:35:LYS:N     | 4:H:35:LYS:HD3   | 2.33                     | 0.42              |
| 1:K:170:ILE:HD11 | 1:K:341:PRO:HB3  | 2.01                     | 0.42              |
| 1:K:96:ILE:O     | 1:K:97:VAL:C     | 2.58                     | 0.42              |
| 1:L:43:VAL:HG21  | 1:L:75:ILE:HD12  | 2.00                     | 0.42              |
| 2:N:432:VAL:HG12 | 2:N:433:ARG:N    | 2.34                     | 0.42              |
| 2:O:256:ASP:HA   | 2:O:257:ASN:HA   | 1.71                     | 0.42              |
| 2:O:140:VAL:CG1  | 2:O:414:LEU:HB3  | 2.49                     | 0.42              |
| 3:P:164:ILE:HD11 | 3:P:182:ILE:HG13 | 2.01                     | 0.42              |
| 1:U:273:LEU:HD11 | 1:U:327:PRO:HB3  | 2.01                     | 0.42              |
| 2:D:170:LEU:O    | 2:D:174:ILE:HG12 | 2.19                     | 0.42              |
| 2:E:281:TYR:CD2  | 2:E:320:PRO:HG2  | 2.55                     | 0.42              |
| 1:B:305:SER:HB2  | 2:F:222:MET:HB2  | 2.02                     | 0.42              |
| 2:F:256:ASP:HA   | 2:F:257:ASN:HA   | 1.78                     | 0.42              |
| 2:F:443:ALA:O    | 2:F:448:LYS:HG3  | 2.19                     | 0.42              |
| 1:J:204:VAL:O    | 1:J:268:ILE:HA   | 2.19                     | 0.42              |
| 1:K:442:GLU:C    | 1:K:445:PRO:HD2  | 2.39                     | 0.42              |
| 1:K:496:LEU:O    | 1:K:500:LYS:HB2  | 2.19                     | 0.42              |
| 2:N:95:ILE:HD11  | 2:N:198:TYR:CG   | 2.55                     | 0.42              |
| 2:O:239:ILE:HG22 | 2:O:243:PHE:CE2  | 2.55                     | 0.42              |
| 1:U:105:LEU:O    | 1:U:108:ARG:HB2  | 2.19                     | 0.42              |
| 1:B:478:HIS:HB3  | 1:B:481:LEU:HG   | 2.01                     | 0.42              |
| 1:C:42:ARG:NE    | 1:C:72:GLN:HE22  | 2.17                     | 0.42              |
| 3:G:189:GLU:HG2  | 3:G:206:PRO:HG2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:16:LEU:HB2   | 4:H:19:GLU:O     | 2.19                     | 0.42              |
| 1:J:54:LEU:HD13  | 1:J:97:VAL:HG22  | 2.00                     | 0.42              |
| 1:K:340:ILE:HB   | 1:K:341:PRO:HD3  | 2.01                     | 0.42              |
| 1:K:363:ILE:HA   | 1:K:431:LYS:HE2  | 2.01                     | 0.42              |
| 2:M:25:PHE:HB2   | 2:M:30:LEU:CD2   | 2.49                     | 0.42              |
| 2:N:87:VAL:HG12  | 2:N:239:ILE:HA   | 2.02                     | 0.42              |
| 1:U:221:THR:HG21 | 1:U:435:TYR:CE1  | 2.53                     | 0.42              |
| 1:U:222:LEU:HB2  | 1:U:228:MET:HE1  | 2.02                     | 0.42              |
| 1:U:203:CYS:O    | 1:U:231:SER:HA   | 2.20                     | 0.42              |
| 1:U:272:ASP:HB3  | 1:U:328:VAL:HG12 | 2.01                     | 0.42              |
| 1:A:485:ILE:HG12 | 1:A:491:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:280:TYR:OH   | 1:B:299:ASP:OD2  | 2.32                     | 0.42              |
| 1:C:103:PRO:HD3  | 1:C:258:TRP:CZ2  | 2.54                     | 0.42              |
| 1:C:76:VAL:HB    | 1:C:243:PRO:HG2  | 2.01                     | 0.42              |
| 1:T:455:LEU:HA   | 1:T:458:ILE:HD13 | 2.02                     | 0.42              |
| 1:U:109:VAL:HG22 | 1:U:233:ILE:HB   | 2.01                     | 0.42              |
| 1:U:55:VAL:HG12  | 1:U:92:ARG:HA    | 2.02                     | 0.42              |
| 2:V:15:ALA:O     | 2:V:21:VAL:HA    | 2.19                     | 0.42              |
| 2:V:85:VAL:CG1   | 2:V:235:THR:HG23 | 2.39                     | 0.42              |
| 2:X:49:GLU:O     | 2:X:61:THR:HA    | 2.20                     | 0.42              |
| 1:A:26:ASN:HB3   | 1:A:30:THR:OG1   | 2.20                     | 0.42              |
| 2:E:135:GLU:OE2  | 2:E:433:ARG:HD3  | 2.20                     | 0.42              |
| 1:K:51:ALA:HB2   | 1:K:68:LEU:HD11  | 2.01                     | 0.42              |
| 2:W:50:VAL:HA    | 2:W:61:THR:HG22  | 2.02                     | 0.42              |
| 1:A:242:ALA:N    | 1:A:243:PRO:CD   | 2.83                     | 0.42              |
| 1:B:174:GLN:CA   | 6:B:600:ANP:HNB1 | 2.14                     | 0.42              |
| 1:C:314:LEU:HB3  | 1:C:318:GLU:HB2  | 2.01                     | 0.42              |
| 2:E:156:PHE:HZ   | 2:E:326:PHE:CZ   | 2.38                     | 0.42              |
| 2:F:134:LEU:HD11 | 2:F:174:ILE:HG21 | 2.02                     | 0.42              |
| 2:F:417:PRO:HG2  | 2:F:430:LYS:H    | 1.85                     | 0.42              |
| 1:J:250:PHE:CE1  | 1:J:307:LEU:HB2  | 2.55                     | 0.42              |
| 1:K:341:PRO:O    | 1:K:345:ILE:HG13 | 2.19                     | 0.42              |
| 1:L:354:LEU:HA   | 1:L:366:ALA:O    | 2.20                     | 0.42              |
| 1:T:197:GLU:HG3  | 1:T:200:LYS:HD2  | 2.00                     | 0.42              |
| 1:T:364:ARG:HA   | 1:T:365:PRO:C    | 2.40                     | 0.42              |
| 2:X:37:LEU:HD23  | 2:X:78:ASP:HA    | 2.02                     | 0.42              |
| 3:Y:10:LEU:HG    | 3:Y:14:LYS:HE2   | 2.02                     | 0.42              |
| 1:B:85:LYS:HE2   | 2:E:32:ALA:HB2   | 2.02                     | 0.41              |
| 1:C:177:LYS:HD2  | 1:C:328:VAL:HG13 | 2.02                     | 0.41              |
| 2:D:140:VAL:HA   | 2:D:414:LEU:HD22 | 2.01                     | 0.41              |
| 2:M:344:ILE:HG23 | 2:M:415:SER:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:147:TYR:CE2  | 2:O:153:ILE:HG21 | 2.55                     | 0.41              |
| 2:O:321:ALA:HB3  | 2:O:322:PRO:CD   | 2.49                     | 0.41              |
| 2:O:335:LEU:HA   | 2:O:347:ALA:O    | 2.19                     | 0.41              |
| 1:S:204:VAL:O    | 1:S:268:ILE:HA   | 2.20                     | 0.41              |
| 2:V:384:LEU:O    | 2:V:388:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:285:LEU:HD21 | 1:C:291:PRO:HB3  | 2.02                     | 0.41              |
| 1:C:168:LEU:HD23 | 1:C:351:GLN:HG2  | 2.03                     | 0.41              |
| 2:D:32:ALA:O     | 2:D:35:ASN:HB2   | 2.19                     | 0.41              |
| 2:F:290:GLY:O    | 2:F:294:GLU:HB2  | 2.20                     | 0.41              |
| 2:M:97:ASN:HD22  | 2:M:103:ILE:HG23 | 1.86                     | 0.41              |
| 2:M:237:LEU:HD23 | 2:M:292:LEU:HD12 | 2.02                     | 0.41              |
| 2:M:324:THR:O    | 2:M:324:THR:HG22 | 2.20                     | 0.41              |
| 3:P:188:ILE:O    | 3:P:188:ILE:HG22 | 2.21                     | 0.41              |
| 1:S:145:HIS:H    | 1:S:313:LYS:NZ   | 2.16                     | 0.41              |
| 1:T:212:ARG:HA   | 1:T:237:THR:HG21 | 2.02                     | 0.41              |
| 2:W:262:THR:HG21 | 2:W:321:ALA:HB2  | 2.01                     | 0.41              |
| 3:Y:233:ARG:O    | 3:Y:237:MET:HG2  | 2.21                     | 0.41              |
| 2:M:417:PRO:HD2  | 2:M:460:VAL:O    | 2.20                     | 0.41              |
| 2:O:297:THR:OG1  | 2:O:298:THR:N    | 2.54                     | 0.41              |
| 4:Q:30:VAL:H     | 4:Q:41:VAL:HG12  | 1.85                     | 0.41              |
| 1:B:154:ALA:HB3  | 1:B:367:ILE:HD12 | 2.03                     | 0.41              |
| 3:G:258:THR:O    | 3:G:262:VAL:HG23 | 2.20                     | 0.41              |
| 1:K:302:TYR:HA   | 1:K:305:SER:OG   | 2.20                     | 0.41              |
| 2:O:148:ALA:HB2  | 2:O:357:LEU:HD11 | 2.02                     | 0.41              |
| 1:C:219:VAL:HB   | 1:C:228:MET:CE   | 2.50                     | 0.41              |
| 2:D:64:MET:HE1   | 2:D:228:ALA:HA   | 2.02                     | 0.41              |
| 1:A:138:ILE:HG21 | 2:E:95:ILE:HD13  | 2.02                     | 0.41              |
| 2:F:134:LEU:CD2  | 2:F:305:THR:HG21 | 2.50                     | 0.41              |
| 1:J:73:VAL:HG12  | 1:J:75:ILE:HG13  | 2.02                     | 0.41              |
| 3:P:141:GLN:HE21 | 3:P:141:GLN:HA   | 1.85                     | 0.41              |
| 1:S:173:ARG:NH2  | 2:V:317:LEU:HD13 | 2.36                     | 0.41              |
| 1:U:36:VAL:HG21  | 1:U:84:VAL:HB    | 2.03                     | 0.41              |
| 2:V:16:VAL:HG12  | 2:V:21:VAL:HG22  | 2.02                     | 0.41              |
| 2:X:275:ILE:HA   | 2:X:276:PRO:HD3  | 1.95                     | 0.41              |
| 2:X:255:ILE:HB   | 2:X:308:GLN:HG2  | 2.02                     | 0.41              |
| 1:B:186:LEU:HD22 | 1:B:225:HIS:CB   | 2.50                     | 0.41              |
| 1:B:267:LEU:HD11 | 1:B:326:LEU:HG   | 2.02                     | 0.41              |
| 2:D:152:LYS:HZ3  | 2:D:293:GLN:HB3  | 1.84                     | 0.41              |
| 2:D:335:LEU:HA   | 2:D:347:ALA:O    | 2.21                     | 0.41              |
| 2:F:266:SER:HB3  | 2:F:282:GLN:OE1  | 2.21                     | 0.41              |
| 1:K:54:LEU:HG    | 1:K:97:VAL:HA    | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:356:ALA:HB1  | 1:S:360:TYR:OH   | 2.21                     | 0.41              |
| 1:U:375:ARG:HH12 | 2:V:190:ARG:NH2  | 2.19                     | 0.41              |
| 2:V:372:SER:O    | 2:V:376:GLU:HG3  | 2.20                     | 0.41              |
| 2:W:156:PHE:HB2  | 2:W:334:VAL:HG22 | 2.02                     | 0.41              |
| 2:X:64:MET:O     | 2:X:65:ASP:HB2   | 2.21                     | 0.41              |
| 3:Y:3:LEU:HD11   | 3:Y:259:ARG:HD3  | 2.03                     | 0.41              |
| 1:A:246:TYR:HE1  | 1:A:303:LEU:HD11 | 1.84                     | 0.41              |
| 1:A:166:ARG:HD2  | 1:A:308:LEU:O    | 2.21                     | 0.41              |
| 1:B:101:VAL:HG12 | 1:B:255:ILE:HA   | 2.03                     | 0.41              |
| 1:A:299:ASP:HB3  | 2:E:271:LEU:HD21 | 2.02                     | 0.41              |
| 2:M:266:SER:HB3  | 2:M:282:GLN:OE1  | 2.20                     | 0.41              |
| 2:N:201:MET:HA   | 2:N:204:THR:HG22 | 2.03                     | 0.41              |
| 3:P:14:LYS:HA    | 3:P:248:ILE:HD11 | 2.03                     | 0.41              |
| 1:S:139:LEU:N    | 1:S:140:PRO:CD   | 2.84                     | 0.41              |
| 1:S:139:LEU:N    | 1:S:140:PRO:HD2  | 2.36                     | 0.41              |
| 2:D:165:VAL:HG13 | 2:D:420:VAL:HG12 | 2.03                     | 0.41              |
| 2:F:134:LEU:HD22 | 2:F:305:THR:HG21 | 2.03                     | 0.41              |
| 3:G:14:LYS:HA    | 3:G:248:ILE:CD1  | 2.48                     | 0.41              |
| 1:K:190:ARG:NE   | 1:K:439:ALA:HB2  | 2.35                     | 0.41              |
| 1:L:46:LEU:O     | 1:L:47:ASN:C     | 2.58                     | 0.41              |
| 3:P:149:LYS:HA   | 3:P:152:SER:HB2  | 2.03                     | 0.41              |
| 1:S:99:VAL:HG22  | 1:S:100:PRO:HD2  | 2.02                     | 0.41              |
| 1:U:398:GLN:O    | 1:U:402:VAL:HG23 | 2.21                     | 0.41              |
| 1:U:51:ALA:HB3   | 2:V:67:THR:O     | 2.20                     | 0.41              |
| 2:W:237:LEU:HD21 | 2:W:295:ARG:HB2  | 2.03                     | 0.41              |
| 1:T:166:ARG:HH22 | 2:X:190:ARG:HD3  | 1.86                     | 0.41              |
| 2:X:346:PRO:HB2  | 2:X:348:VAL:HG23 | 2.03                     | 0.41              |
| 1:B:308:LEU:HB2  | 1:B:347:ILE:HG21 | 2.03                     | 0.41              |
| 1:C:248:ALA:HB3  | 1:C:249:PRO:HD3  | 2.03                     | 0.41              |
| 2:E:193:GLU:HA   | 2:E:196:ASP:HB2  | 2.03                     | 0.41              |
| 1:J:138:ILE:HG22 | 1:J:139:LEU:HD12 | 2.02                     | 0.41              |
| 1:S:271:ASP:HA   | 1:S:272:ASP:HA   | 1.84                     | 0.41              |
| 1:T:168:LEU:HB2  | 1:T:348:THR:HG21 | 2.02                     | 0.41              |
| 1:A:98:ASP:C     | 1:A:98:ASP:OD1   | 2.58                     | 0.41              |
| 1:B:309:GLU:HG3  | 2:F:222:MET:HG3  | 2.02                     | 0.41              |
| 1:L:389:ALA:O    | 1:L:390:GLY:O    | 2.39                     | 0.41              |
| 1:L:138:ILE:HD12 | 2:M:191:THR:HG23 | 2.02                     | 0.41              |
| 2:N:185:THR:OG1  | 2:N:236:GLY:HA3  | 2.21                     | 0.41              |
| 2:O:440:SER:OG   | 2:O:463:ILE:HB   | 2.21                     | 0.41              |
| 1:S:355:GLU:HB2  | 1:S:358:LEU:HD12 | 2.03                     | 0.41              |
| 1:S:426:LEU:O    | 1:S:430:LEU:HG   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:153:ILE:C    | 2:V:329:LEU:HD22 | 2.41                     | 0.41              |
| 2:W:185:THR:HA   | 2:W:218:VAL:O    | 2.21                     | 0.41              |
| 2:W:244:ARG:HG3  | 2:W:303:SER:N    | 2.36                     | 0.41              |
| 1:A:142:ARG:HG3  | 1:A:142:ARG:HH11 | 1.86                     | 0.41              |
| 2:D:201:MET:CE   | 2:D:215:VAL:HG11 | 2.50                     | 0.41              |
| 2:E:462:GLY:O    | 2:E:464:GLU:N    | 2.54                     | 0.41              |
| 1:J:316:GLU:HA   | 1:J:320:SER:OG   | 2.21                     | 0.41              |
| 1:K:161:ILE:HD13 | 1:K:326:LEU:HD21 | 2.03                     | 0.41              |
| 1:K:168:LEU:HD13 | 1:K:344:VAL:HG11 | 2.02                     | 0.41              |
| 2:M:134:LEU:HD11 | 2:M:174:ILE:HD12 | 2.03                     | 0.41              |
| 2:N:25:PHE:O     | 2:N:57:ASN:HB3   | 2.21                     | 0.41              |
| 1:T:211:LYS:HB2  | 1:T:214:THR:OG1  | 2.20                     | 0.41              |
| 2:V:97:ASN:ND2   | 2:V:101:GLU:HB2  | 2.34                     | 0.41              |
| 2:V:132:GLU:HB3  | 2:V:149:ARG:HB2  | 2.03                     | 0.41              |
| 2:V:377:THR:HG22 | 2:V:407:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:99:VAL:CG1   | 1:B:251:THR:HB   | 2.51                     | 0.40              |
| 3:G:86:SER:O     | 3:G:90:GLN:HG2   | 2.21                     | 0.40              |
| 1:K:141:ARG:HB2  | 2:O:195:ASN:ND2  | 2.36                     | 0.40              |
| 1:K:206:VAL:HG13 | 1:K:234:VAL:HB   | 2.02                     | 0.40              |
| 2:M:117:ILE:HD12 | 2:M:234:LEU:HB2  | 2.03                     | 0.40              |
| 1:L:82:ARG:HG2   | 2:O:34:LEU:HD12  | 2.03                     | 0.40              |
| 2:D:222:MET:HA   | 2:D:229:ARG:HD2  | 2.03                     | 0.40              |
| 2:E:185:THR:HG21 | 2:E:233:ALA:HA   | 2.03                     | 0.40              |
| 2:E:201:MET:HG2  | 2:E:206:VAL:CG2  | 2.51                     | 0.40              |
| 1:K:249:PRO:HG2  | 1:K:276:GLN:NE2  | 2.36                     | 0.40              |
| 1:L:329:ILE:HD11 | 1:L:344:VAL:HG21 | 2.03                     | 0.40              |
| 2:N:168:GLN:HE21 | 2:N:201:MET:CG   | 2.35                     | 0.40              |
| 1:S:96:ILE:HB    | 1:S:130:ARG:HD2  | 2.02                     | 0.40              |
| 1:T:174:GLN:HA   | 6:T:600:ANP:HNB1 | 1.86                     | 0.40              |
| 2:X:37:LEU:HD12  | 2:X:61:THR:HG21  | 2.02                     | 0.40              |
| 1:A:491:LEU:HD13 | 1:A:496:LEU:HD23 | 2.03                     | 0.40              |
| 2:D:93:GLY:HA2   | 2:D:207:ILE:HG12 | 2.03                     | 0.40              |
| 2:D:440:SER:OG   | 2:D:463:ILE:HB   | 2.22                     | 0.40              |
| 3:G:96:ARG:HE    | 3:G:121:THR:HG21 | 1.85                     | 0.40              |
| 1:J:168:LEU:HB2  | 1:J:348:THR:HG21 | 2.03                     | 0.40              |
| 1:K:161:ILE:HA   | 1:K:165:GLN:OE1  | 2.21                     | 0.40              |
| 1:K:212:ARG:NH1  | 2:N:123:SER:HA   | 2.36                     | 0.40              |
| 2:O:410:ILE:HG23 | 2:O:441:PHE:HE2  | 1.86                     | 0.40              |
| 3:P:75:VAL:HG22  | 3:P:108:VAL:HB   | 2.03                     | 0.40              |
| 3:P:74:ILE:O     | 3:P:107:ILE:HA   | 2.21                     | 0.40              |
| 1:T:109:VAL:HG13 | 1:T:233:ILE:HB   | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:53:GLU:HG2   | 1:T:54:LEU:H     | 1.87                     | 0.40              |
| 2:V:324:THR:HG22 | 2:V:324:THR:O    | 2.22                     | 0.40              |
| 1:S:347:ILE:HA   | 2:W:222:MET:SD   | 2.62                     | 0.40              |
| 1:B:139:LEU:HA   | 1:B:139:LEU:HD12 | 1.83                     | 0.40              |
| 1:B:382:VAL:HG11 | 1:B:440:THR:HG21 | 2.03                     | 0.40              |
| 2:F:449:TYR:HB3  | 2:F:452:ILE:HD12 | 2.02                     | 0.40              |
| 3:G:78:THR:HG23  | 3:G:91:LEU:HD23  | 2.03                     | 0.40              |
| 4:H:14:PHE:HB2   | 4:H:22:TYR:HB2   | 2.02                     | 0.40              |
| 2:N:32:ALA:O     | 2:N:35:ASN:HB2   | 2.22                     | 0.40              |
| 1:K:50:GLN:NE2   | 2:O:69:GLY:HA2   | 2.37                     | 0.40              |
| 1:S:237:THR:N    | 1:S:240:GLU:OE1  | 2.55                     | 0.40              |
| 2:V:239:ILE:O    | 2:V:243:PHE:HD2  | 2.05                     | 0.40              |
| 1:U:337:SER:HB3  | 2:V:314:ALA:HB1  | 2.02                     | 0.40              |
| 1:B:282:GLN:OE1  | 2:E:284:THR:HA   | 2.21                     | 0.40              |
| 2:D:348:VAL:O    | 2:D:350:PRO:HD3  | 2.21                     | 0.40              |
| 2:M:237:LEU:CD2  | 2:M:292:LEU:HD12 | 2.51                     | 0.40              |
| 1:S:49:ILE:HG23  | 1:S:68:LEU:HD22  | 2.04                     | 0.40              |
| 1:U:260:ARG:O    | 1:U:321:GLY:HA3  | 2.22                     | 0.40              |
| 1:U:69:GLU:HB3   | 1:U:70:PRO:HD2   | 2.03                     | 0.40              |
| 2:V:258:ILE:HG13 | 2:V:258:ILE:O    | 2.21                     | 0.40              |
| 2:W:183:VAL:HG11 | 2:W:236:GLY:O    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 478/510 (94%) | 454 (95%) | 23 (5%) | 1 (0%)   | 47          | 82 |
| 1   | B     | 479/510 (94%) | 448 (94%) | 30 (6%) | 1 (0%)   | 47          | 82 |
| 1   | C     | 482/510 (94%) | 453 (94%) | 28 (6%) | 1 (0%)   | 47          | 82 |
| 1   | J     | 477/510 (94%) | 460 (96%) | 16 (3%) | 1 (0%)   | 47          | 82 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | K     | 482/510 (94%)    | 442 (92%)  | 35 (7%)  | 5 (1%)   | 15          | 53  |
| 1   | L     | 478/510 (94%)    | 450 (94%)  | 27 (6%)  | 1 (0%)   | 47          | 82  |
| 1   | S     | 474/510 (93%)    | 447 (94%)  | 25 (5%)  | 2 (0%)   | 34          | 72  |
| 1   | T     | 475/510 (93%)    | 438 (92%)  | 33 (7%)  | 4 (1%)   | 19          | 57  |
| 1   | U     | 477/510 (94%)    | 432 (91%)  | 39 (8%)  | 6 (1%)   | 12          | 45  |
| 2   | D     | 468/484 (97%)    | 439 (94%)  | 28 (6%)  | 1 (0%)   | 47          | 82  |
| 2   | E     | 466/484 (96%)    | 436 (94%)  | 28 (6%)  | 2 (0%)   | 34          | 72  |
| 2   | F     | 467/484 (96%)    | 435 (93%)  | 27 (6%)  | 5 (1%)   | 14          | 50  |
| 2   | M     | 468/484 (97%)    | 437 (93%)  | 30 (6%)  | 1 (0%)   | 47          | 82  |
| 2   | N     | 468/484 (97%)    | 431 (92%)  | 33 (7%)  | 4 (1%)   | 17          | 55  |
| 2   | O     | 466/484 (96%)    | 442 (95%)  | 24 (5%)  | 0        | 100         | 100 |
| 2   | V     | 468/484 (97%)    | 423 (90%)  | 38 (8%)  | 7 (2%)   | 10          | 42  |
| 2   | W     | 465/484 (96%)    | 432 (93%)  | 30 (6%)  | 3 (1%)   | 25          | 64  |
| 2   | X     | 467/484 (96%)    | 432 (92%)  | 33 (7%)  | 2 (0%)   | 34          | 72  |
| 3   | G     | 262/278 (94%)    | 245 (94%)  | 17 (6%)  | 0        | 100         | 100 |
| 3   | P     | 234/278 (84%)    | 210 (90%)  | 19 (8%)  | 5 (2%)   | 7           | 33  |
| 3   | Y     | 189/278 (68%)    | 176 (93%)  | 13 (7%)  | 0        | 100         | 100 |
| 4   | H     | 110/138 (80%)    | 89 (81%)   | 19 (17%) | 2 (2%)   | 8           | 37  |
| 4   | Q     | 74/138 (54%)     | 61 (82%)   | 13 (18%) | 0        | 100         | 100 |
| 4   | Z     | 15/138 (11%)     | 11 (73%)   | 3 (20%)  | 1 (7%)   | 1           | 6   |
| 5   | 1     | 23/61 (38%)      | 19 (83%)   | 3 (13%)  | 1 (4%)   | 2           | 15  |
| 5   | I     | 43/61 (70%)      | 33 (77%)   | 6 (14%)  | 4 (9%)   | 0           | 3   |
| 5   | R     | 30/61 (49%)      | 25 (83%)   | 5 (17%)  | 0        | 100         | 100 |
| All | All   | 9485/10377 (91%) | 8800 (93%) | 625 (7%) | 60 (1%)  | 25          | 64  |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 101 | ILE  |
| 5   | I     | 55  | GLU  |
| 1   | L     | 390 | GLY  |
| 2   | N     | 221 | GLN  |
| 2   | V     | 347 | ALA  |
| 2   | W     | 54  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 390 | GLY  |
| 2   | D     | 27  | GLN  |
| 2   | E     | 463 | ILE  |
| 1   | K     | 412 | LEU  |
| 3   | P     | 134 | GLY  |
| 1   | T     | 46  | LEU  |
| 1   | U     | 97  | VAL  |
| 1   | U     | 298 | GLY  |
| 2   | V     | 27  | GLN  |
| 2   | V     | 68  | GLU  |
| 2   | F     | 315 | ASP  |
| 5   | I     | 29  | LEU  |
| 1   | J     | 403 | ALA  |
| 1   | K     | 316 | GLU  |
| 1   | K     | 373 | VAL  |
| 3   | P     | 202 | ASP  |
| 1   | S     | 406 | ALA  |
| 2   | W     | 28  | SER  |
| 1   | B     | 363 | ILE  |
| 2   | F     | 34  | LEU  |
| 2   | F     | 83  | ILE  |
| 2   | F     | 105 | GLU  |
| 1   | K     | 457 | GLY  |
| 1   | T     | 59  | SER  |
| 1   | T     | 60  | GLY  |
| 1   | U     | 226 | ASP  |
| 1   | U     | 406 | ALA  |
| 2   | X     | 390 | ILE  |
| 4   | Z     | 120 | ALA  |
| 2   | E     | 455 | HIS  |
| 4   | H     | 36  | SER  |
| 1   | K     | 97  | VAL  |
| 2   | M     | 460 | VAL  |
| 3   | P     | 205 | VAL  |
| 1   | U     | 46  | LEU  |
| 2   | V     | 28  | SER  |
| 2   | V     | 34  | LEU  |
| 2   | W     | 158 | GLY  |
| 1   | A     | 70  | PRO  |
| 2   | F     | 347 | ALA  |
| 5   | I     | 28  | GLU  |
| 1   | U     | 140 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | X     | 18  | GLY  |
| 2   | N     | 108 | PRO  |
| 3   | P     | 133 | ILE  |
| 5   | I     | 56  | PRO  |
| 3   | P     | 95  | VAL  |
| 2   | V     | 346 | PRO  |
| 5   | 1     | 21  | ILE  |
| 1   | T     | 390 | GLY  |
| 2   | N     | 158 | GLY  |
| 1   | S     | 97  | VAL  |
| 2   | V     | 82  | PRO  |
| 2   | N     | 428 | 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     | 388/412 (94%) | 369 (95%) | 19 (5%)  | 25          | 61 |
| 1   | B     | 388/412 (94%) | 373 (96%) | 15 (4%)  | 32          | 69 |
| 1   | C     | 390/412 (95%) | 378 (97%) | 12 (3%)  | 40          | 75 |
| 1   | J     | 387/412 (94%) | 372 (96%) | 15 (4%)  | 32          | 69 |
| 1   | K     | 390/412 (95%) | 372 (95%) | 18 (5%)  | 27          | 64 |
| 1   | L     | 388/412 (94%) | 365 (94%) | 23 (6%)  | 19          | 54 |
| 1   | S     | 385/412 (93%) | 365 (95%) | 20 (5%)  | 23          | 59 |
| 1   | T     | 386/412 (94%) | 371 (96%) | 15 (4%)  | 32          | 69 |
| 1   | U     | 387/412 (94%) | 376 (97%) | 11 (3%)  | 43          | 77 |
| 2   | D     | 379/390 (97%) | 362 (96%) | 17 (4%)  | 27          | 64 |
| 2   | E     | 370/390 (95%) | 354 (96%) | 16 (4%)  | 29          | 66 |
| 2   | F     | 375/390 (96%) | 358 (96%) | 17 (4%)  | 27          | 64 |
| 2   | M     | 378/390 (97%) | 360 (95%) | 18 (5%)  | 25          | 62 |
| 2   | N     | 378/390 (97%) | 357 (94%) | 21 (6%)  | 21          | 56 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2   | O     | 378/390 (97%)   | 366 (97%)  | 12 (3%)  | 39          | 74  |
| 2   | V     | 379/390 (97%)   | 364 (96%)  | 15 (4%)  | 31          | 68  |
| 2   | W     | 378/390 (97%)   | 360 (95%)  | 18 (5%)  | 25          | 62  |
| 2   | X     | 379/390 (97%)   | 364 (96%)  | 15 (4%)  | 31          | 68  |
| 3   | G     | 226/236 (96%)   | 210 (93%)  | 16 (7%)  | 14          | 46  |
| 3   | P     | 200/236 (85%)   | 184 (92%)  | 16 (8%)  | 12          | 40  |
| 3   | Y     | 164/236 (70%)   | 150 (92%)  | 14 (8%)  | 10          | 38  |
| 4   | H     | 64/112 (57%)    | 54 (84%)   | 10 (16%) | 2           | 13  |
| 4   | Q     | 11/112 (10%)    | 9 (82%)    | 2 (18%)  | 1           | 9   |
| 5   | 1     | 2/48 (4%)       | 2 (100%)   | 0        | 100         | 100 |
| 5   | I     | 28/48 (58%)     | 25 (89%)   | 3 (11%)  | 6           | 26  |
| 5   | R     | 5/48 (10%)      | 4 (80%)    | 1 (20%)  | 1           | 7   |
| All | All   | 7583/8294 (91%) | 7224 (95%) | 359 (5%) | 26          | 63  |

All (359) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | PRO  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 142 | ARG  |
| 1   | A     | 166 | ARG  |
| 1   | A     | 246 | TYR  |
| 1   | A     | 251 | THR  |
| 1   | A     | 284 | SER  |
| 1   | A     | 288 | ARG  |
| 1   | A     | 373 | VAL  |
| 1   | A     | 378 | SER  |
| 1   | A     | 413 | ASP  |
| 1   | A     | 436 | SER  |
| 1   | A     | 458 | ILE  |
| 1   | A     | 460 | LEU  |
| 1   | A     | 472 | SER  |
| 1   | A     | 480 | GLU  |
| 1   | A     | 481 | LEU  |
| 1   | A     | 499 | LEU  |
| 1   | A     | 509 | THR  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 30  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 91  | LYS  |
| 1   | B     | 99  | VAL  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 159 | VAL  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 197 | GLU  |
| 1   | B     | 204 | VAL  |
| 1   | B     | 212 | ARG  |
| 1   | B     | 283 | LEU  |
| 1   | B     | 309 | GLU  |
| 1   | B     | 400 | ARG  |
| 1   | B     | 468 | SER  |
| 1   | B     | 509 | THR  |
| 1   | C     | 69  | GLU  |
| 1   | C     | 99  | VAL  |
| 1   | C     | 166 | ARG  |
| 1   | C     | 198 | SER  |
| 1   | C     | 220 | GLN  |
| 1   | C     | 283 | LEU  |
| 1   | C     | 293 | ARG  |
| 1   | C     | 346 | SER  |
| 1   | C     | 364 | ARG  |
| 1   | C     | 375 | ARG  |
| 1   | C     | 394 | LEU  |
| 1   | C     | 465 | GLU  |
| 2   | D     | 7   | THR  |
| 2   | D     | 58  | THR  |
| 2   | D     | 89  | ARG  |
| 2   | D     | 132 | GLU  |
| 2   | D     | 210 | GLU  |
| 2   | D     | 251 | VAL  |
| 2   | D     | 274 | ARG  |
| 2   | D     | 287 | THR  |
| 2   | D     | 299 | THR  |
| 2   | D     | 303 | SER  |
| 2   | D     | 322 | PRO  |
| 2   | D     | 386 | ASP  |
| 2   | D     | 398 | GLU  |
| 2   | D     | 413 | PHE  |
| 2   | D     | 431 | LEU  |
| 2   | D     | 464 | GLU  |
| 2   | D     | 467 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 43  | GLN  |
| 2   | E     | 58  | THR  |
| 2   | E     | 68  | GLU  |
| 2   | E     | 111 | SER  |
| 2   | E     | 115 | LYS  |
| 2   | E     | 140 | VAL  |
| 2   | E     | 204 | THR  |
| 2   | E     | 210 | GLU  |
| 2   | E     | 232 | VAL  |
| 2   | E     | 269 | SER  |
| 2   | E     | 337 | ARG  |
| 2   | E     | 352 | ASP  |
| 2   | E     | 356 | ARG  |
| 2   | E     | 390 | ILE  |
| 2   | E     | 402 | LEU  |
| 2   | E     | 436 | ASP  |
| 2   | F     | 27  | GLN  |
| 2   | F     | 28  | SER  |
| 2   | F     | 45  | LYS  |
| 2   | F     | 68  | GLU  |
| 2   | F     | 113 | LEU  |
| 2   | F     | 132 | GLU  |
| 2   | F     | 133 | ILE  |
| 2   | F     | 140 | VAL  |
| 2   | F     | 201 | MET  |
| 2   | F     | 208 | ASN  |
| 2   | F     | 297 | THR  |
| 2   | F     | 303 | SER  |
| 2   | F     | 336 | SER  |
| 2   | F     | 355 | SER  |
| 2   | F     | 403 | THR  |
| 2   | F     | 420 | VAL  |
| 2   | F     | 464 | GLU  |
| 3   | G     | 3   | LEU  |
| 3   | G     | 9   | ARG  |
| 3   | G     | 11  | LYS  |
| 3   | G     | 21  | LYS  |
| 3   | G     | 48  | GLU  |
| 3   | G     | 53  | LYS  |
| 3   | G     | 77  | ILE  |
| 3   | G     | 97  | ARG  |
| 3   | G     | 118 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 133 | ILE  |
| 3   | G     | 150 | LEU  |
| 3   | G     | 153 | VAL  |
| 3   | G     | 235 | ASN  |
| 3   | G     | 239 | ASN  |
| 3   | G     | 252 | SER  |
| 3   | G     | 276 | SER  |
| 4   | H     | 14  | PHE  |
| 4   | H     | 20  | THR  |
| 4   | H     | 22  | TYR  |
| 4   | H     | 27  | VAL  |
| 4   | H     | 35  | LYS  |
| 4   | H     | 36  | SER  |
| 4   | H     | 39  | ILE  |
| 4   | H     | 46  | VAL  |
| 4   | H     | 48  | THR  |
| 4   | H     | 70  | ILE  |
| 5   | I     | 27  | THR  |
| 5   | I     | 35  | LEU  |
| 5   | I     | 57  | THR  |
| 1   | J     | 26  | ASN  |
| 1   | J     | 27  | LEU  |
| 1   | J     | 134 | LYS  |
| 1   | J     | 166 | ARG  |
| 1   | J     | 175 | THR  |
| 1   | J     | 183 | ASP  |
| 1   | J     | 237 | THR  |
| 1   | J     | 373 | VAL  |
| 1   | J     | 418 | GLN  |
| 1   | J     | 429 | LEU  |
| 1   | J     | 440 | THR  |
| 1   | J     | 468 | SER  |
| 1   | J     | 469 | SER  |
| 1   | J     | 481 | LEU  |
| 1   | J     | 509 | THR  |
| 1   | K     | 23  | ASP  |
| 1   | K     | 40  | ILE  |
| 1   | K     | 58  | SER  |
| 1   | K     | 68  | LEU  |
| 1   | K     | 99  | VAL  |
| 1   | K     | 106 | LEU  |
| 1   | K     | 134 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 143 | SER  |
| 1   | K     | 166 | ARG  |
| 1   | K     | 199 | LYS  |
| 1   | K     | 246 | TYR  |
| 1   | K     | 309 | GLU  |
| 1   | K     | 320 | SER  |
| 1   | K     | 371 | LEU  |
| 1   | K     | 399 | TYR  |
| 1   | K     | 411 | ASP  |
| 1   | K     | 462 | ARG  |
| 1   | K     | 504 | GLU  |
| 1   | L     | 99  | VAL  |
| 1   | L     | 132 | GLN  |
| 1   | L     | 142 | ARG  |
| 1   | L     | 163 | ARG  |
| 1   | L     | 166 | ARG  |
| 1   | L     | 189 | LYS  |
| 1   | L     | 198 | SER  |
| 1   | L     | 220 | GLN  |
| 1   | L     | 231 | SER  |
| 1   | L     | 267 | LEU  |
| 1   | L     | 284 | SER  |
| 1   | L     | 293 | ARG  |
| 1   | L     | 342 | THR  |
| 1   | L     | 400 | ARG  |
| 1   | L     | 405 | PHE  |
| 1   | L     | 419 | THR  |
| 1   | L     | 436 | SER  |
| 1   | L     | 465 | GLU  |
| 1   | L     | 468 | SER  |
| 1   | L     | 469 | SER  |
| 1   | L     | 476 | SER  |
| 1   | L     | 480 | GLU  |
| 1   | L     | 481 | LEU  |
| 2   | M     | 57  | ASN  |
| 2   | M     | 89  | ARG  |
| 2   | M     | 90  | GLU  |
| 2   | M     | 132 | GLU  |
| 2   | M     | 182 | SER  |
| 2   | M     | 206 | VAL  |
| 2   | M     | 210 | GLU  |
| 2   | M     | 224 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 250 | ASP  |
| 2   | M     | 261 | PHE  |
| 2   | M     | 342 | LEU  |
| 2   | M     | 359 | ASP  |
| 2   | M     | 385 | GLN  |
| 2   | M     | 386 | ASP  |
| 2   | M     | 394 | ASP  |
| 2   | M     | 413 | PHE  |
| 2   | M     | 434 | LEU  |
| 2   | M     | 460 | VAL  |
| 2   | N     | 68  | GLU  |
| 2   | N     | 113 | LEU  |
| 2   | N     | 126 | GLU  |
| 2   | N     | 130 | SER  |
| 2   | N     | 132 | GLU  |
| 2   | N     | 140 | VAL  |
| 2   | N     | 152 | LYS  |
| 2   | N     | 212 | GLU  |
| 2   | N     | 221 | GLN  |
| 2   | N     | 232 | VAL  |
| 2   | N     | 318 | THR  |
| 2   | N     | 330 | ASP  |
| 2   | N     | 376 | GLU  |
| 2   | N     | 386 | ASP  |
| 2   | N     | 387 | ILE  |
| 2   | N     | 393 | MET  |
| 2   | N     | 423 | VAL  |
| 2   | N     | 450 | ASP  |
| 2   | N     | 458 | TYR  |
| 2   | N     | 463 | ILE  |
| 2   | N     | 465 | ASP  |
| 2   | O     | 30  | LEU  |
| 2   | O     | 77  | LEU  |
| 2   | O     | 84  | SER  |
| 2   | O     | 140 | VAL  |
| 2   | O     | 149 | ARG  |
| 2   | O     | 167 | ILE  |
| 2   | O     | 192 | ARG  |
| 2   | O     | 274 | ARG  |
| 2   | O     | 297 | THR  |
| 2   | O     | 402 | LEU  |
| 2   | O     | 413 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 455 | HIS  |
| 3   | P     | 3   | LEU  |
| 3   | P     | 11  | LYS  |
| 3   | P     | 35  | GLU  |
| 3   | P     | 42  | LYS  |
| 3   | P     | 99  | LEU  |
| 3   | P     | 107 | ILE  |
| 3   | P     | 130 | ILE  |
| 3   | P     | 133 | ILE  |
| 3   | P     | 136 | ASP  |
| 3   | P     | 141 | GLN  |
| 3   | P     | 155 | LYS  |
| 3   | P     | 178 | SER  |
| 3   | P     | 186 | LYS  |
| 3   | P     | 189 | GLU  |
| 3   | P     | 218 | MET  |
| 3   | P     | 220 | THR  |
| 4   | Q     | 39  | ILE  |
| 4   | Q     | 45  | HIS  |
| 5   | R     | 31  | THR  |
| 1   | S     | 32  | ARG  |
| 1   | S     | 105 | LEU  |
| 1   | S     | 111 | ASP  |
| 1   | S     | 115 | ASN  |
| 1   | S     | 123 | ILE  |
| 1   | S     | 124 | ASP  |
| 1   | S     | 134 | LYS  |
| 1   | S     | 139 | LEU  |
| 1   | S     | 189 | LYS  |
| 1   | S     | 267 | LEU  |
| 1   | S     | 318 | GLU  |
| 1   | S     | 360 | TYR  |
| 1   | S     | 373 | VAL  |
| 1   | S     | 383 | LYS  |
| 1   | S     | 441 | GLU  |
| 1   | S     | 459 | GLU  |
| 1   | S     | 490 | GLU  |
| 1   | S     | 496 | LEU  |
| 1   | S     | 504 | GLU  |
| 1   | S     | 505 | SER  |
| 1   | T     | 26  | ASN  |
| 1   | T     | 67  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 95  | ASN  |
| 1   | T     | 99  | VAL  |
| 1   | T     | 138 | ILE  |
| 1   | T     | 159 | VAL  |
| 1   | T     | 246 | TYR  |
| 1   | T     | 371 | LEU  |
| 1   | T     | 373 | VAL  |
| 1   | T     | 401 | GLU  |
| 1   | T     | 427 | THR  |
| 1   | T     | 428 | GLN  |
| 1   | T     | 465 | GLU  |
| 1   | T     | 469 | SER  |
| 1   | T     | 483 | THR  |
| 1   | U     | 82  | ARG  |
| 1   | U     | 88  | GLU  |
| 1   | U     | 172 | ASP  |
| 1   | U     | 174 | GLN  |
| 1   | U     | 304 | HIS  |
| 1   | U     | 339 | TYR  |
| 1   | U     | 383 | LYS  |
| 1   | U     | 388 | VAL  |
| 1   | U     | 394 | LEU  |
| 1   | U     | 419 | THR  |
| 1   | U     | 440 | THR  |
| 2   | V     | 46  | LEU  |
| 2   | V     | 133 | ILE  |
| 2   | V     | 149 | ARG  |
| 2   | V     | 192 | ARG  |
| 2   | V     | 204 | THR  |
| 2   | V     | 250 | ASP  |
| 2   | V     | 268 | VAL  |
| 2   | V     | 354 | LYS  |
| 2   | V     | 357 | LEU  |
| 2   | V     | 386 | ASP  |
| 2   | V     | 387 | ILE  |
| 2   | V     | 413 | PHE  |
| 2   | V     | 423 | VAL  |
| 2   | V     | 425 | THR  |
| 2   | V     | 460 | VAL  |
| 2   | W     | 27  | GLN  |
| 2   | W     | 65  | ASP  |
| 2   | W     | 106 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | W     | 109 | ILE  |
| 2   | W     | 140 | VAL  |
| 2   | W     | 204 | THR  |
| 2   | W     | 210 | GLU  |
| 2   | W     | 232 | VAL  |
| 2   | W     | 257 | ASN  |
| 2   | W     | 284 | THR  |
| 2   | W     | 324 | THR  |
| 2   | W     | 352 | ASP  |
| 2   | W     | 373 | LYS  |
| 2   | W     | 386 | ASP  |
| 2   | W     | 387 | ILE  |
| 2   | W     | 393 | MET  |
| 2   | W     | 433 | ARG  |
| 2   | W     | 448 | LYS  |
| 2   | X     | 14  | THR  |
| 2   | X     | 22  | ASP  |
| 2   | X     | 27  | GLN  |
| 2   | X     | 29  | GLU  |
| 2   | X     | 46  | LEU  |
| 2   | X     | 84  | SER  |
| 2   | X     | 155 | LEU  |
| 2   | X     | 167 | ILE  |
| 2   | X     | 208 | ASN  |
| 2   | X     | 250 | ASP  |
| 2   | X     | 274 | ARG  |
| 2   | X     | 336 | SER  |
| 2   | X     | 356 | ARG  |
| 2   | X     | 427 | ILE  |
| 2   | X     | 454 | GLU  |
| 3   | Y     | 15  | ASN  |
| 3   | Y     | 19  | ILE  |
| 3   | Y     | 101 | ASP  |
| 3   | Y     | 112 | ASP  |
| 3   | Y     | 119 | LEU  |
| 3   | Y     | 121 | THR  |
| 3   | Y     | 131 | ASN  |
| 3   | Y     | 136 | ASP  |
| 3   | Y     | 142 | GLU  |
| 3   | Y     | 162 | ILE  |
| 3   | Y     | 167 | ASN  |
| 3   | Y     | 216 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Y     | 267 | LEU  |
| 3   | Y     | 271 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | HIS  |
| 1   | A     | 418 | GLN  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 428 | GLN  |
| 1   | C     | 72  | GLN  |
| 1   | C     | 174 | GLN  |
| 1   | C     | 210 | GLN  |
| 1   | C     | 418 | GLN  |
| 2   | D     | 178 | HIS  |
| 2   | D     | 208 | ASN  |
| 2   | D     | 375 | GLN  |
| 2   | E     | 168 | GLN  |
| 2   | F     | 27  | GLN  |
| 2   | F     | 208 | ASN  |
| 3   | G     | 49  | GLN  |
| 3   | G     | 59  | ASN  |
| 3   | G     | 102 | GLN  |
| 3   | G     | 117 | GLN  |
| 3   | G     | 216 | ASN  |
| 3   | G     | 235 | ASN  |
| 4   | H     | 45  | HIS  |
| 4   | H     | 51  | GLN  |
| 1   | J     | 26  | ASN  |
| 1   | J     | 174 | GLN  |
| 1   | J     | 262 | ASN  |
| 1   | J     | 351 | GLN  |
| 1   | J     | 479 | ASN  |
| 1   | K     | 50  | GLN  |
| 1   | K     | 217 | GLN  |
| 1   | K     | 265 | HIS  |
| 1   | K     | 428 | GLN  |
| 1   | L     | 132 | GLN  |
| 1   | L     | 174 | GLN  |
| 1   | L     | 217 | GLN  |
| 1   | L     | 220 | GLN  |
| 1   | L     | 398 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 195 | ASN  |
| 2   | M     | 367 | HIS  |
| 2   | M     | 375 | GLN  |
| 2   | N     | 168 | GLN  |
| 2   | O     | 27  | GLN  |
| 2   | O     | 208 | ASN  |
| 2   | O     | 328 | HIS  |
| 3   | P     | 88  | HIS  |
| 3   | P     | 141 | GLN  |
| 4   | Q     | 51  | GLN  |
| 1   | T     | 67  | ASN  |
| 1   | T     | 145 | HIS  |
| 1   | T     | 149 | GLN  |
| 1   | T     | 217 | GLN  |
| 1   | T     | 304 | HIS  |
| 1   | T     | 387 | GLN  |
| 1   | U     | 225 | HIS  |
| 1   | U     | 262 | ASN  |
| 1   | U     | 387 | GLN  |
| 1   | U     | 479 | ASN  |
| 2   | V     | 118 | HIS  |
| 2   | V     | 168 | GLN  |
| 2   | W     | 27  | GLN  |
| 2   | W     | 385 | GLN  |
| 2   | X     | 27  | GLN  |
| 2   | X     | 43  | GLN  |
| 2   | X     | 118 | HIS  |
| 2   | X     | 263 | GLN  |
| 2   | X     | 328 | HIS  |
| 2   | X     | 365 | GLN  |
| 3   | Y     | 100 | ASN  |
| 3   | Y     | 122 | HIS  |
| 3   | Y     | 260 | GLN  |
| 3   | Y     | 265 | 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 6   | ANP  | X     | 600 | 7    | 29,33,33     | 1.77 | 6 (20%)     | 31,52,52    | 2.17 | 8 (25%)     |
| 6   | ANP  | C     | 600 | 7    | 29,33,33     | 1.85 | 9 (31%)     | 31,52,52    | 2.01 | 8 (25%)     |
| 6   | ANP  | D     | 600 | 7    | 29,33,33     | 1.71 | 7 (24%)     | 31,52,52    | 1.77 | 8 (25%)     |
| 6   | ANP  | F     | 600 | 7    | 29,33,33     | 1.78 | 7 (24%)     | 31,52,52    | 1.95 | 8 (25%)     |
| 6   | ANP  | A     | 600 | 7    | 29,33,33     | 1.88 | 8 (27%)     | 31,52,52    | 1.87 | 5 (16%)     |
| 6   | ANP  | B     | 600 | 7    | 29,33,33     | 1.78 | 6 (20%)     | 31,52,52    | 1.93 | 6 (19%)     |
| 6   | ANP  | K     | 600 | 7    | 29,33,33     | 1.81 | 7 (24%)     | 31,52,52    | 2.12 | 9 (29%)     |
| 6   | ANP  | L     | 600 | 7    | 29,33,33     | 1.95 | 8 (27%)     | 31,52,52    | 1.86 | 7 (22%)     |
| 6   | ANP  | M     | 600 | 7    | 29,33,33     | 1.68 | 5 (17%)     | 31,52,52    | 2.21 | 6 (19%)     |
| 6   | ANP  | J     | 600 | 7    | 29,33,33     | 1.77 | 6 (20%)     | 31,52,52    | 1.97 | 7 (22%)     |
| 6   | ANP  | S     | 600 | 7    | 29,33,33     | 1.89 | 7 (24%)     | 31,52,52    | 1.93 | 8 (25%)     |
| 6   | ANP  | T     | 600 | 7    | 29,33,33     | 1.90 | 6 (20%)     | 31,52,52    | 1.97 | 8 (25%)     |
| 6   | ANP  | U     | 600 | 7    | 29,33,33     | 1.81 | 7 (24%)     | 31,52,52    | 2.15 | 8 (25%)     |
| 6   | ANP  | V     | 600 | 7    | 29,33,33     | 1.76 | 6 (20%)     | 31,52,52    | 2.10 | 8 (25%)     |
| 6   | ANP  | O     | 600 | 7    | 29,33,33     | 1.77 | 6 (20%)     | 31,52,52    | 1.97 | 7 (22%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | ANP  | X     | 600 | 7    | -       | 8/14/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | ANP  | C     | 600 | 7    | -       | 3/14/38/38 | 0/3/3/3 |
| 6   | ANP  | D     | 600 | 7    | -       | 4/14/38/38 | 0/3/3/3 |
| 6   | ANP  | F     | 600 | 7    | -       | 3/14/38/38 | 0/3/3/3 |
| 6   | ANP  | A     | 600 | 7    | -       | 2/14/38/38 | 0/3/3/3 |
| 6   | ANP  | B     | 600 | 7    | -       | 2/14/38/38 | 0/3/3/3 |
| 6   | ANP  | K     | 600 | 7    | -       | 9/14/38/38 | 0/3/3/3 |
| 6   | ANP  | L     | 600 | 7    | -       | 2/14/38/38 | 0/3/3/3 |
| 6   | ANP  | M     | 600 | 7    | -       | 4/14/38/38 | 0/3/3/3 |
| 6   | ANP  | J     | 600 | 7    | -       | 2/14/38/38 | 0/3/3/3 |
| 6   | ANP  | S     | 600 | 7    | -       | 4/14/38/38 | 0/3/3/3 |
| 6   | ANP  | T     | 600 | 7    | -       | 2/14/38/38 | 0/3/3/3 |
| 6   | ANP  | U     | 600 | 7    | -       | 4/14/38/38 | 0/3/3/3 |
| 6   | ANP  | V     | 600 | 7    | -       | 7/14/38/38 | 0/3/3/3 |
| 6   | ANP  | O     | 600 | 7    | -       | 3/14/38/38 | 0/3/3/3 |

All (101) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 6   | S     | 600 | ANP  | PG-N3B | 4.80 | 1.75        | 1.63     |
| 6   | L     | 600 | ANP  | PG-N3B | 4.79 | 1.75        | 1.63     |
| 6   | T     | 600 | ANP  | PG-N3B | 4.64 | 1.75        | 1.63     |
| 6   | T     | 600 | ANP  | PB-N3B | 4.55 | 1.75        | 1.63     |
| 6   | X     | 600 | ANP  | PB-N3B | 4.51 | 1.75        | 1.63     |
| 6   | A     | 600 | ANP  | PG-N3B | 4.47 | 1.75        | 1.63     |
| 6   | S     | 600 | ANP  | PB-N3B | 4.47 | 1.75        | 1.63     |
| 6   | C     | 600 | ANP  | PB-N3B | 4.41 | 1.74        | 1.63     |
| 6   | C     | 600 | ANP  | PG-N3B | 4.38 | 1.74        | 1.63     |
| 6   | U     | 600 | ANP  | PB-N3B | 4.37 | 1.74        | 1.63     |
| 6   | L     | 600 | ANP  | PB-N3B | 4.34 | 1.74        | 1.63     |
| 6   | X     | 600 | ANP  | PG-N3B | 4.22 | 1.74        | 1.63     |
| 6   | J     | 600 | ANP  | PB-N3B | 4.21 | 1.74        | 1.63     |
| 6   | B     | 600 | ANP  | PG-N3B | 4.19 | 1.74        | 1.63     |
| 6   | V     | 600 | ANP  | PG-N3B | 4.17 | 1.74        | 1.63     |
| 6   | D     | 600 | ANP  | PG-N3B | 4.16 | 1.74        | 1.63     |
| 6   | F     | 600 | ANP  | PG-N3B | 4.14 | 1.74        | 1.63     |
| 6   | F     | 600 | ANP  | PB-N3B | 4.12 | 1.74        | 1.63     |
| 6   | D     | 600 | ANP  | PB-N3B | 4.12 | 1.74        | 1.63     |
| 6   | B     | 600 | ANP  | PB-N3B | 4.08 | 1.74        | 1.63     |
| 6   | J     | 600 | ANP  | PG-N3B | 4.04 | 1.73        | 1.63     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 6   | A     | 600 | ANP  | PB-N3B | 4.04 | 1.73        | 1.63     |
| 6   | U     | 600 | ANP  | PG-N3B | 4.02 | 1.73        | 1.63     |
| 6   | T     | 600 | ANP  | PG-O1G | 4.00 | 1.52        | 1.46     |
| 6   | O     | 600 | ANP  | PB-N3B | 3.95 | 1.73        | 1.63     |
| 6   | O     | 600 | ANP  | PG-N3B | 3.93 | 1.73        | 1.63     |
| 6   | K     | 600 | ANP  | PB-N3B | 3.90 | 1.73        | 1.63     |
| 6   | V     | 600 | ANP  | PB-N3B | 3.89 | 1.73        | 1.63     |
| 6   | M     | 600 | ANP  | PB-N3B | 3.88 | 1.73        | 1.63     |
| 6   | A     | 600 | ANP  | PB-O1B | 3.62 | 1.51        | 1.46     |
| 6   | K     | 600 | ANP  | PG-N3B | 3.62 | 1.72        | 1.63     |
| 6   | K     | 600 | ANP  | PB-O3A | 3.48 | 1.63        | 1.59     |
| 6   | S     | 600 | ANP  | PG-O1G | 3.47 | 1.51        | 1.46     |
| 6   | U     | 600 | ANP  | PG-O1G | 3.46 | 1.51        | 1.46     |
| 6   | M     | 600 | ANP  | PG-N3B | 3.46 | 1.72        | 1.63     |
| 6   | M     | 600 | ANP  | PB-O1B | 3.46 | 1.51        | 1.46     |
| 6   | A     | 600 | ANP  | PG-O1G | 3.45 | 1.51        | 1.46     |
| 6   | M     | 600 | ANP  | PG-O1G | 3.34 | 1.51        | 1.46     |
| 6   | B     | 600 | ANP  | PG-O1G | 3.34 | 1.51        | 1.46     |
| 6   | K     | 600 | ANP  | PG-O1G | 3.32 | 1.51        | 1.46     |
| 6   | C     | 600 | ANP  | PB-O1B | 3.30 | 1.51        | 1.46     |
| 6   | V     | 600 | ANP  | PB-O1B | 3.28 | 1.51        | 1.46     |
| 6   | T     | 600 | ANP  | PB-O1B | 3.28 | 1.51        | 1.46     |
| 6   | K     | 600 | ANP  | PB-O1B | 3.26 | 1.51        | 1.46     |
| 6   | J     | 600 | ANP  | PG-O1G | 3.22 | 1.51        | 1.46     |
| 6   | C     | 600 | ANP  | PG-O1G | 3.21 | 1.51        | 1.46     |
| 6   | D     | 600 | ANP  | PG-O1G | 3.18 | 1.51        | 1.46     |
| 6   | O     | 600 | ANP  | PG-O1G | 3.17 | 1.51        | 1.46     |
| 6   | F     | 600 | ANP  | PG-O1G | 3.15 | 1.51        | 1.46     |
| 6   | V     | 600 | ANP  | PG-O1G | 3.13 | 1.51        | 1.46     |
| 6   | U     | 600 | ANP  | PB-O1B | 3.13 | 1.51        | 1.46     |
| 6   | L     | 600 | ANP  | PB-O1B | 3.10 | 1.51        | 1.46     |
| 6   | X     | 600 | ANP  | PB-O1B | 3.05 | 1.51        | 1.46     |
| 6   | L     | 600 | ANP  | PB-O3A | 3.02 | 1.62        | 1.59     |
| 6   | O     | 600 | ANP  | PB-O3A | 3.02 | 1.62        | 1.59     |
| 6   | F     | 600 | ANP  | PB-O1B | 2.99 | 1.50        | 1.46     |
| 6   | S     | 600 | ANP  | PB-O1B | 2.99 | 1.50        | 1.46     |
| 6   | A     | 600 | ANP  | PB-O3A | 2.98 | 1.62        | 1.59     |
| 6   | L     | 600 | ANP  | PG-O1G | 2.97 | 1.50        | 1.46     |
| 6   | X     | 600 | ANP  | PG-O1G | 2.86 | 1.50        | 1.46     |
| 6   | B     | 600 | ANP  | PB-O1B | 2.79 | 1.50        | 1.46     |
| 6   | F     | 600 | ANP  | PB-O3A | 2.78 | 1.62        | 1.59     |
| 6   | K     | 600 | ANP  | C5-C4  | 2.78 | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | X     | 600 | ANP  | C5-C4   | 2.76  | 1.48        | 1.40     |
| 6   | J     | 600 | ANP  | PB-O3A  | 2.75  | 1.62        | 1.59     |
| 6   | J     | 600 | ANP  | PB-O1B  | 2.72  | 1.50        | 1.46     |
| 6   | B     | 600 | ANP  | C5-C4   | 2.70  | 1.48        | 1.40     |
| 6   | L     | 600 | ANP  | PG-O2G  | -2.65 | 1.49        | 1.56     |
| 6   | L     | 600 | ANP  | C5-C4   | 2.62  | 1.47        | 1.40     |
| 6   | T     | 600 | ANP  | C5-C4   | 2.61  | 1.47        | 1.40     |
| 6   | O     | 600 | ANP  | PB-O1B  | 2.61  | 1.50        | 1.46     |
| 6   | A     | 600 | ANP  | PG-O2G  | -2.61 | 1.49        | 1.56     |
| 6   | S     | 600 | ANP  | PB-O3A  | 2.59  | 1.62        | 1.59     |
| 6   | F     | 600 | ANP  | C5-C4   | 2.56  | 1.47        | 1.40     |
| 6   | U     | 600 | ANP  | PB-O3A  | 2.56  | 1.62        | 1.59     |
| 6   | O     | 600 | ANP  | C5-C4   | 2.52  | 1.47        | 1.40     |
| 6   | J     | 600 | ANP  | C5-C4   | 2.52  | 1.47        | 1.40     |
| 6   | V     | 600 | ANP  | C5-C4   | 2.50  | 1.47        | 1.40     |
| 6   | D     | 600 | ANP  | C5-C4   | 2.49  | 1.47        | 1.40     |
| 6   | U     | 600 | ANP  | C5-C4   | 2.48  | 1.47        | 1.40     |
| 6   | D     | 600 | ANP  | PB-O1B  | 2.45  | 1.50        | 1.46     |
| 6   | C     | 600 | ANP  | C5-C4   | 2.42  | 1.47        | 1.40     |
| 6   | S     | 600 | ANP  | C5-C4   | 2.42  | 1.47        | 1.40     |
| 6   | S     | 600 | ANP  | C2-N3   | 2.39  | 1.35        | 1.32     |
| 6   | V     | 600 | ANP  | C2-N3   | 2.31  | 1.35        | 1.32     |
| 6   | T     | 600 | ANP  | PB-O3A  | 2.27  | 1.61        | 1.59     |
| 6   | L     | 600 | ANP  | PG-O3G  | -2.27 | 1.50        | 1.56     |
| 6   | A     | 600 | ANP  | C5-C4   | 2.27  | 1.46        | 1.40     |
| 6   | C     | 600 | ANP  | C2-N3   | 2.25  | 1.35        | 1.32     |
| 6   | D     | 600 | ANP  | PB-O2B  | -2.23 | 1.50        | 1.56     |
| 6   | M     | 600 | ANP  | C5-C4   | 2.20  | 1.46        | 1.40     |
| 6   | A     | 600 | ANP  | O4'-C1' | 2.18  | 1.44        | 1.41     |
| 6   | B     | 600 | ANP  | PB-O3A  | 2.17  | 1.61        | 1.59     |
| 6   | X     | 600 | ANP  | PB-O3A  | 2.15  | 1.61        | 1.59     |
| 6   | U     | 600 | ANP  | C2-N3   | 2.15  | 1.35        | 1.32     |
| 6   | K     | 600 | ANP  | C2-N3   | 2.09  | 1.35        | 1.32     |
| 6   | C     | 600 | ANP  | PG-O3G  | -2.08 | 1.51        | 1.56     |
| 6   | C     | 600 | ANP  | PG-O2G  | -2.05 | 1.51        | 1.56     |
| 6   | F     | 600 | ANP  | PG-O3G  | -2.03 | 1.51        | 1.56     |
| 6   | C     | 600 | ANP  | O4'-C1' | 2.02  | 1.43        | 1.41     |
| 6   | D     | 600 | ANP  | PG-O3G  | -2.01 | 1.51        | 1.56     |

All (111) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | M     | 600 | ANP  | O1G-PG-N3B | -7.65 | 100.51      | 111.77   |
| 6   | K     | 600 | ANP  | O1G-PG-N3B | -6.50 | 102.20      | 111.77   |
| 6   | J     | 600 | ANP  | O1G-PG-N3B | -6.49 | 102.21      | 111.77   |
| 6   | A     | 600 | ANP  | O1G-PG-N3B | -6.31 | 102.47      | 111.77   |
| 6   | X     | 600 | ANP  | O1G-PG-N3B | -6.27 | 102.54      | 111.77   |
| 6   | V     | 600 | ANP  | O1G-PG-N3B | -6.12 | 102.76      | 111.77   |
| 6   | B     | 600 | ANP  | O1G-PG-N3B | -6.10 | 102.79      | 111.77   |
| 6   | C     | 600 | ANP  | O2B-PB-O1B | 5.98  | 122.45      | 109.92   |
| 6   | M     | 600 | ANP  | O2B-PB-O1B | 5.81  | 122.10      | 109.92   |
| 6   | F     | 600 | ANP  | O1G-PG-N3B | -5.78 | 103.26      | 111.77   |
| 6   | T     | 600 | ANP  | O1G-PG-N3B | -5.78 | 103.26      | 111.77   |
| 6   | U     | 600 | ANP  | O1G-PG-N3B | -5.69 | 103.39      | 111.77   |
| 6   | C     | 600 | ANP  | O1G-PG-N3B | -5.28 | 103.99      | 111.77   |
| 6   | U     | 600 | ANP  | O2B-PB-O1B | 5.28  | 120.98      | 109.92   |
| 6   | O     | 600 | ANP  | O1G-PG-N3B | -5.15 | 104.18      | 111.77   |
| 6   | L     | 600 | ANP  | O2B-PB-O1B | 4.79  | 119.96      | 109.92   |
| 6   | O     | 600 | ANP  | O1B-PB-N3B | -4.68 | 104.88      | 111.77   |
| 6   | V     | 600 | ANP  | O2B-PB-O1B | 4.67  | 119.72      | 109.92   |
| 6   | F     | 600 | ANP  | O2B-PB-O1B | 4.55  | 119.47      | 109.92   |
| 6   | S     | 600 | ANP  | O1G-PG-N3B | -4.54 | 105.09      | 111.77   |
| 6   | J     | 600 | ANP  | O2B-PB-O1B | 4.51  | 119.38      | 109.92   |
| 6   | L     | 600 | ANP  | O1G-PG-N3B | -4.49 | 105.16      | 111.77   |
| 6   | X     | 600 | ANP  | O2B-PB-O1B | 4.48  | 119.30      | 109.92   |
| 6   | B     | 600 | ANP  | O2B-PB-O1B | 4.47  | 119.30      | 109.92   |
| 6   | U     | 600 | ANP  | O1B-PB-N3B | -4.42 | 105.26      | 111.77   |
| 6   | A     | 600 | ANP  | O2B-PB-O1B | 4.35  | 119.04      | 109.92   |
| 6   | X     | 600 | ANP  | O1B-PB-N3B | -4.33 | 105.40      | 111.77   |
| 6   | D     | 600 | ANP  | O1G-PG-N3B | -4.13 | 105.69      | 111.77   |
| 6   | O     | 600 | ANP  | O2B-PB-O1B | 4.10  | 118.53      | 109.92   |
| 6   | T     | 600 | ANP  | O1B-PB-N3B | -4.10 | 105.73      | 111.77   |
| 6   | T     | 600 | ANP  | O2B-PB-O1B | 3.95  | 118.20      | 109.92   |
| 6   | L     | 600 | ANP  | O1B-PB-N3B | -3.92 | 105.99      | 111.77   |
| 6   | X     | 600 | ANP  | PA-O3A-PB  | -3.81 | 119.22      | 132.62   |
| 6   | S     | 600 | ANP  | O2B-PB-O1B | 3.79  | 117.86      | 109.92   |
| 6   | K     | 600 | ANP  | O2B-PB-O1B | 3.71  | 117.69      | 109.92   |
| 6   | B     | 600 | ANP  | N3-C2-N1   | -3.69 | 122.91      | 128.68   |
| 6   | S     | 600 | ANP  | PA-O3A-PB  | -3.61 | 119.92      | 132.62   |
| 6   | D     | 600 | ANP  | O2B-PB-O1B | 3.61  | 117.48      | 109.92   |
| 6   | D     | 600 | ANP  | N3-C2-N1   | -3.60 | 123.05      | 128.68   |
| 6   | D     | 600 | ANP  | O3G-PG-O2G | 3.54  | 117.06      | 107.64   |
| 6   | K     | 600 | ANP  | O1B-PB-N3B | -3.54 | 106.56      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | U     | 600 | ANP  | N3-C2-N1    | -3.54 | 123.15      | 128.68   |
| 6   | T     | 600 | ANP  | N3-C2-N1    | -3.48 | 123.23      | 128.68   |
| 6   | F     | 600 | ANP  | O1B-PB-N3B  | -3.42 | 106.73      | 111.77   |
| 6   | C     | 600 | ANP  | N3-C2-N1    | -3.41 | 123.36      | 128.68   |
| 6   | S     | 600 | ANP  | N3-C2-N1    | -3.40 | 123.37      | 128.68   |
| 6   | V     | 600 | ANP  | O1B-PB-N3B  | -3.39 | 106.78      | 111.77   |
| 6   | J     | 600 | ANP  | N3-C2-N1    | -3.39 | 123.38      | 128.68   |
| 6   | F     | 600 | ANP  | N3-C2-N1    | -3.36 | 123.42      | 128.68   |
| 6   | L     | 600 | ANP  | N3-C2-N1    | -3.35 | 123.44      | 128.68   |
| 6   | M     | 600 | ANP  | O1B-PB-N3B  | -3.31 | 106.89      | 111.77   |
| 6   | S     | 600 | ANP  | O1B-PB-N3B  | -3.31 | 106.90      | 111.77   |
| 6   | V     | 600 | ANP  | N3-C2-N1    | -3.29 | 123.53      | 128.68   |
| 6   | X     | 600 | ANP  | N3-C2-N1    | -3.28 | 123.56      | 128.68   |
| 6   | K     | 600 | ANP  | N3-C2-N1    | -3.27 | 123.57      | 128.68   |
| 6   | O     | 600 | ANP  | N3-C2-N1    | -3.26 | 123.58      | 128.68   |
| 6   | V     | 600 | ANP  | PA-O3A-PB   | -3.21 | 121.30      | 132.62   |
| 6   | A     | 600 | ANP  | N3-C2-N1    | -3.20 | 123.67      | 128.68   |
| 6   | X     | 600 | ANP  | C3'-C2'-C1' | 3.17  | 105.75      | 100.98   |
| 6   | S     | 600 | ANP  | O3G-PG-O2G  | 3.16  | 116.06      | 107.64   |
| 6   | T     | 600 | ANP  | PA-O3A-PB   | -3.06 | 121.84      | 132.62   |
| 6   | K     | 600 | ANP  | O2B-PB-O3A  | 2.99  | 114.61      | 104.64   |
| 6   | O     | 600 | ANP  | C3'-C2'-C1' | 2.96  | 105.44      | 100.98   |
| 6   | U     | 600 | ANP  | PA-O3A-PB   | -2.94 | 122.26      | 132.62   |
| 6   | X     | 600 | ANP  | O3G-PG-O2G  | 2.93  | 115.43      | 107.64   |
| 6   | V     | 600 | ANP  | C3'-C2'-C1' | 2.92  | 105.38      | 100.98   |
| 6   | F     | 600 | ANP  | O3G-PG-O2G  | 2.88  | 115.30      | 107.64   |
| 6   | B     | 600 | ANP  | O3G-PG-O2G  | 2.87  | 115.29      | 107.64   |
| 6   | V     | 600 | ANP  | C4-C5-N7    | -2.87 | 106.41      | 109.40   |
| 6   | K     | 600 | ANP  | C3'-C2'-C1' | 2.85  | 105.27      | 100.98   |
| 6   | M     | 600 | ANP  | N3-C2-N1    | -2.81 | 124.28      | 128.68   |
| 6   | S     | 600 | ANP  | C3'-C2'-C1' | 2.80  | 105.20      | 100.98   |
| 6   | C     | 600 | ANP  | O3G-PG-O2G  | 2.80  | 115.08      | 107.64   |
| 6   | D     | 600 | ANP  | PA-O3A-PB   | -2.79 | 122.78      | 132.62   |
| 6   | U     | 600 | ANP  | C4-C5-N7    | -2.77 | 106.51      | 109.40   |
| 6   | U     | 600 | ANP  | O3G-PG-O2G  | 2.76  | 115.00      | 107.64   |
| 6   | J     | 600 | ANP  | C4-C5-N7    | -2.74 | 106.55      | 109.40   |
| 6   | K     | 600 | ANP  | C4-C5-N7    | -2.71 | 106.58      | 109.40   |
| 6   | M     | 600 | ANP  | C4-C5-N7    | -2.70 | 106.59      | 109.40   |
| 6   | C     | 600 | ANP  | PA-O3A-PB   | -2.69 | 123.13      | 132.62   |
| 6   | V     | 600 | ANP  | O3G-PG-O2G  | 2.69  | 114.80      | 107.64   |
| 6   | U     | 600 | ANP  | C3'-C2'-C1' | 2.69  | 105.02      | 100.98   |
| 6   | K     | 600 | ANP  | PA-O3A-PB   | -2.68 | 123.19      | 132.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 600 | ANP  | PA-O3A-PB   | -2.57 | 123.56      | 132.62   |
| 6   | O     | 600 | ANP  | C4-C5-N7    | -2.55 | 106.74      | 109.40   |
| 6   | A     | 600 | ANP  | C4-C5-N7    | -2.52 | 106.78      | 109.40   |
| 6   | D     | 600 | ANP  | C3'-C2'-C1' | 2.52  | 104.77      | 100.98   |
| 6   | L     | 600 | ANP  | C4-C5-N7    | -2.51 | 106.79      | 109.40   |
| 6   | K     | 600 | ANP  | O3G-PG-O2G  | 2.49  | 114.27      | 107.64   |
| 6   | T     | 600 | ANP  | O3G-PG-O2G  | 2.48  | 114.23      | 107.64   |
| 6   | B     | 600 | ANP  | C4-C5-N7    | -2.47 | 106.83      | 109.40   |
| 6   | M     | 600 | ANP  | C3'-C2'-C1' | 2.45  | 104.67      | 100.98   |
| 6   | F     | 600 | ANP  | O2B-PB-O3A  | 2.39  | 112.63      | 104.64   |
| 6   | X     | 600 | ANP  | C4-C5-N7    | -2.37 | 106.92      | 109.40   |
| 6   | L     | 600 | ANP  | O3G-PG-O2G  | 2.33  | 113.84      | 107.64   |
| 6   | C     | 600 | ANP  | C4-C5-N7    | -2.32 | 106.98      | 109.40   |
| 6   | J     | 600 | ANP  | O3G-PG-O2G  | 2.30  | 113.77      | 107.64   |
| 6   | C     | 600 | ANP  | O1B-PB-N3B  | -2.29 | 108.40      | 111.77   |
| 6   | T     | 600 | ANP  | C4-C5-N7    | -2.29 | 107.02      | 109.40   |
| 6   | J     | 600 | ANP  | PA-O3A-PB   | -2.29 | 124.56      | 132.62   |
| 6   | S     | 600 | ANP  | C4-C5-N7    | -2.23 | 107.08      | 109.40   |
| 6   | F     | 600 | ANP  | PA-O3A-PB   | -2.22 | 124.79      | 132.62   |
| 6   | A     | 600 | ANP  | O1B-PB-N3B  | -2.21 | 108.52      | 111.77   |
| 6   | D     | 600 | ANP  | C4-C5-N7    | -2.19 | 107.12      | 109.40   |
| 6   | O     | 600 | ANP  | O3G-PG-O2G  | 2.15  | 113.37      | 107.64   |
| 6   | C     | 600 | ANP  | O4'-C1'-C2' | -2.11 | 103.85      | 106.93   |
| 6   | D     | 600 | ANP  | C2-N1-C6    | 2.10  | 122.35      | 118.75   |
| 6   | L     | 600 | ANP  | O3A-PB-N3B  | 2.10  | 112.42      | 106.59   |
| 6   | T     | 600 | ANP  | C3'-C2'-C1' | 2.07  | 104.10      | 100.98   |
| 6   | F     | 600 | ANP  | N6-C6-N1    | 2.06  | 122.85      | 118.57   |
| 6   | J     | 600 | ANP  | C3'-C2'-C1' | 2.04  | 104.05      | 100.98   |

There are no chirality outliers.

All (59) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 6   | K     | 600 | ANP  | PB-N3B-PG-O1G  |
| 6   | K     | 600 | ANP  | PG-N3B-PB-O1B  |
| 6   | K     | 600 | ANP  | PG-N3B-PB-O3A  |
| 6   | K     | 600 | ANP  | C5'-O5'-PA-O2A |
| 6   | O     | 600 | ANP  | PB-N3B-PG-O1G  |
| 6   | O     | 600 | ANP  | PG-N3B-PB-O1B  |
| 6   | O     | 600 | ANP  | PG-N3B-PB-O3A  |
| 6   | M     | 600 | ANP  | PB-N3B-PG-O1G  |
| 6   | M     | 600 | ANP  | PG-N3B-PB-O1B  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | M     | 600 | ANP  | PA-O3A-PB-O1B   |
| 6   | C     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | C     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | S     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | S     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | S     | 600 | ANP  | PA-O3A-PB-O1B   |
| 6   | S     | 600 | ANP  | PA-O3A-PB-O2B   |
| 6   | T     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | T     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | X     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | X     | 600 | ANP  | PA-O3A-PB-O1B   |
| 6   | X     | 600 | ANP  | PA-O3A-PB-O2B   |
| 6   | X     | 600 | ANP  | C5'-O5'-PA-O1A  |
| 6   | X     | 600 | ANP  | C5'-O5'-PA-O2A  |
| 6   | X     | 600 | ANP  | O4'-C4'-C5'-O5' |
| 6   | X     | 600 | ANP  | C3'-C4'-C5'-O5' |
| 6   | F     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | F     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | F     | 600 | ANP  | PG-N3B-PB-O3A   |
| 6   | L     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | L     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | J     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | J     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | U     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | U     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | U     | 600 | ANP  | PG-N3B-PB-O3A   |
| 6   | U     | 600 | ANP  | PA-O3A-PB-O1B   |
| 6   | V     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | V     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | V     | 600 | ANP  | PG-N3B-PB-O3A   |
| 6   | V     | 600 | ANP  | PA-O3A-PB-O1B   |
| 6   | V     | 600 | ANP  | PA-O3A-PB-O2B   |
| 6   | D     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | D     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | D     | 600 | ANP  | PG-N3B-PB-O3A   |
| 6   | A     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | A     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | B     | 600 | ANP  | PB-N3B-PG-O1G   |
| 6   | B     | 600 | ANP  | PG-N3B-PB-O1B   |
| 6   | V     | 600 | ANP  | O4'-C4'-C5'-O5' |
| 6   | V     | 600 | ANP  | C3'-C4'-C5'-O5' |
| 6   | K     | 600 | ANP  | C5'-O5'-PA-O3A  |

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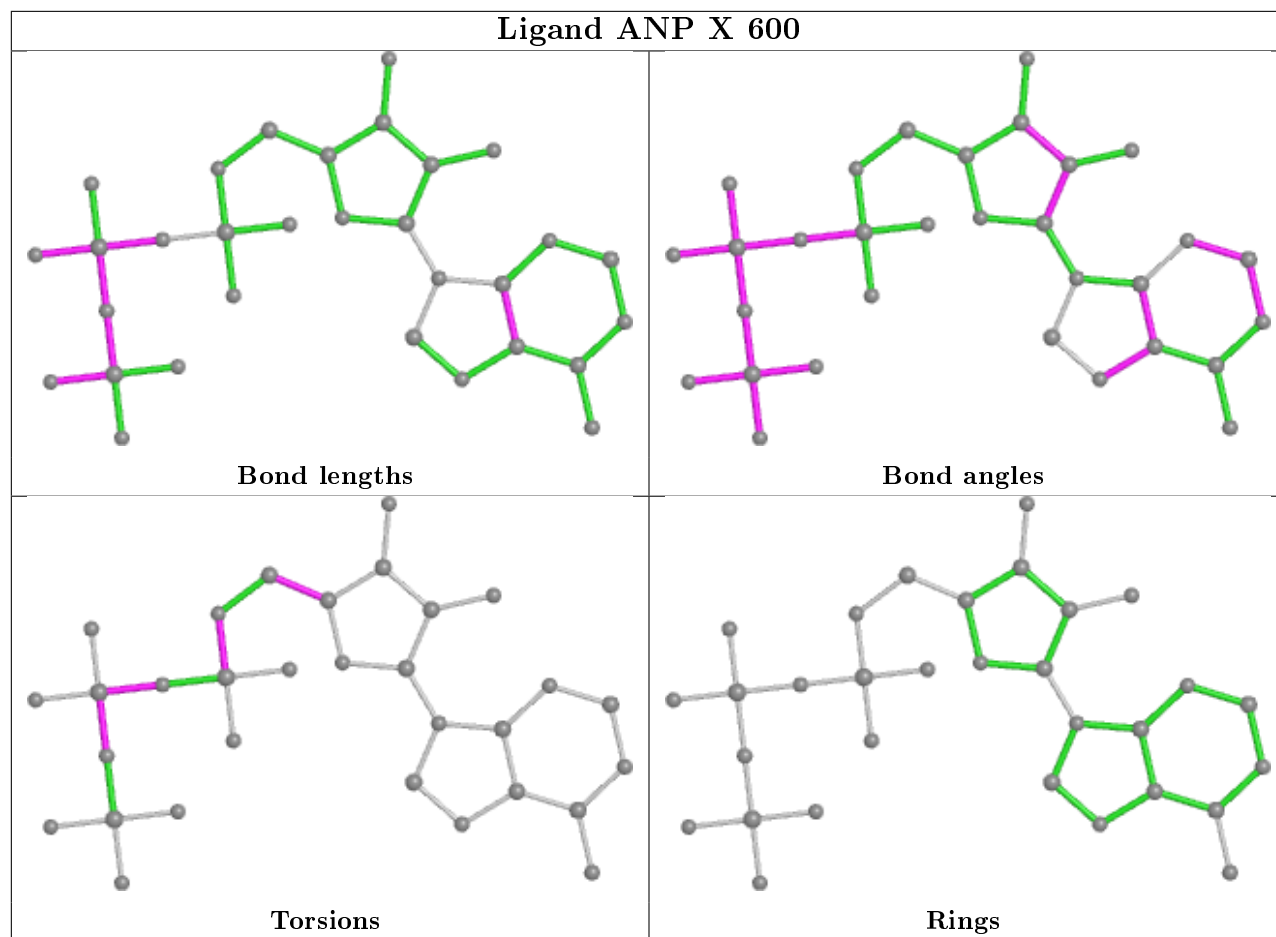
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | K     | 600 | ANP  | C5'-O5'-PA-O1A  |
| 6   | K     | 600 | ANP  | O4'-C4'-C5'-O5' |
| 6   | K     | 600 | ANP  | C3'-C4'-C5'-O5' |
| 6   | K     | 600 | ANP  | PB-O3A-PA-O2A   |
| 6   | M     | 600 | ANP  | O4'-C4'-C5'-O5' |
| 6   | D     | 600 | ANP  | PA-O3A-PB-O2B   |
| 6   | C     | 600 | ANP  | PB-O3A-PA-O1A   |
| 6   | X     | 600 | ANP  | C5'-O5'-PA-O3A  |

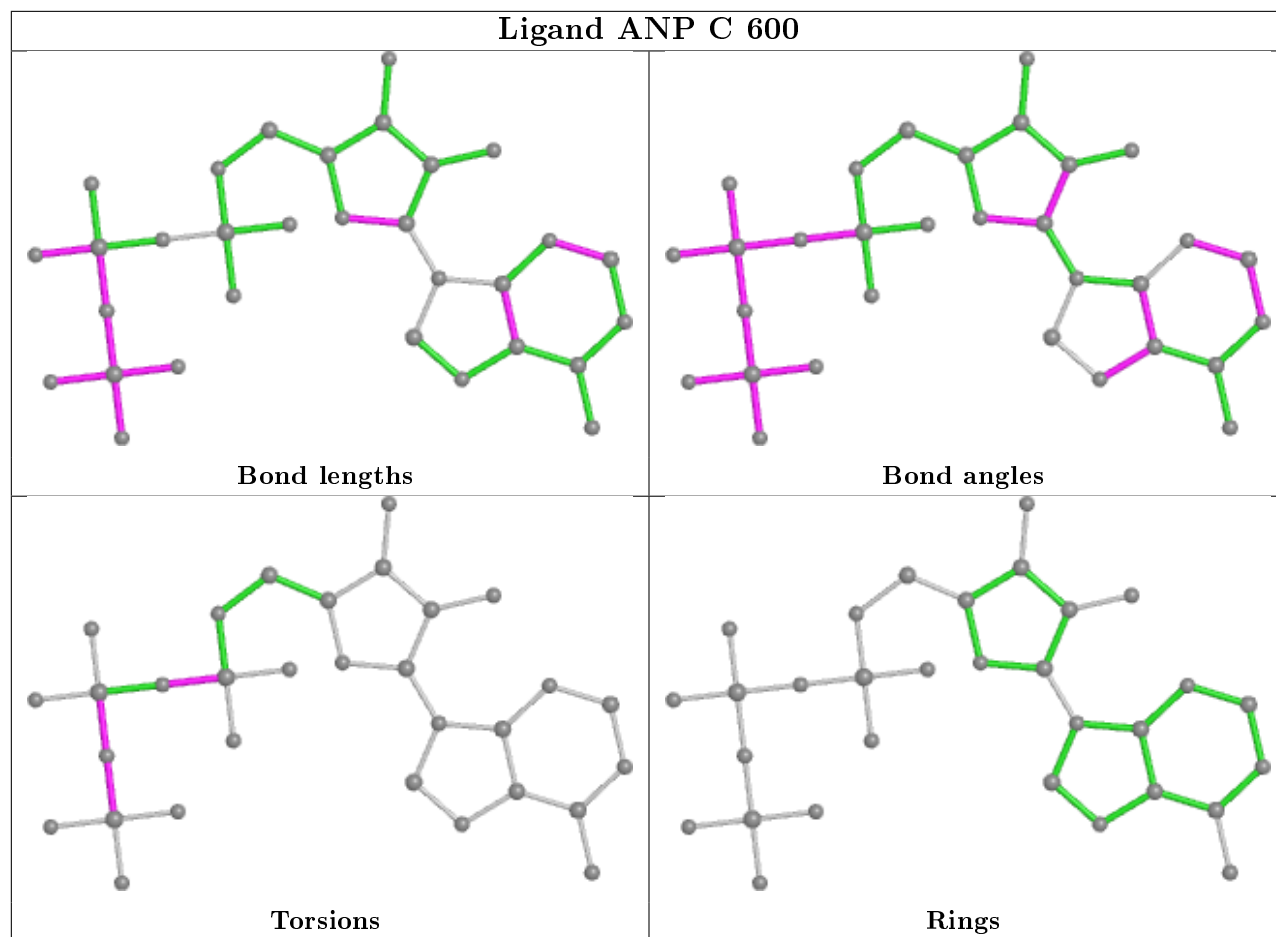
There are no ring outliers.

12 monomers are involved in 25 short contacts:

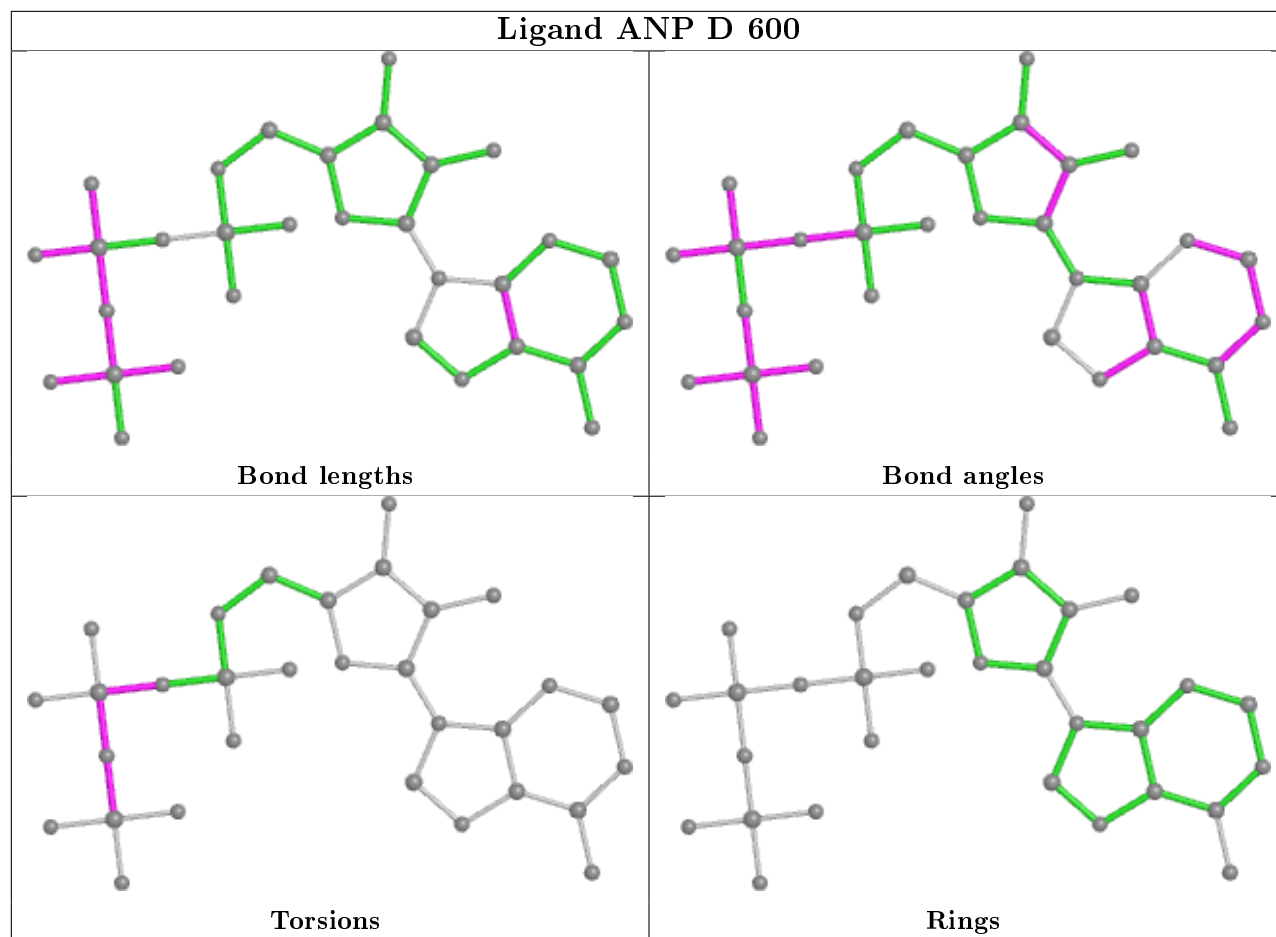
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | X     | 600 | ANP  | 4       | 0            |
| 6   | F     | 600 | ANP  | 1       | 0            |
| 6   | A     | 600 | ANP  | 1       | 0            |
| 6   | B     | 600 | ANP  | 4       | 0            |
| 6   | K     | 600 | ANP  | 3       | 0            |
| 6   | L     | 600 | ANP  | 1       | 0            |
| 6   | M     | 600 | ANP  | 4       | 0            |
| 6   | J     | 600 | ANP  | 1       | 0            |
| 6   | T     | 600 | ANP  | 1       | 0            |
| 6   | U     | 600 | ANP  | 1       | 0            |
| 6   | V     | 600 | ANP  | 1       | 0            |
| 6   | O     | 600 | ANP  | 3       | 0            |

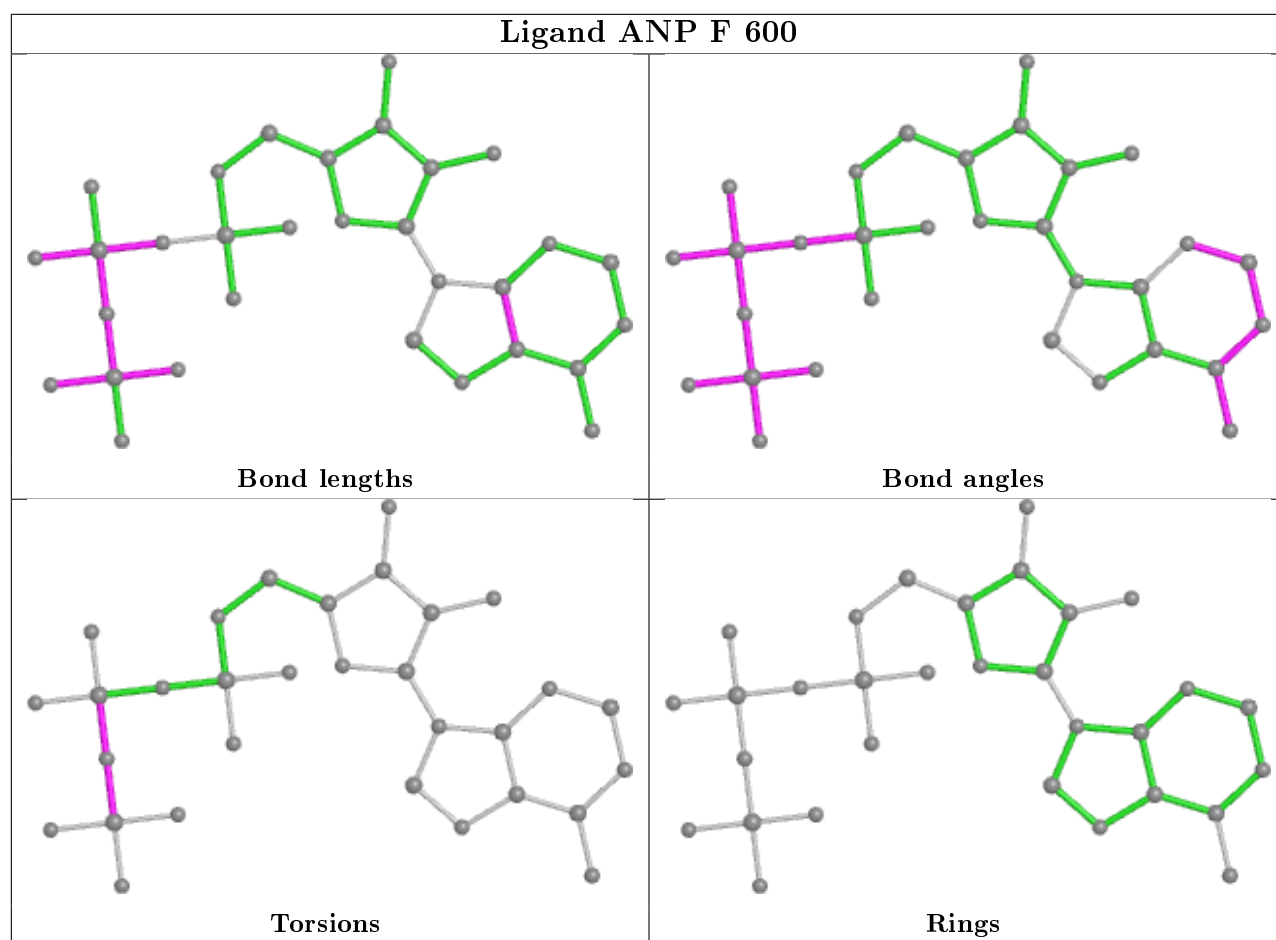
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

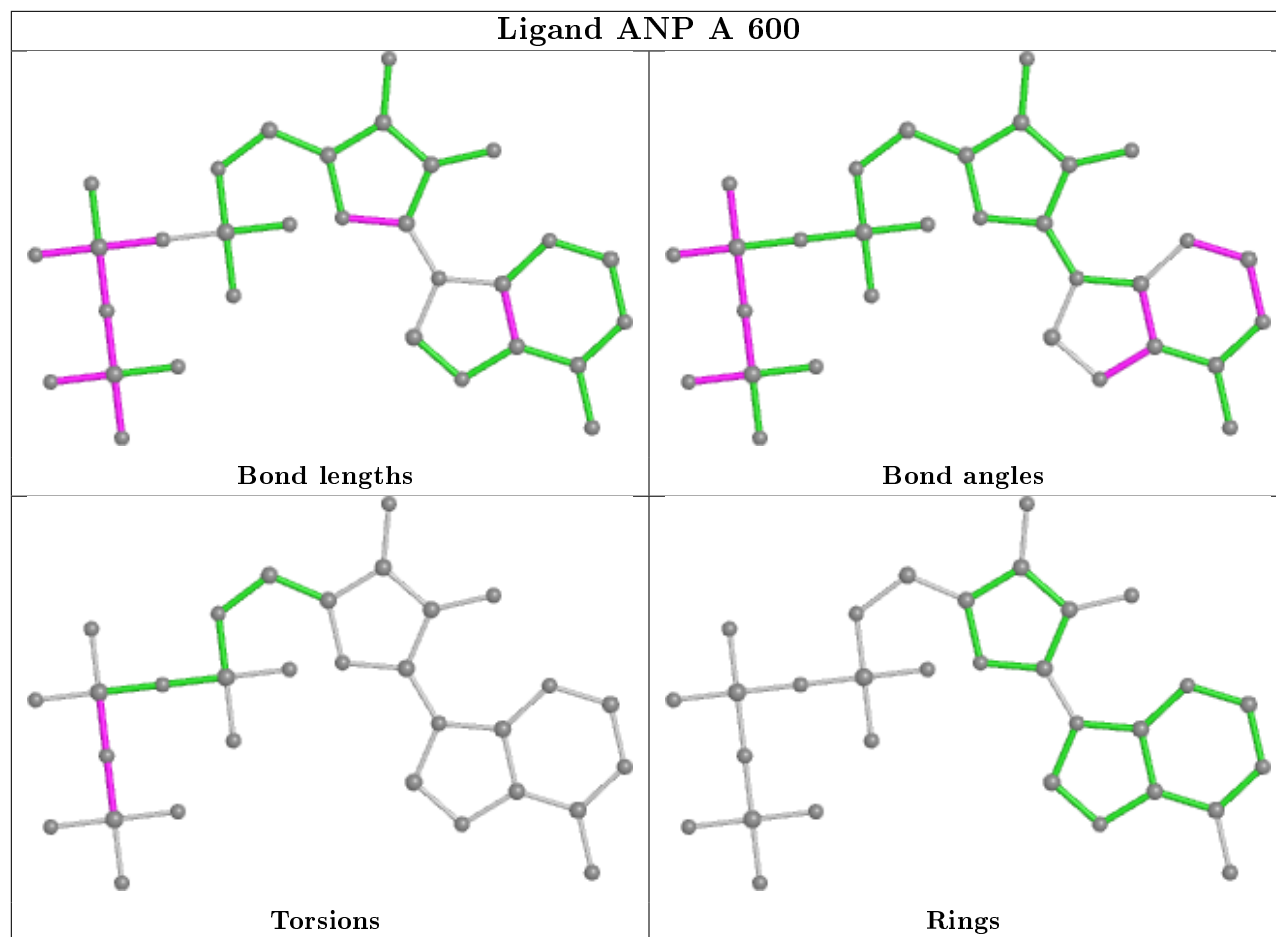


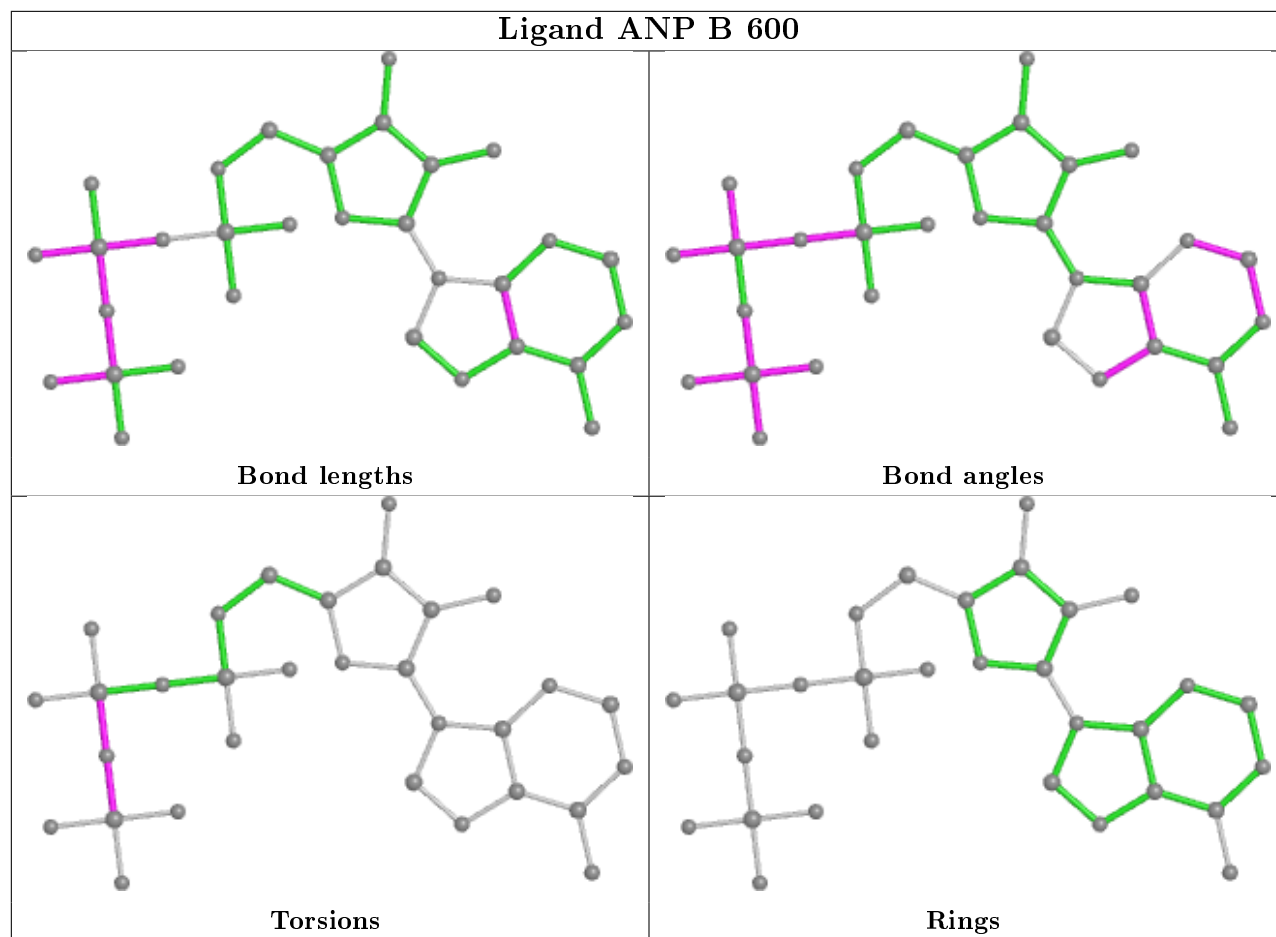


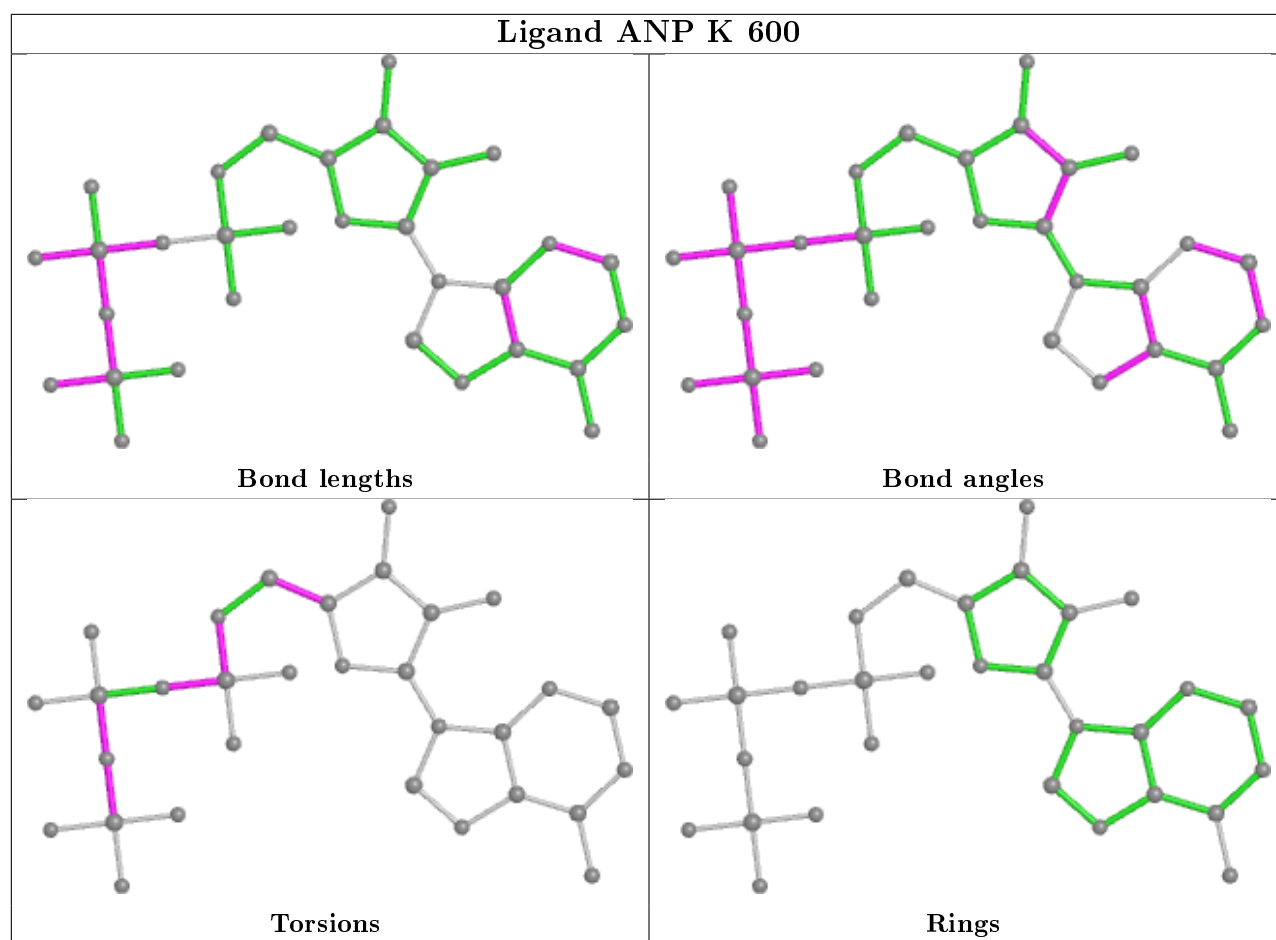


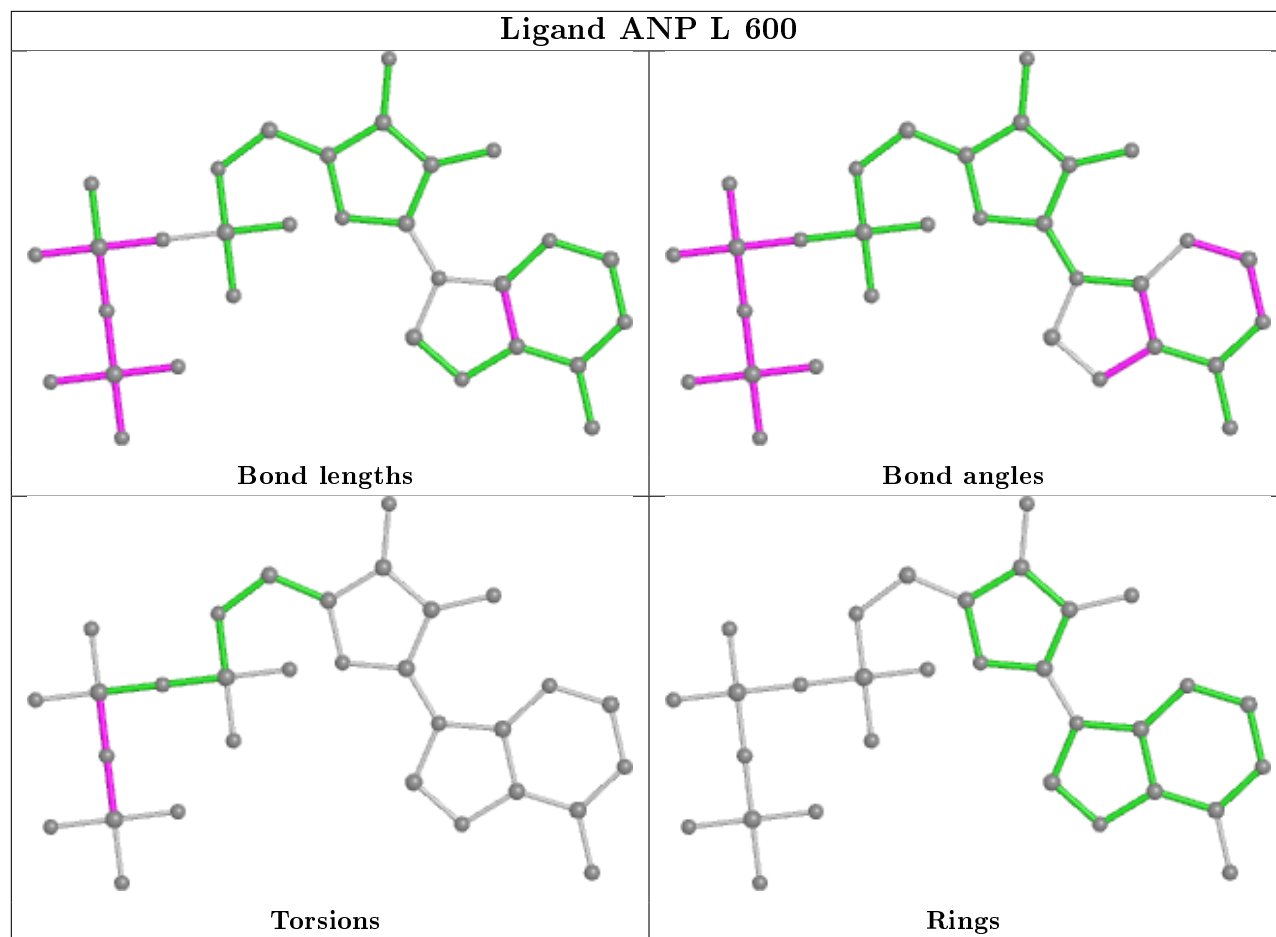


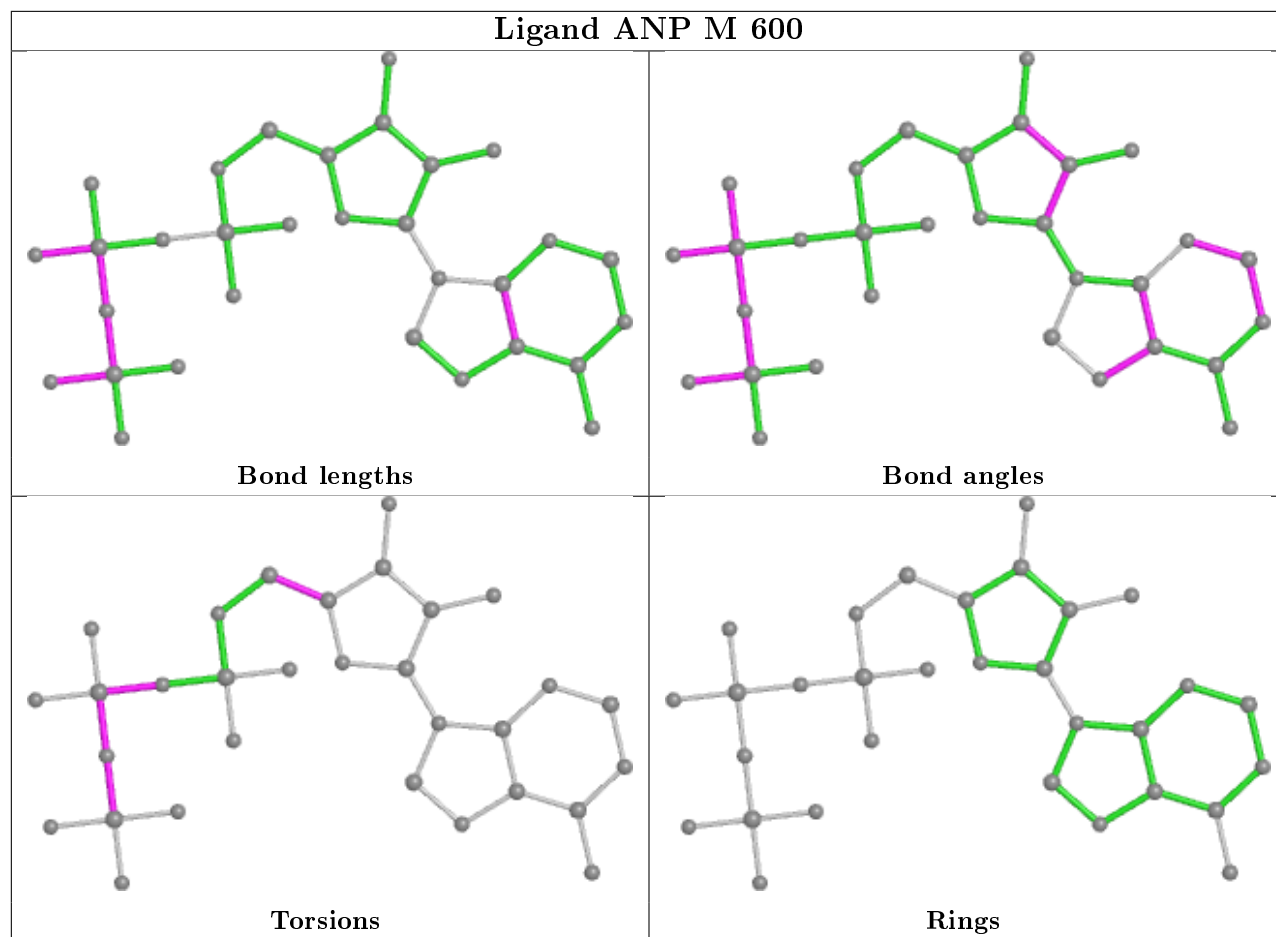




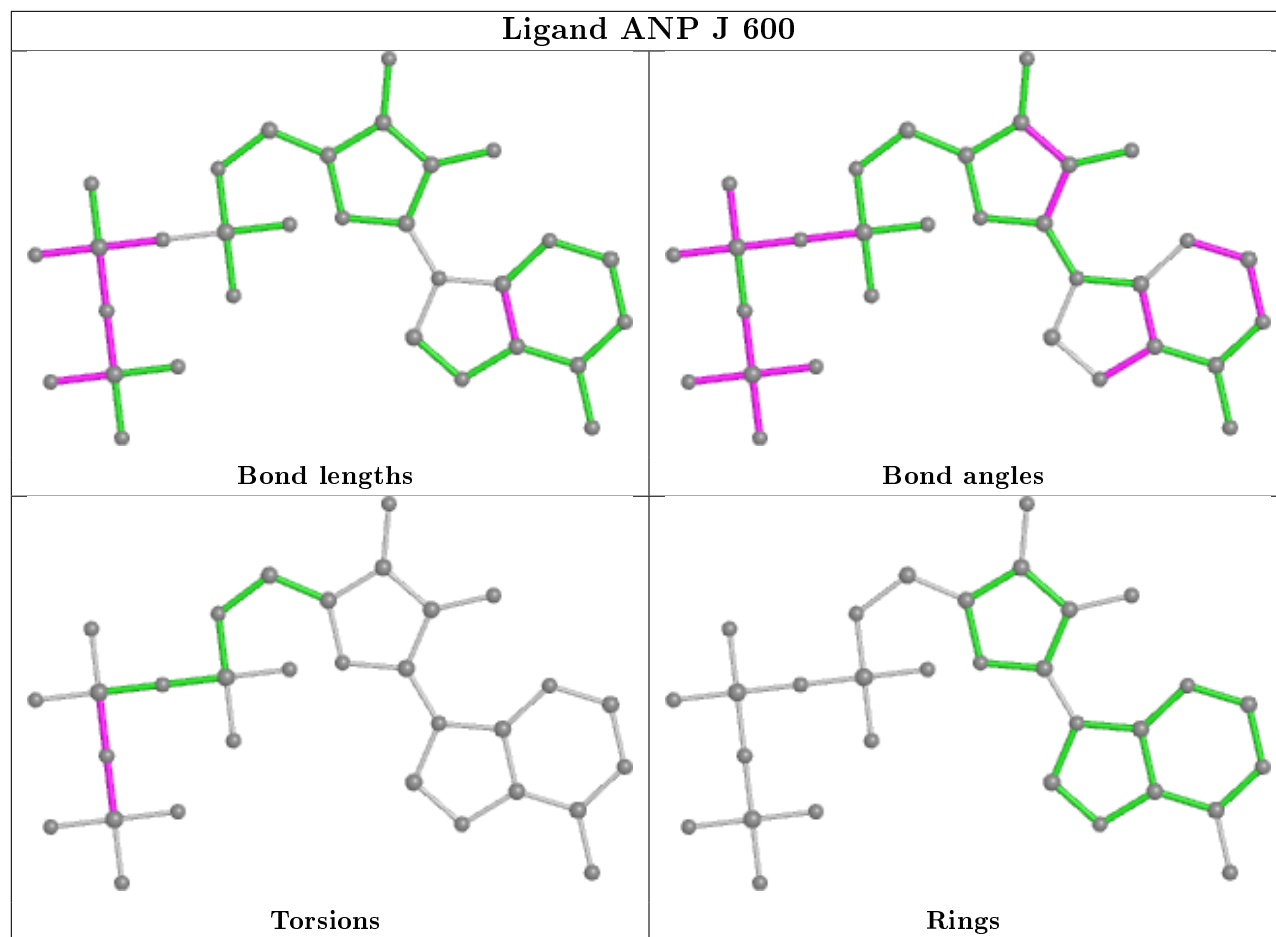




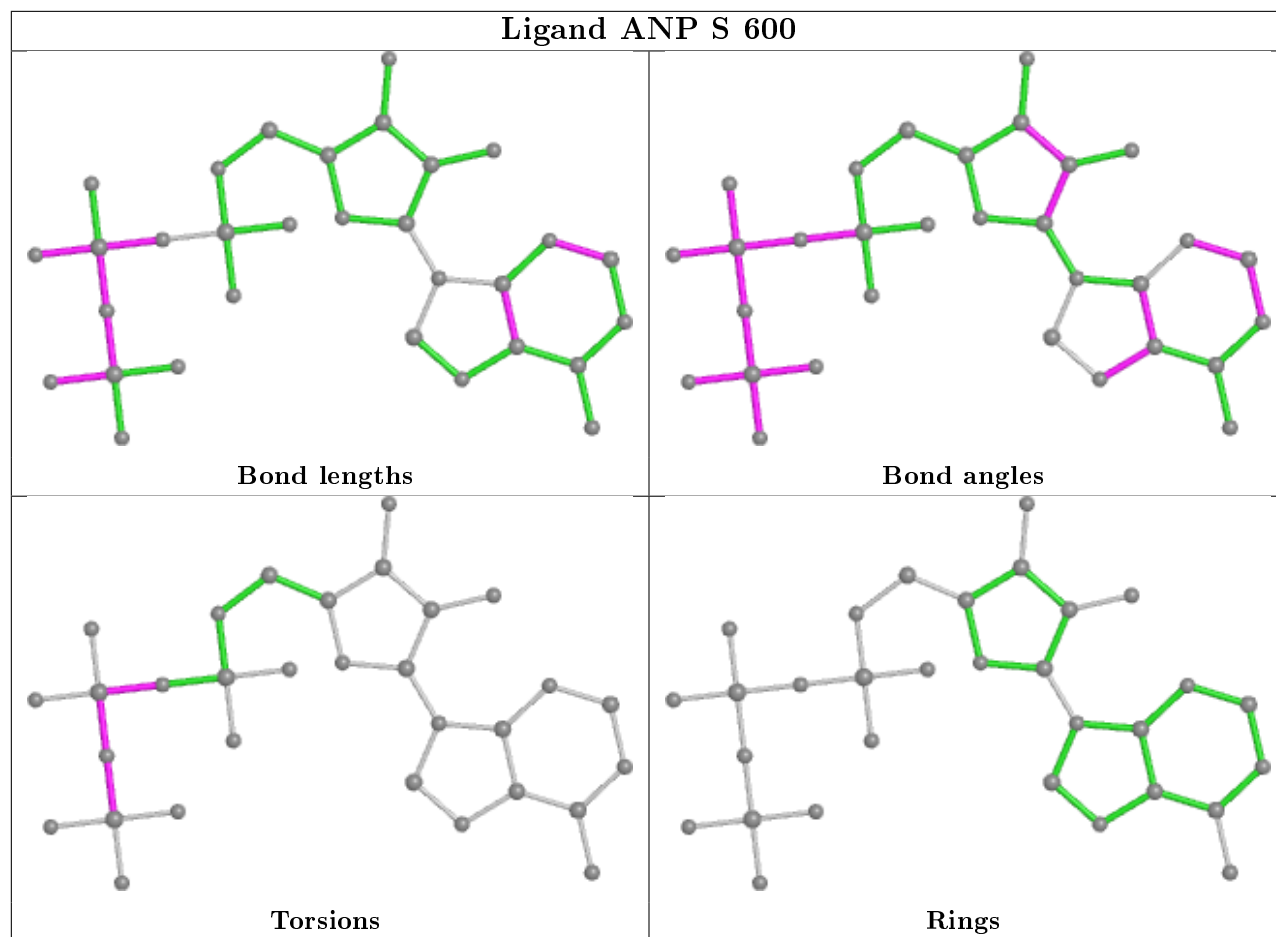


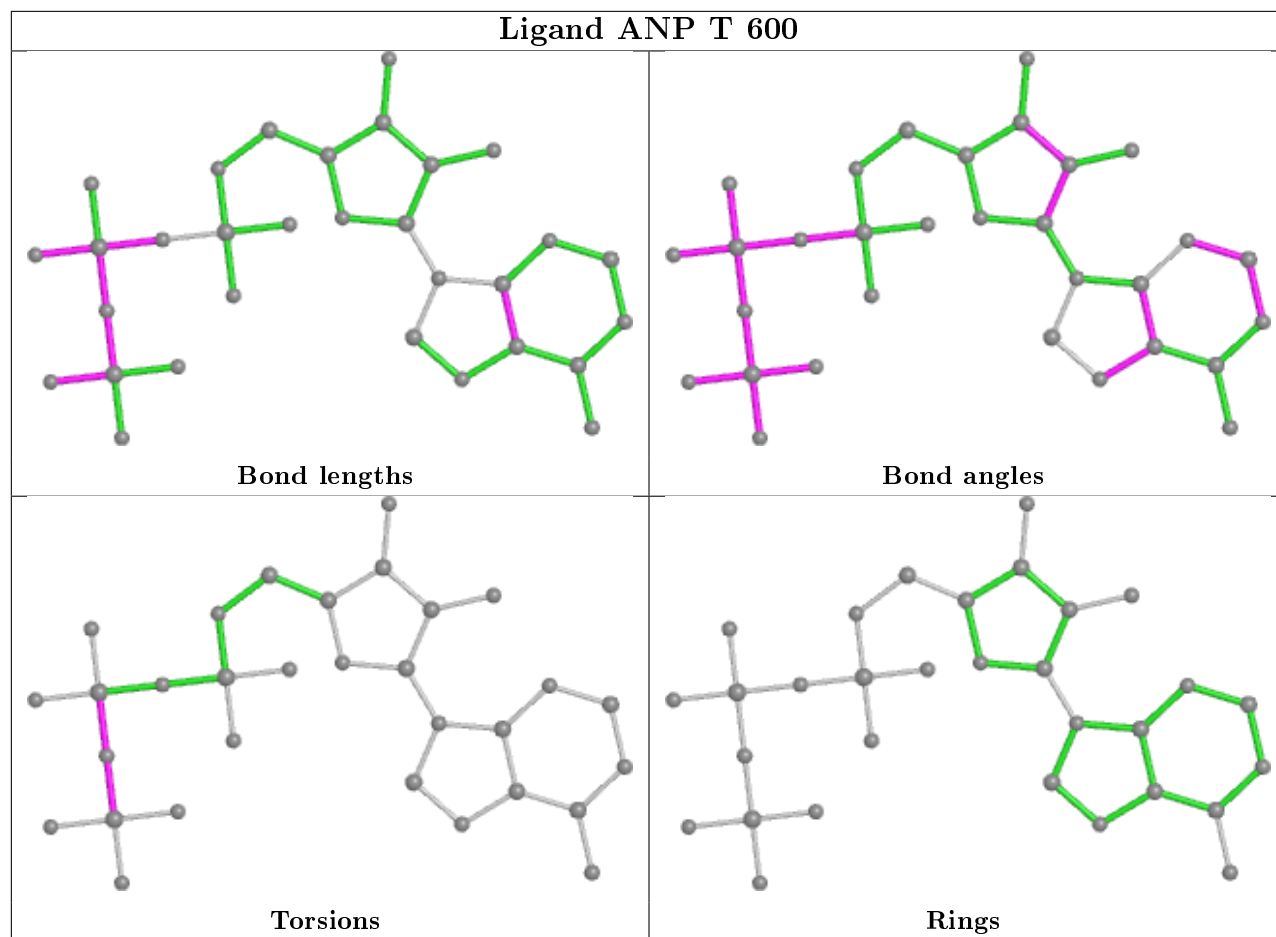


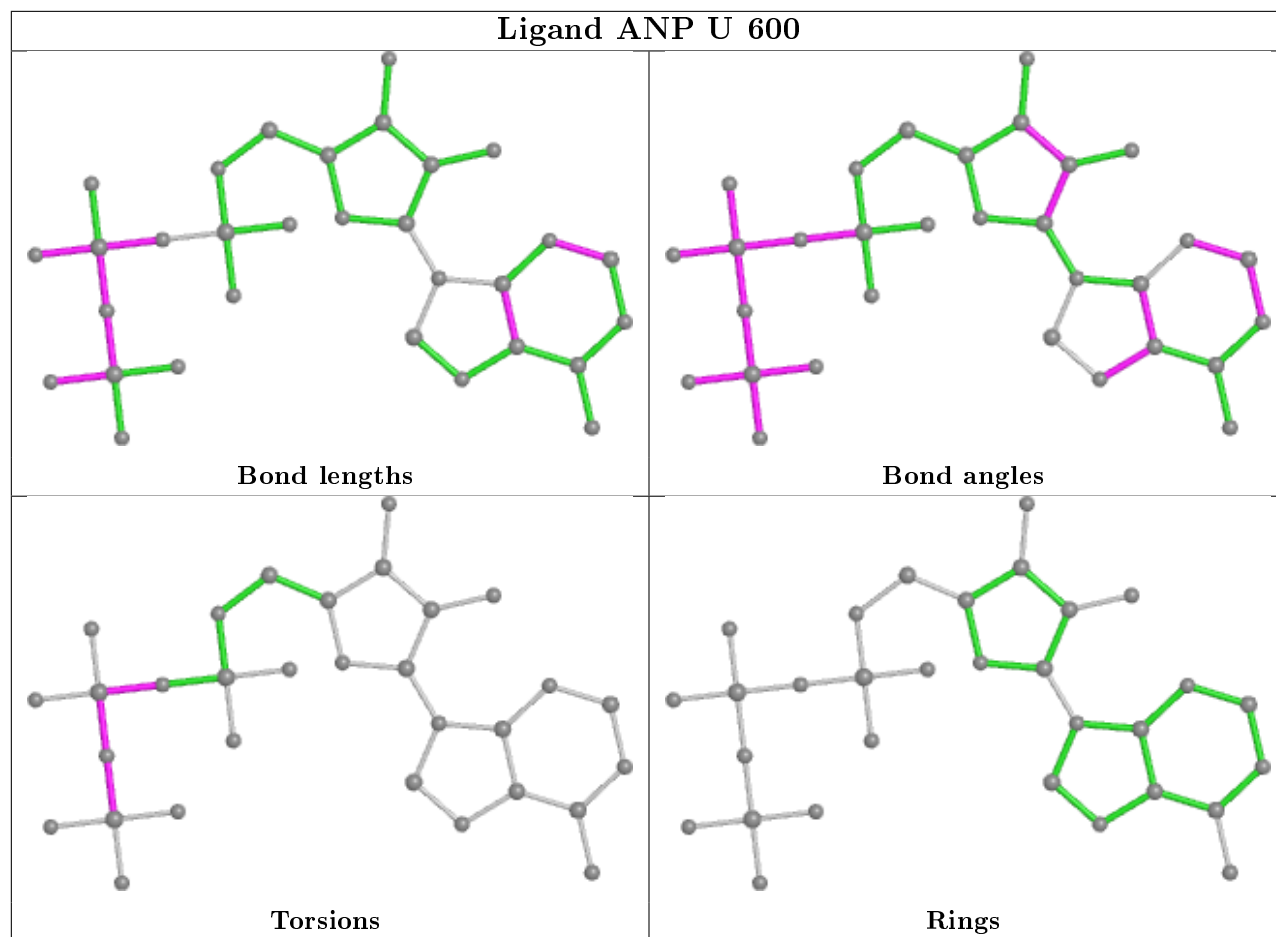
## Ligand ANP J 600

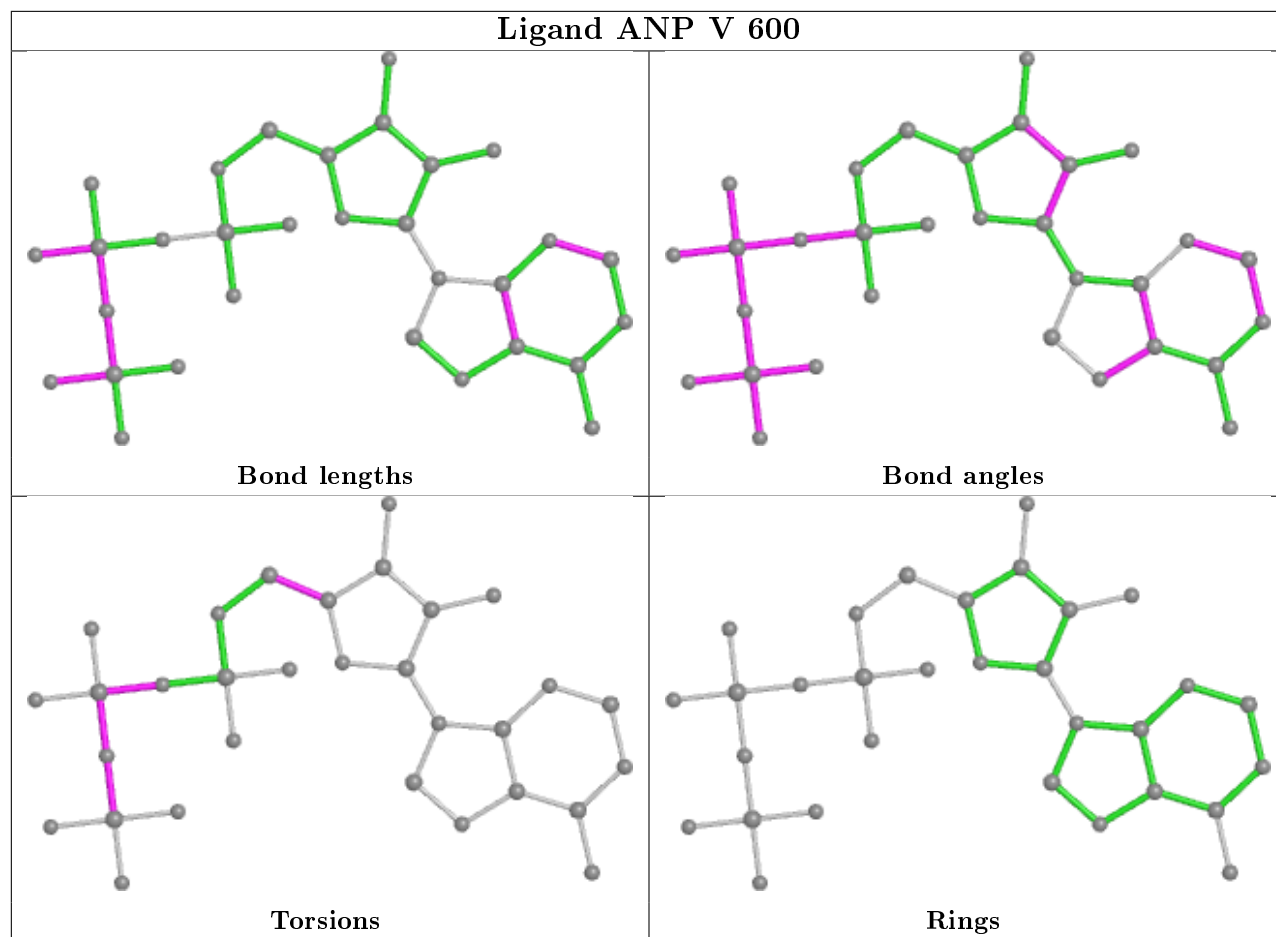


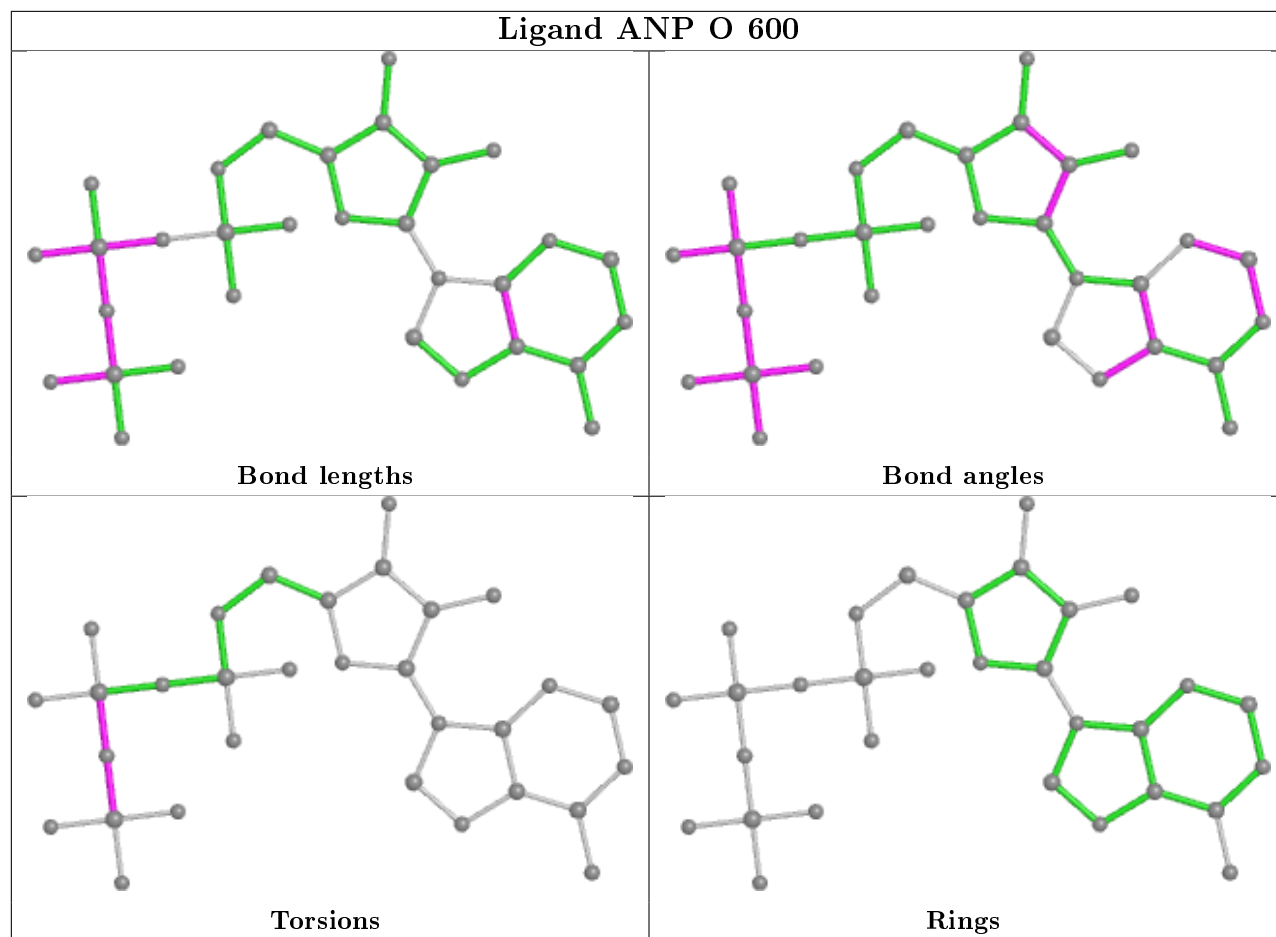












## 5.7 Other polymers [i](#)

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     | 482/510 (94%) | -0.49  | 0 100 100     | 41, 63, 99, 156       | 0     |
| 1   | B     | 483/510 (94%) | -0.23  | 3 (0%) 89 72  | 48, 92, 148, 188      | 0     |
| 1   | C     | 484/510 (94%) | -0.41  | 0 100 100     | 43, 73, 129, 177      | 0     |
| 1   | J     | 481/510 (94%) | -0.26  | 2 (0%) 92 79  | 60, 100, 149, 206     | 0     |
| 1   | K     | 486/510 (95%) | -0.06  | 16 (3%) 46 20 | 78, 126, 187, 217     | 0     |
| 1   | L     | 482/510 (94%) | -0.40  | 0 100 100     | 47, 68, 137, 194      | 0     |
| 1   | S     | 478/510 (93%) | -0.21  | 8 (1%) 70 41  | 77, 109, 153, 179     | 0     |
| 1   | T     | 479/510 (93%) | 0.21   | 29 (6%) 21 7  | 103, 151, 186, 202    | 0     |
| 1   | U     | 481/510 (94%) | 0.19   | 31 (6%) 19 6  | 104, 150, 181, 217    | 0     |
| 2   | D     | 470/484 (97%) | -0.44  | 1 (0%) 95 87  | 42, 70, 123, 181      | 0     |
| 2   | E     | 468/484 (96%) | -0.23  | 9 (1%) 66 37  | 46, 86, 161, 211      | 0     |
| 2   | F     | 469/484 (96%) | -0.31  | 0 100 100     | 48, 89, 129, 169      | 0     |
| 2   | M     | 470/484 (97%) | -0.32  | 2 (0%) 92 79  | 55, 86, 134, 180      | 0     |
| 2   | N     | 470/484 (97%) | 0.06   | 18 (3%) 40 16 | 71, 133, 199, 229     | 0     |
| 2   | O     | 468/484 (96%) | -0.30  | 0 100 100     | 54, 94, 141, 175      | 0     |
| 2   | V     | 470/484 (97%) | 0.10   | 26 (5%) 25 9  | 93, 138, 180, 210     | 0     |
| 2   | W     | 467/484 (96%) | -0.07  | 14 (2%) 50 22 | 89, 117, 164, 189     | 0     |
| 2   | X     | 469/484 (96%) | 0.06   | 20 (4%) 35 13 | 93, 134, 185, 234     | 0     |
| 3   | G     | 266/278 (95%) | -0.24  | 2 (0%) 86 65  | 63, 103, 140, 167     | 0     |
| 3   | P     | 246/278 (88%) | 0.22   | 13 (5%) 26 10 | 69, 131, 195, 237     | 0     |
| 3   | Y     | 201/278 (72%) | 0.43   | 19 (9%) 8 3   | 107, 146, 192, 232    | 0     |
| 4   | H     | 116/138 (84%) | -0.05  | 6 (5%) 27 10  | 82, 127, 216, 236     | 0     |
| 4   | Q     | 84/138 (60%)  | 0.01   | 3 (3%) 42 17  | 109, 150, 208, 214    | 0     |
| 4   | Z     | 17/138 (12%)  | 2.21   | 11 (64%) 0 0  | 190, 210, 236, 245    | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 5   | 1     | 27/61 (44%)      | 1.54   | 9 (33%) 0 0    | 159, 168, 187, 210    | 0     |
| 5   | I     | 49/61 (80%)      | -0.08  | 1 (2%) 65 36   | 97, 127, 178, 217     | 0     |
| 5   | R     | 34/61 (55%)      | -0.33  | 1 (2%) 51 23   | 108, 122, 187, 200    | 0     |
| All | All   | 9597/10377 (92%) | -0.14  | 244 (2%) 57 29 | 41, 108, 176, 245     | 0     |

All (244) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | U     | 26  | ASN  | 6.3  |
| 1   | T     | 491 | LEU  | 5.3  |
| 2   | X     | 7   | THR  | 5.2  |
| 5   | 1     | 33  | SER  | 4.9  |
| 2   | X     | 90  | GLU  | 4.8  |
| 3   | P     | 170 | VAL  | 4.7  |
| 3   | Y     | 140 | PHE  | 4.7  |
| 1   | U     | 63  | GLY  | 4.4  |
| 2   | W     | 474 | ALA  | 4.4  |
| 2   | N     | 387 | ILE  | 4.4  |
| 3   | Y     | 170 | VAL  | 4.3  |
| 2   | V     | 214 | LYS  | 4.3  |
| 1   | U     | 62  | LYS  | 4.3  |
| 2   | D     | 6   | SER  | 4.2  |
| 2   | X     | 30  | LEU  | 4.2  |
| 1   | T     | 27  | LEU  | 4.1  |
| 4   | Z     | 121 | ALA  | 4.1  |
| 2   | N     | 457 | PHE  | 4.0  |
| 1   | T     | 485 | ILE  | 4.0  |
| 2   | X     | 28  | SER  | 3.9  |
| 2   | V     | 213 | SER  | 3.9  |
| 1   | T     | 35  | ALA  | 3.9  |
| 3   | P     | 54  | ASN  | 3.9  |
| 2   | X     | 9   | ILE  | 3.9  |
| 1   | T     | 46  | LEU  | 3.8  |
| 2   | X     | 55  | GLY  | 3.8  |
| 2   | N     | 453 | PRO  | 3.8  |
| 1   | K     | 494 | GLU  | 3.8  |
| 1   | U     | 43  | VAL  | 3.8  |
| 1   | K     | 503 | THR  | 3.7  |
| 2   | N     | 6   | SER  | 3.6  |
| 4   | H     | 90  | ALA  | 3.6  |
| 1   | S     | 87  | GLY  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | Y     | 41  | ALA  | 3.5  |
| 1   | B     | 491 | LEU  | 3.5  |
| 2   | X     | 8   | PRO  | 3.5  |
| 3   | P     | 169 | PRO  | 3.5  |
| 2   | V     | 110 | LYS  | 3.5  |
| 2   | N     | 475 | ALA  | 3.4  |
| 1   | T     | 202 | TYR  | 3.4  |
| 2   | V     | 57  | ASN  | 3.4  |
| 2   | E     | 457 | PHE  | 3.4  |
| 2   | N     | 23  | VAL  | 3.4  |
| 2   | V     | 28  | SER  | 3.3  |
| 4   | Q     | 81  | SER  | 3.3  |
| 2   | X     | 76  | VAL  | 3.3  |
| 1   | U     | 122 | PRO  | 3.2  |
| 4   | Z     | 135 | SER  | 3.2  |
| 1   | T     | 32  | ARG  | 3.2  |
| 1   | T     | 54  | LEU  | 3.2  |
| 1   | K     | 457 | GLY  | 3.2  |
| 1   | K     | 195 | SER  | 3.1  |
| 5   | 1     | 11  | ALA  | 3.1  |
| 2   | X     | 249 | GLN  | 3.1  |
| 2   | V     | 9   | ILE  | 3.1  |
| 2   | E     | 391 | LEU  | 3.1  |
| 1   | U     | 489 | GLY  | 3.1  |
| 1   | U     | 446 | LEU  | 3.1  |
| 4   | H     | 111 | ASN  | 3.1  |
| 1   | T     | 55  | VAL  | 3.1  |
| 1   | K     | 454 | HIS  | 3.1  |
| 1   | T     | 26  | ASN  | 3.0  |
| 3   | Y     | 91  | LEU  | 3.0  |
| 4   | Z     | 128 | GLU  | 3.0  |
| 1   | U     | 52  | GLU  | 3.0  |
| 5   | 1     | 22  | ARG  | 3.0  |
| 1   | S     | 89  | LEU  | 3.0  |
| 1   | T     | 30  | THR  | 3.0  |
| 2   | X     | 31  | PRO  | 3.0  |
| 1   | S     | 37  | GLY  | 2.9  |
| 1   | U     | 30  | THR  | 2.9  |
| 2   | V     | 108 | PRO  | 2.9  |
| 1   | T     | 314 | LEU  | 2.9  |
| 2   | W     | 470 | ALA  | 2.9  |
| 4   | Z     | 129 | VAL  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | H     | 103 | ASN  | 2.9  |
| 1   | U     | 114 | GLY  | 2.9  |
| 3   | Y     | 45  | ASP  | 2.9  |
| 2   | X     | 11  | GLY  | 2.9  |
| 2   | X     | 77  | LEU  | 2.9  |
| 1   | U     | 491 | LEU  | 2.9  |
| 1   | U     | 455 | LEU  | 2.8  |
| 2   | V     | 27  | GLN  | 2.8  |
| 3   | P     | 105 | ALA  | 2.8  |
| 4   | Z     | 124 | ALA  | 2.8  |
| 5   | 1     | 18  | ALA  | 2.8  |
| 2   | M     | 6   | SER  | 2.8  |
| 2   | V     | 210 | GLU  | 2.8  |
| 2   | N     | 8   | PRO  | 2.8  |
| 2   | W     | 437 | THR  | 2.8  |
| 2   | X     | 10  | THR  | 2.8  |
| 2   | V     | 102 | PRO  | 2.8  |
| 1   | B     | 485 | ILE  | 2.7  |
| 4   | Z     | 132 | ASN  | 2.7  |
| 2   | X     | 75  | LYS  | 2.7  |
| 2   | V     | 71  | VAL  | 2.7  |
| 3   | P     | 106 | ASP  | 2.7  |
| 1   | T     | 320 | SER  | 2.7  |
| 2   | W     | 390 | ILE  | 2.7  |
| 1   | S     | 30  | THR  | 2.7  |
| 2   | X     | 32  | ALA  | 2.7  |
| 1   | T     | 63  | GLY  | 2.7  |
| 2   | W     | 463 | ILE  | 2.7  |
| 1   | K     | 474 | LEU  | 2.7  |
| 1   | T     | 49  | ILE  | 2.7  |
| 1   | U     | 123 | ILE  | 2.6  |
| 1   | K     | 505 | SER  | 2.6  |
| 5   | 1     | 15  | ASN  | 2.6  |
| 2   | W     | 394 | ASP  | 2.6  |
| 2   | V     | 475 | ALA  | 2.6  |
| 4   | Z     | 134 | GLN  | 2.6  |
| 2   | N     | 7   | THR  | 2.6  |
| 2   | N     | 302 | GLY  | 2.6  |
| 2   | N     | 409 | LYS  | 2.6  |
| 4   | H     | 113 | SER  | 2.6  |
| 1   | T     | 199 | LYS  | 2.6  |
| 2   | W     | 473 | LEU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | W     | 453 | PRO  | 2.6  |
| 4   | Z     | 130 | LEU  | 2.6  |
| 1   | T     | 321 | GLY  | 2.6  |
| 1   | U     | 442 | GLU  | 2.6  |
| 5   | I     | 23  | SER  | 2.6  |
| 3   | P     | 161 | LYS  | 2.5  |
| 1   | U     | 509 | THR  | 2.5  |
| 1   | T     | 489 | GLY  | 2.5  |
| 2   | W     | 395 | GLU  | 2.5  |
| 1   | U     | 507 | VAL  | 2.5  |
| 2   | N     | 445 | LEU  | 2.5  |
| 1   | T     | 412 | LEU  | 2.5  |
| 3   | Y     | 223 | ALA  | 2.5  |
| 4   | H     | 112 | VAL  | 2.5  |
| 2   | N     | 451 | ASN  | 2.5  |
| 1   | T     | 313 | LYS  | 2.5  |
| 3   | Y     | 165 | PHE  | 2.5  |
| 1   | U     | 143 | SER  | 2.5  |
| 2   | W     | 387 | ILE  | 2.5  |
| 3   | Y     | 124 | ASN  | 2.5  |
| 2   | V     | 31  | PRO  | 2.5  |
| 3   | P     | 39  | ILE  | 2.5  |
| 3   | Y     | 219 | LEU  | 2.4  |
| 2   | E     | 474 | ALA  | 2.4  |
| 3   | P     | 46  | GLU  | 2.4  |
| 3   | Y     | 141 | GLN  | 2.4  |
| 2   | N     | 402 | LEU  | 2.4  |
| 5   | R     | 27  | THR  | 2.4  |
| 3   | G     | 172 | SER  | 2.4  |
| 1   | T     | 200 | LYS  | 2.4  |
| 2   | V     | 29  | GLU  | 2.4  |
| 3   | P     | 164 | ILE  | 2.4  |
| 3   | Y     | 119 | LEU  | 2.4  |
| 4   | Q     | 80  | ASP  | 2.3  |
| 1   | T     | 197 | GLU  | 2.3  |
| 1   | U     | 424 | GLU  | 2.3  |
| 4   | Z     | 126 | GLN  | 2.3  |
| 2   | E     | 451 | ASN  | 2.3  |
| 1   | J     | 481 | LEU  | 2.3  |
| 3   | G     | 60  | LEU  | 2.3  |
| 1   | U     | 44  | PHE  | 2.3  |
| 2   | N     | 456 | ALA  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 410 | ILE  | 2.3  |
| 1   | S     | 507 | VAL  | 2.3  |
| 2   | V     | 467 | VAL  | 2.3  |
| 2   | V     | 302 | GLY  | 2.2  |
| 3   | Y     | 39  | ILE  | 2.2  |
| 2   | E     | 405 | GLU  | 2.2  |
| 1   | T     | 122 | PRO  | 2.2  |
| 1   | B     | 489 | GLY  | 2.2  |
| 2   | V     | 212 | GLU  | 2.2  |
| 3   | Y     | 169 | PRO  | 2.2  |
| 1   | K     | 499 | LEU  | 2.2  |
| 1   | U     | 58  | SER  | 2.2  |
| 1   | K     | 491 | LEU  | 2.2  |
| 4   | H     | 49  | VAL  | 2.2  |
| 1   | U     | 48  | ASN  | 2.2  |
| 1   | U     | 476 | SER  | 2.2  |
| 1   | U     | 411 | ASP  | 2.2  |
| 1   | S     | 36  | VAL  | 2.2  |
| 2   | V     | 23  | VAL  | 2.2  |
| 1   | U     | 469 | SER  | 2.2  |
| 2   | E     | 407 | ALA  | 2.2  |
| 1   | U     | 304 | HIS  | 2.2  |
| 2   | V     | 90  | GLU  | 2.2  |
| 1   | T     | 482 | LEU  | 2.2  |
| 2   | V     | 8   | PRO  | 2.2  |
| 2   | V     | 427 | ILE  | 2.2  |
| 5   | 1     | 16  | VAL  | 2.2  |
| 2   | X     | 248 | GLY  | 2.2  |
| 5   | 1     | 13  | TYR  | 2.2  |
| 3   | Y     | 40  | SER  | 2.2  |
| 1   | K     | 418 | GLN  | 2.2  |
| 1   | U     | 29  | GLU  | 2.2  |
| 2   | N     | 395 | GLU  | 2.2  |
| 2   | E     | 445 | LEU  | 2.1  |
| 1   | K     | 149 | GLN  | 2.1  |
| 3   | P     | 91  | LEU  | 2.1  |
| 1   | U     | 33  | VAL  | 2.1  |
| 2   | N     | 390 | ILE  | 2.1  |
| 4   | Z     | 133 | LEU  | 2.1  |
| 5   | 1     | 17  | ALA  | 2.1  |
| 1   | U     | 116 | PRO  | 2.1  |
| 1   | T     | 123 | ILE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | T     | 490 | GLU  | 2.1  |
| 1   | U     | 86  | GLU  | 2.1  |
| 3   | P     | 126 | ILE  | 2.1  |
| 1   | K     | 460 | LEU  | 2.1  |
| 4   | Q     | 97  | SER  | 2.1  |
| 2   | V     | 109 | ILE  | 2.1  |
| 2   | W     | 58  | THR  | 2.1  |
| 1   | T     | 264 | LYS  | 2.1  |
| 1   | S     | 44  | PHE  | 2.1  |
| 2   | X     | 42  | PRO  | 2.1  |
| 1   | K     | 508 | ALA  | 2.1  |
| 3   | Y     | 212 | TYR  | 2.1  |
| 2   | V     | 26  | GLU  | 2.1  |
| 3   | P     | 101 | ASP  | 2.1  |
| 2   | E     | 452 | ILE  | 2.1  |
| 1   | T     | 103 | PRO  | 2.1  |
| 4   | Z     | 120 | ALA  | 2.1  |
| 1   | K     | 458 | ILE  | 2.1  |
| 2   | W     | 72  | ARG  | 2.1  |
| 2   | V     | 211 | GLY  | 2.1  |
| 2   | X     | 112 | LYS  | 2.1  |
| 2   | W     | 391 | LEU  | 2.1  |
| 3   | Y     | 44  | MET  | 2.1  |
| 1   | T     | 48  | ASN  | 2.1  |
| 2   | V     | 45  | LYS  | 2.1  |
| 5   | 1     | 34  | VAL  | 2.1  |
| 2   | M     | 27  | GLN  | 2.0  |
| 2   | N     | 394 | ASP  | 2.0  |
| 1   | K     | 448 | TYR  | 2.0  |
| 1   | J     | 496 | LEU  | 2.0  |
| 2   | N     | 11  | GLY  | 2.0  |
| 3   | Y     | 145 | LEU  | 2.0  |
| 2   | V     | 25  | PHE  | 2.0  |
| 2   | W     | 457 | PHE  | 2.0  |
| 1   | U     | 49  | ILE  | 2.0  |
| 2   | X     | 12  | LYS  | 2.0  |
| 3   | Y     | 224 | GLN  | 2.0  |
| 1   | K     | 455 | LEU  | 2.0  |
| 3   | P     | 107 | ILE  | 2.0  |
| 3   | Y     | 36  | LYS  | 2.0  |
| 1   | U     | 78  | PHE  | 2.0  |
| 2   | X     | 25  | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | S     | 83  | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

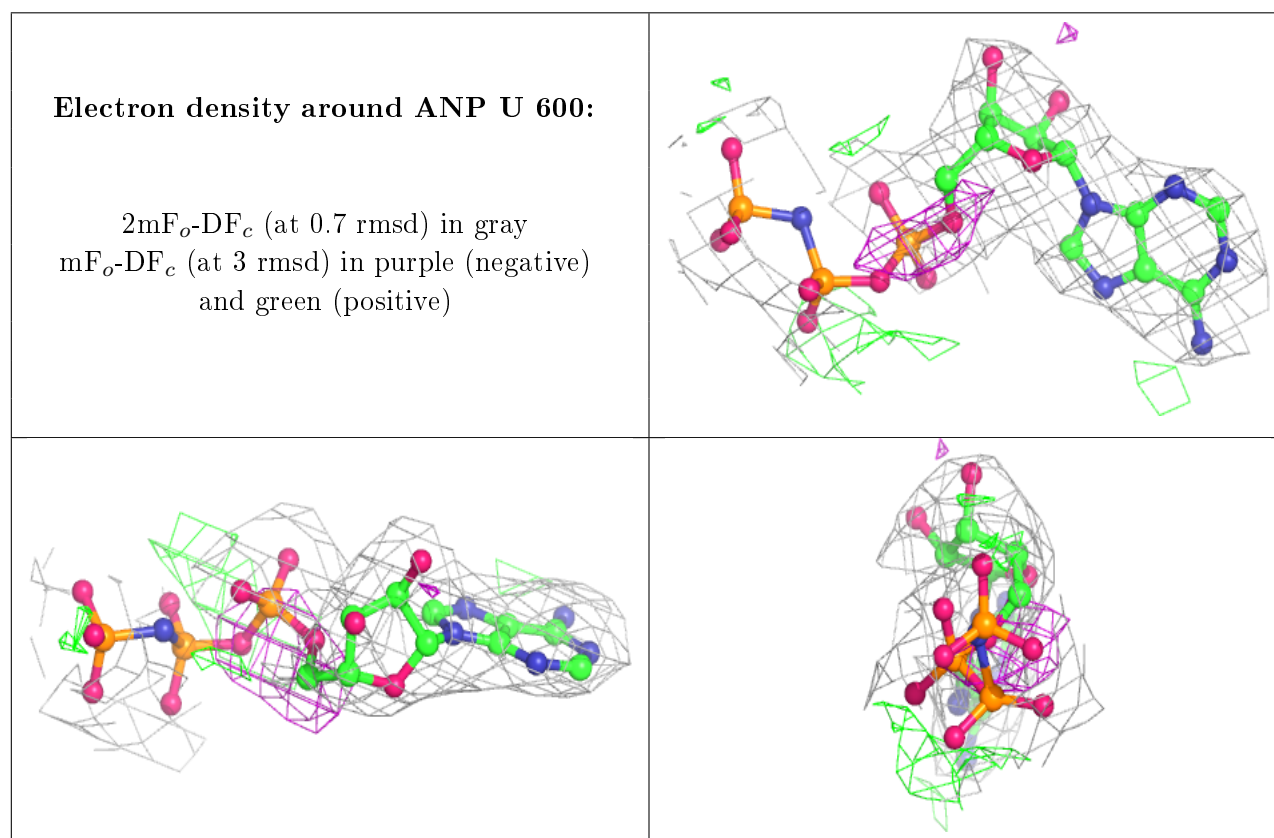
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 7   | MG   | J     | 700 | 1/1   | 0.88 | 0.24 | 51,51,51,51                | 0     |
| 6   | ANP  | U     | 600 | 31/31 | 0.89 | 0.20 | 73,79,82,82                | 0     |
| 6   | ANP  | K     | 600 | 31/31 | 0.91 | 0.19 | 79,96,100,101              | 0     |
| 6   | ANP  | T     | 600 | 31/31 | 0.92 | 0.17 | 81,102,107,108             | 0     |
| 7   | MG   | M     | 700 | 1/1   | 0.92 | 0.35 | 53,53,53,53                | 0     |
| 7   | MG   | T     | 700 | 1/1   | 0.93 | 0.28 | 62,62,62,62                | 0     |
| 6   | ANP  | J     | 600 | 31/31 | 0.94 | 0.17 | 60,74,82,83                | 0     |
| 7   | MG   | D     | 700 | 1/1   | 0.94 | 0.29 | 48,48,48,48                | 0     |
| 7   | MG   | L     | 700 | 1/1   | 0.95 | 0.33 | 48,48,48,48                | 0     |
| 7   | MG   | O     | 700 | 1/1   | 0.95 | 0.11 | 61,61,61,61                | 0     |
| 6   | ANP  | V     | 600 | 31/31 | 0.95 | 0.20 | 80,100,102,102             | 0     |
| 6   | ANP  | B     | 600 | 31/31 | 0.95 | 0.16 | 66,79,81,82                | 0     |
| 6   | ANP  | C     | 600 | 31/31 | 0.96 | 0.20 | 57,68,75,75                | 0     |
| 6   | ANP  | X     | 600 | 31/31 | 0.96 | 0.17 | 83,95,97,97                | 0     |
| 6   | ANP  | F     | 600 | 31/31 | 0.96 | 0.20 | 65,79,84,85                | 0     |
| 7   | MG   | S     | 700 | 1/1   | 0.96 | 0.27 | 53,53,53,53                | 0     |
| 6   | ANP  | L     | 600 | 31/31 | 0.96 | 0.19 | 49,62,70,70                | 0     |
| 6   | ANP  | S     | 600 | 31/31 | 0.96 | 0.14 | 64,78,80,80                | 0     |
| 7   | MG   | V     | 700 | 1/1   | 0.97 | 0.21 | 61,61,61,61                | 0     |
| 6   | ANP  | O     | 600 | 31/31 | 0.97 | 0.18 | 69,79,81,82                | 0     |
| 7   | MG   | C     | 700 | 1/1   | 0.97 | 0.37 | 52,52,52,52                | 0     |
| 7   | MG   | K     | 700 | 1/1   | 0.97 | 0.19 | 66,66,66,66                | 0     |

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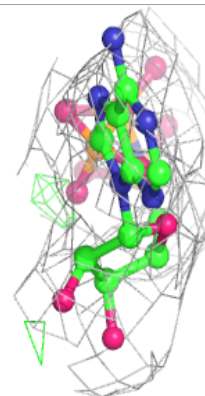
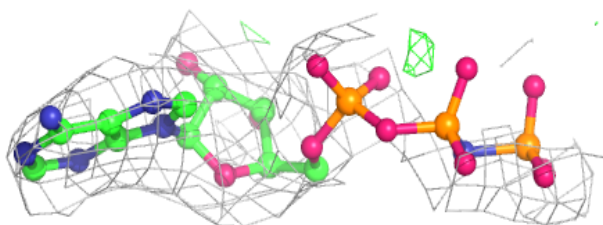
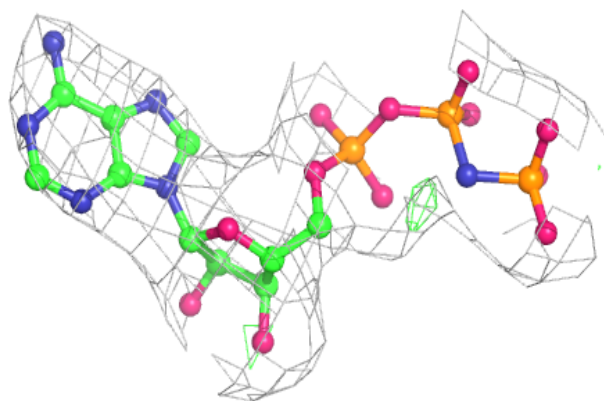
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 7   | MG   | F     | 700 | 1/1   | 0.97 | 0.33 | 55,55,55,55                 | 0     |
| 6   | ANP  | D     | 600 | 31/31 | 0.98 | 0.19 | 55,65,68,69                 | 0     |
| 7   | MG   | A     | 700 | 1/1   | 0.98 | 0.32 | 41,41,41,41                 | 0     |
| 7   | MG   | B     | 700 | 1/1   | 0.98 | 0.32 | 57,57,57,57                 | 0     |
| 6   | ANP  | A     | 600 | 31/31 | 0.98 | 0.19 | 44,57,61,63                 | 0     |
| 7   | MG   | X     | 700 | 1/1   | 0.98 | 0.15 | 70,70,70,70                 | 0     |
| 6   | ANP  | M     | 600 | 31/31 | 0.98 | 0.20 | 60,70,73,74                 | 0     |
| 7   | MG   | U     | 700 | 1/1   | 0.99 | 0.30 | 61,61,61,61                 | 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.

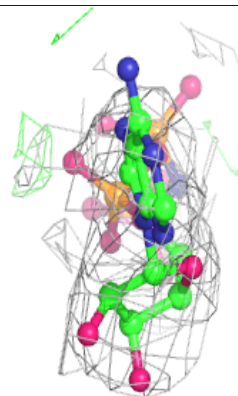
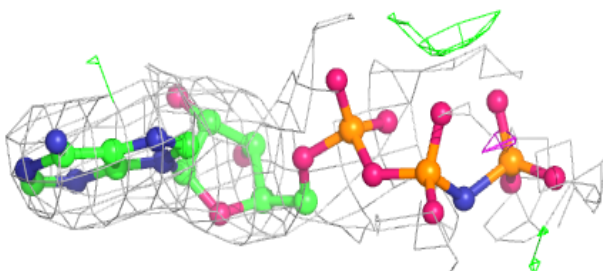
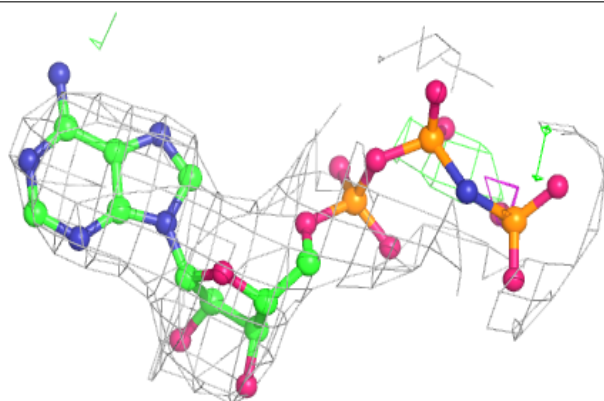


**Electron density around ANP K 600:**

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

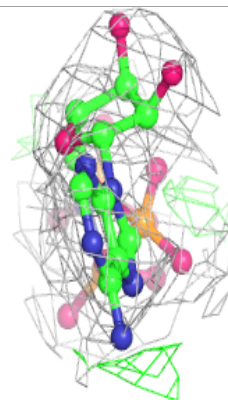
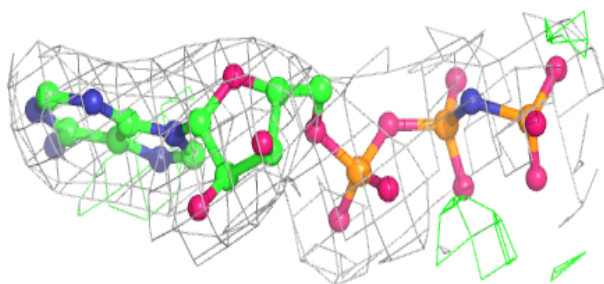
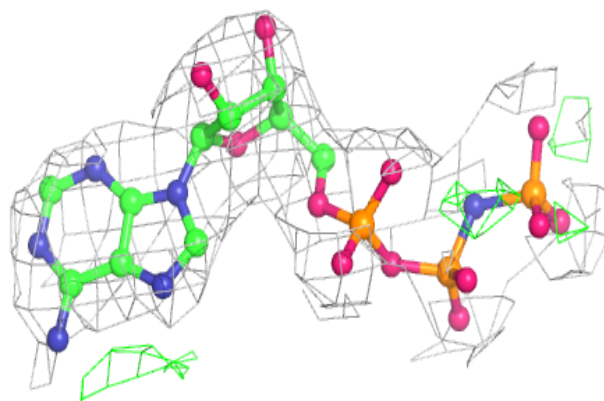
**Electron density around ANP T 600:**

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

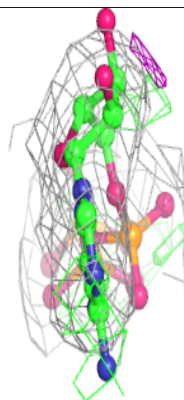
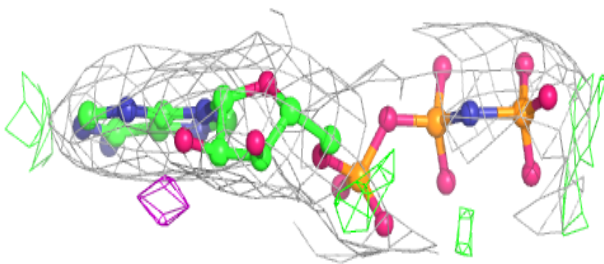
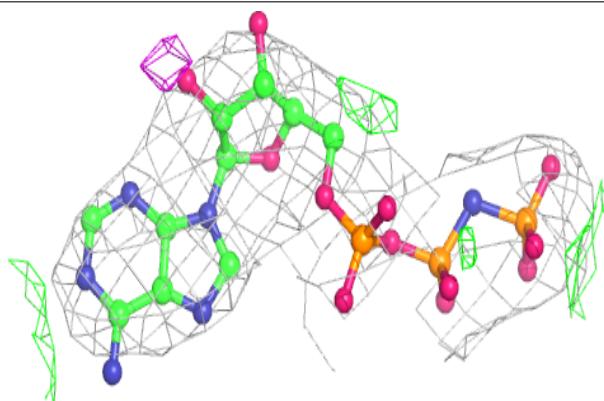


**Electron density around ANP J 600:**

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

**Electron density around ANP V 600:**

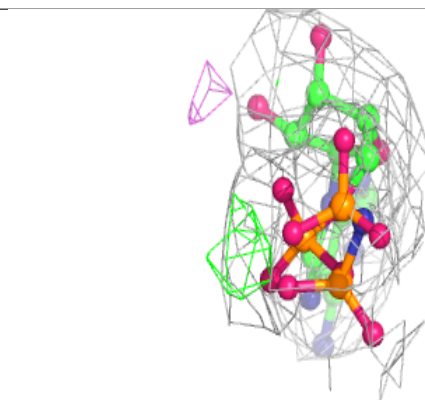
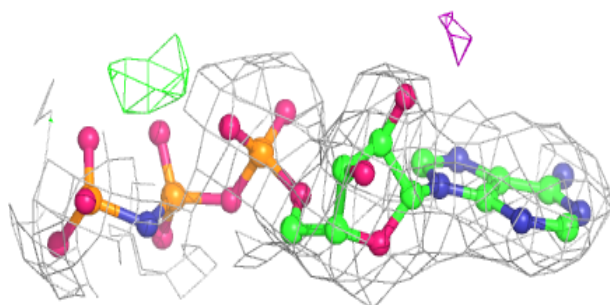
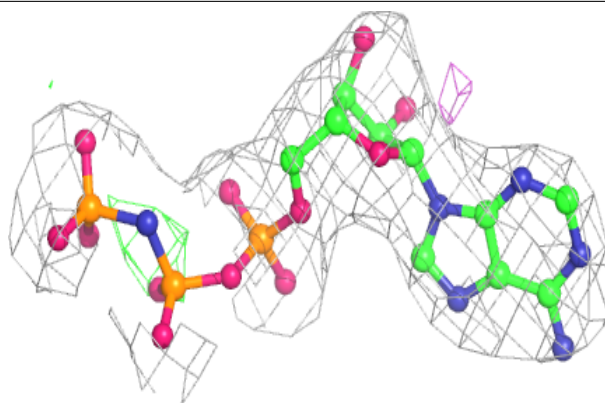
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



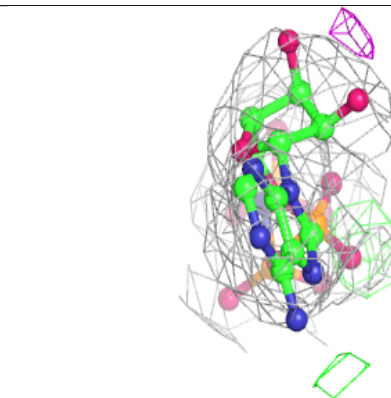
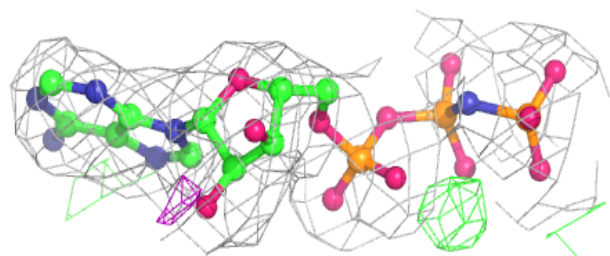
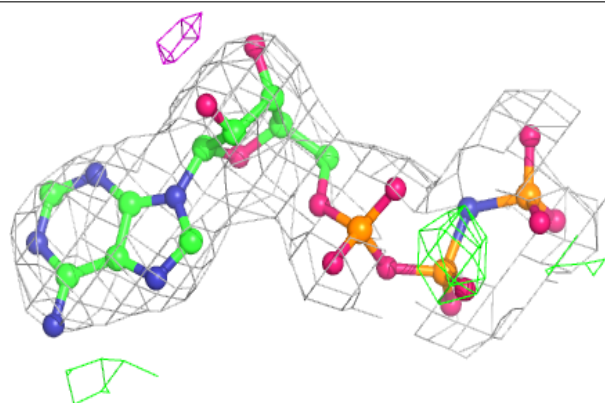


**Electron density around ANP B 600:**

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and green (positive)

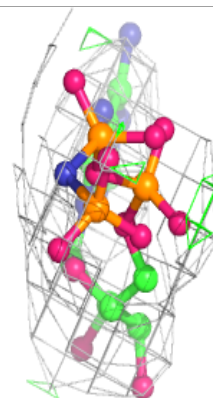
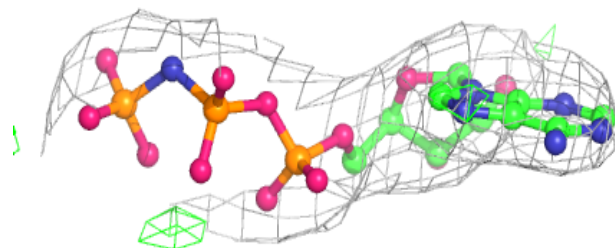
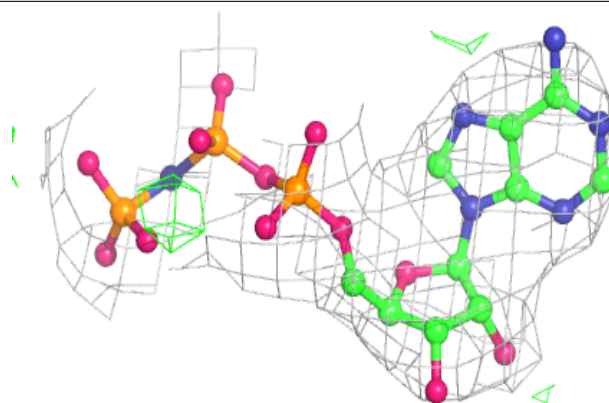
**Electron density around ANP C 600:**

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and green (positive)

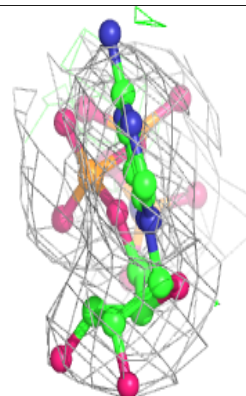
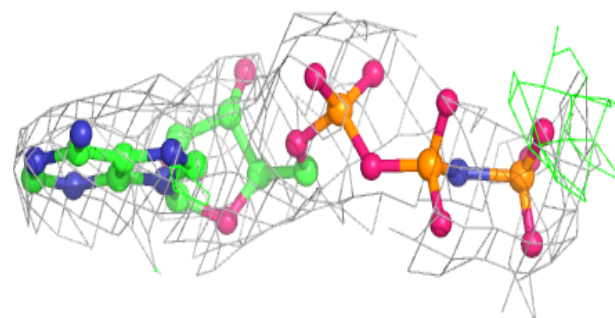
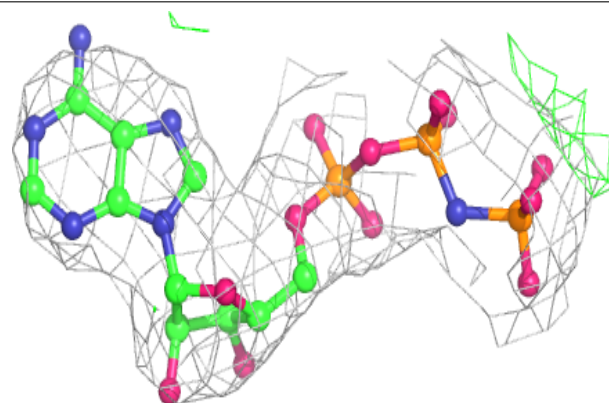


**Electron density around ANP X 600:**

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

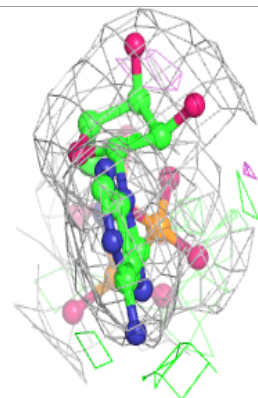
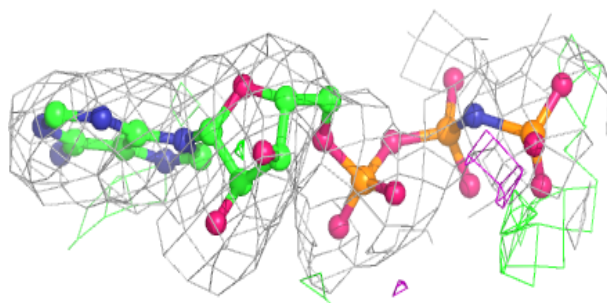
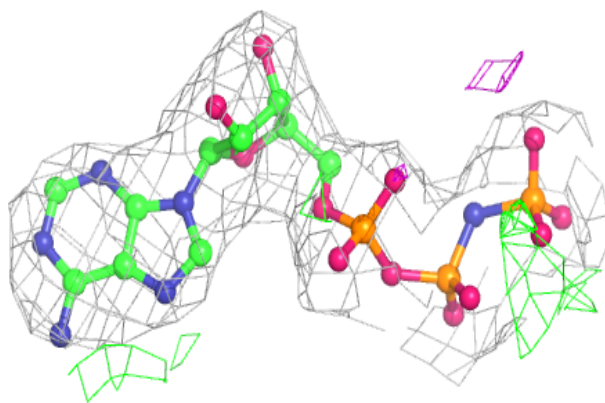
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and green (positive)

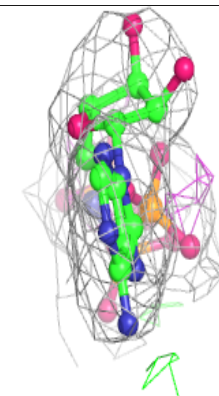
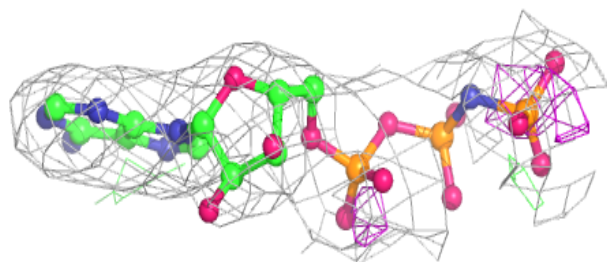
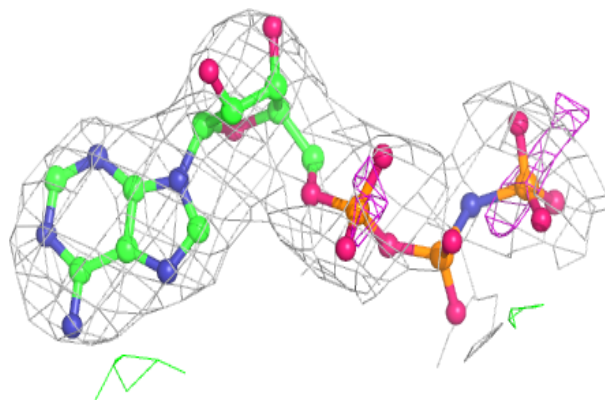


**Electron density around ANP L 600:**

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and green (positive)

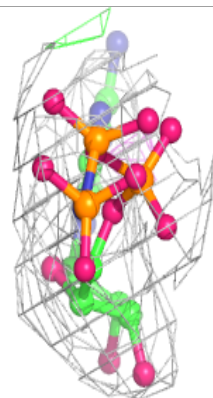
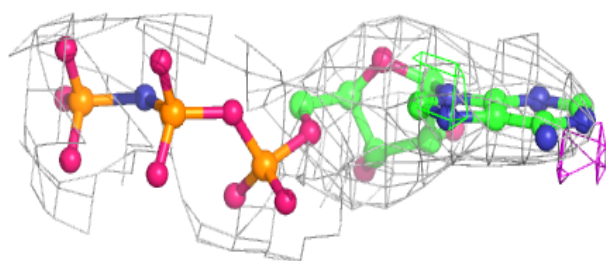
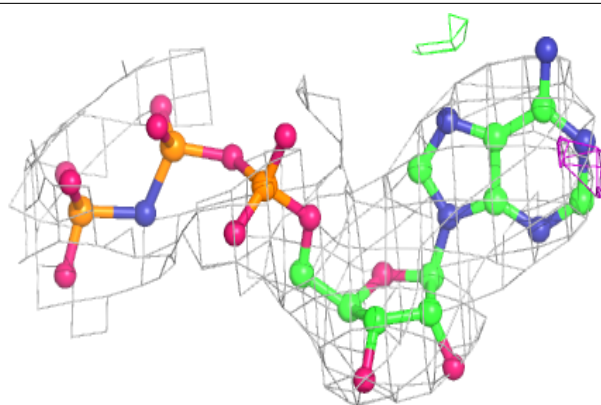
**Electron density around ANP S 600:**

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and green (positive)

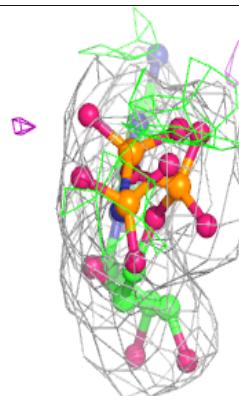
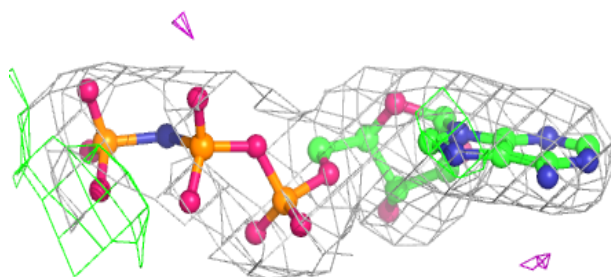
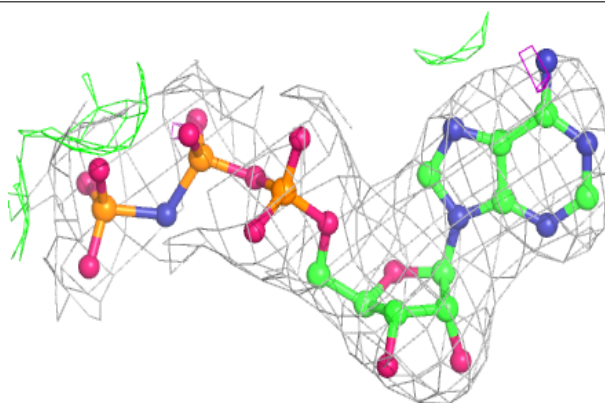


**Electron density around ANP O 600:**

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

**Electron density around ANP D 600:**

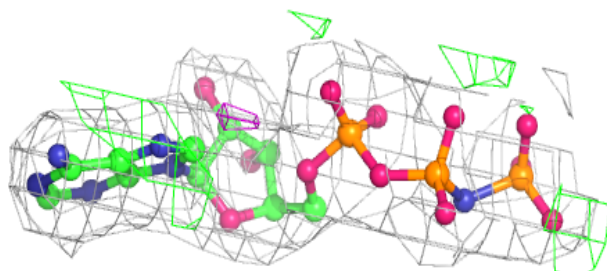
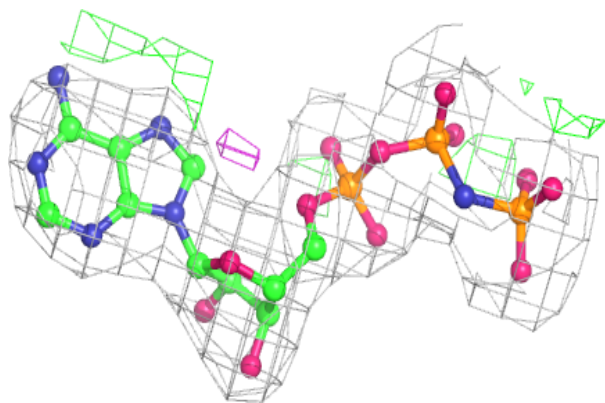
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



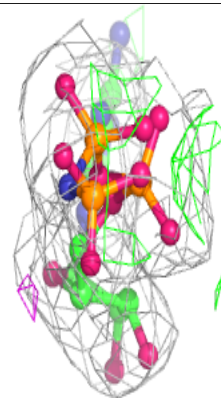
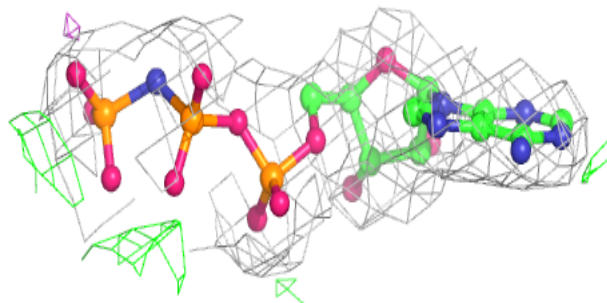
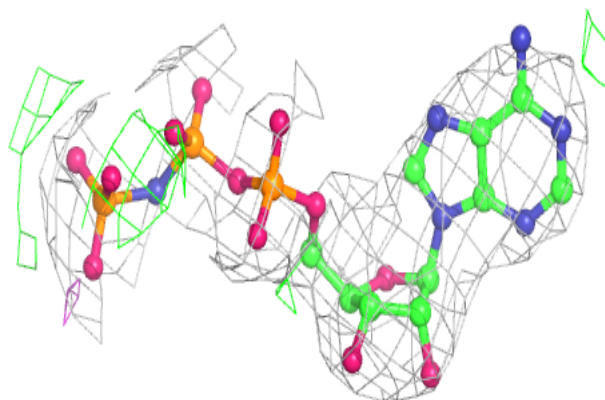


**Electron density around ANP A 600:**

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

**Electron density around ANP M 600:**

$2mF_o-DF_c$  (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.