



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 2XOK / pdb\_00002xok  
Title : Refined structure of yeast F1c10 ATPase complex to 3 Å resolution  
Authors : Stock, D.; W Leslie, A.G.; Walker, J.E.  
Deposited on : 2010-08-18  
Resolution : 3.01 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

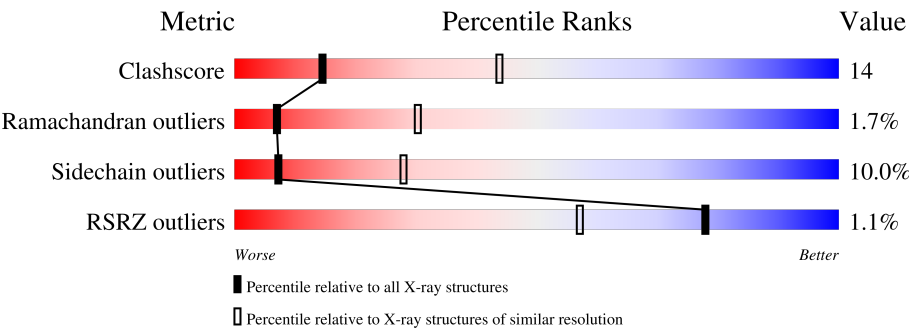
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 3444 (3.04-3.00)                                      |
| Ramachandran outliers | 187476                      | 3319 (3.04-3.00)                                      |
| Sidechain outliers    | 187428                      | 3322 (3.04-3.00)                                      |
| RSRZ outliers         | 180081                      | 3130 (3.04-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                                         |
|-----|-------|--------|----------------------------------------------------------|
| 1   | A     | 545    | <div><div></div><div>60%27%11%</div></div>               |
| 1   | B     | 545    | <div>%<div><div></div><div>55%29%5%11%</div></div></div> |
| 1   | C     | 545    | <div><div></div><div>59%27%11%</div></div>               |
| 2   | D     | 511    | <div><div></div><div>65%25%8%</div></div>                |
| 2   | E     | 511    | <div><div></div><div>60%30%8%</div></div>                |
| 2   | F     | 511    | <div><div></div><div>59%30%8%</div></div>                |
| 3   | G     | 311    | <div>%<div><div></div><div>54%24%6%14%</div></div></div> |

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| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 4   | H     | 160    | <br>48% 20% 6% 26%  |
| 5   | I     | 61     | <br>41% 26% 11% 20% |
| 6   | K     | 76     | <br>57% 30% 9%      |
| 6   | L     | 76     | <br>62% 28% 5% 5%   |
| 6   | M     | 76     | <br>63% 25% 8%      |
| 6   | N     | 76     | <br>58% 28% 11%     |
| 6   | O     | 76     | <br>61% 29% 8%      |
| 6   | P     | 76     | <br>63% 26% 9%      |
| 6   | Q     | 76     | <br>55% 33% 11%     |
| 6   | R     | 76     | <br>62% 28% 5%      |
| 6   | S     | 76     | <br>62% 29% 5%      |
| 6   | T     | 76     | <br>58% 30% 8%      |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 30113 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, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 483      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3665  | 2314 | 649 | 699 | 3 |         |         |       |
| 1   | B     | 484      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3670  | 2317 | 650 | 700 | 3 |         |         |       |
| 1   | C     | 485      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3674  | 2319 | 651 | 701 | 3 |         |         |       |

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | D     | 471      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3550  | 2250 | 605 | 689 | 6 |         |         |       |
| 2   | E     | 469      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3537  | 2243 | 603 | 685 | 6 |         |         |       |
| 2   | F     | 470      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3544  | 2247 | 604 | 687 | 6 |         |         |       |

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | G     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 2031  | 1277 | 356 | 388 | 10 |         |         |       |

- Molecule 4 is a protein called ATP SYNTHASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | H     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 751   | 470 | 133 | 146 | 2 |         |         |       |

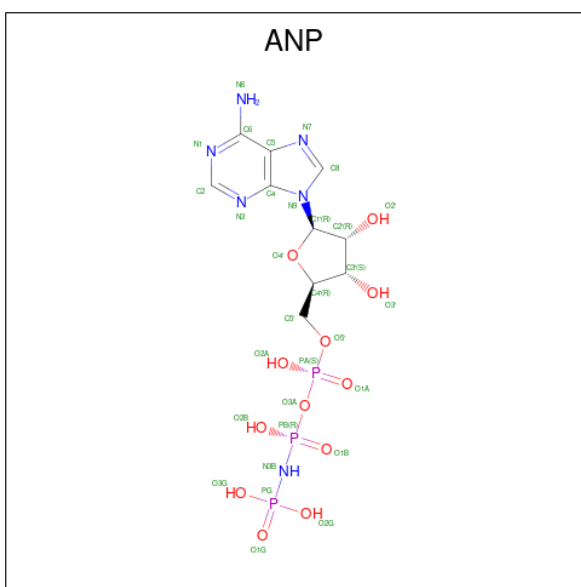
- Molecule 5 is a protein called ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUB-UNIT.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 5   | I     | 49       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 325   | 201 | 57 | 67 |         |         |       |

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | K     | 73       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 517   | 347 | 80 | 87 | 3 |         |         |       |
| 6   | L     | 72       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 507   | 337 | 80 | 87 | 3 |         |         |       |
| 6   | M     | 73       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 515   | 342 | 81 | 88 | 4 |         |         |       |
| 6   | N     | 73       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 515   | 342 | 81 | 88 | 4 |         |         |       |
| 6   | O     | 74       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 523   | 348 | 82 | 89 | 4 |         |         |       |
| 6   | P     | 75       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 534   | 357 | 83 | 90 | 4 |         |         |       |
| 6   | Q     | 75       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 534   | 357 | 83 | 90 | 4 |         |         |       |
| 6   | R     | 74       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 523   | 348 | 82 | 89 | 4 |         |         |       |
| 6   | S     | 74       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 523   | 348 | 82 | 89 | 4 |         |         |       |
| 6   | T     | 73       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 515   | 343 | 81 | 88 | 3 |         |         |       |

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: 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 |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 7   | A     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 7   | B     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 7   | C     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 7   | D     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 7   | F     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |

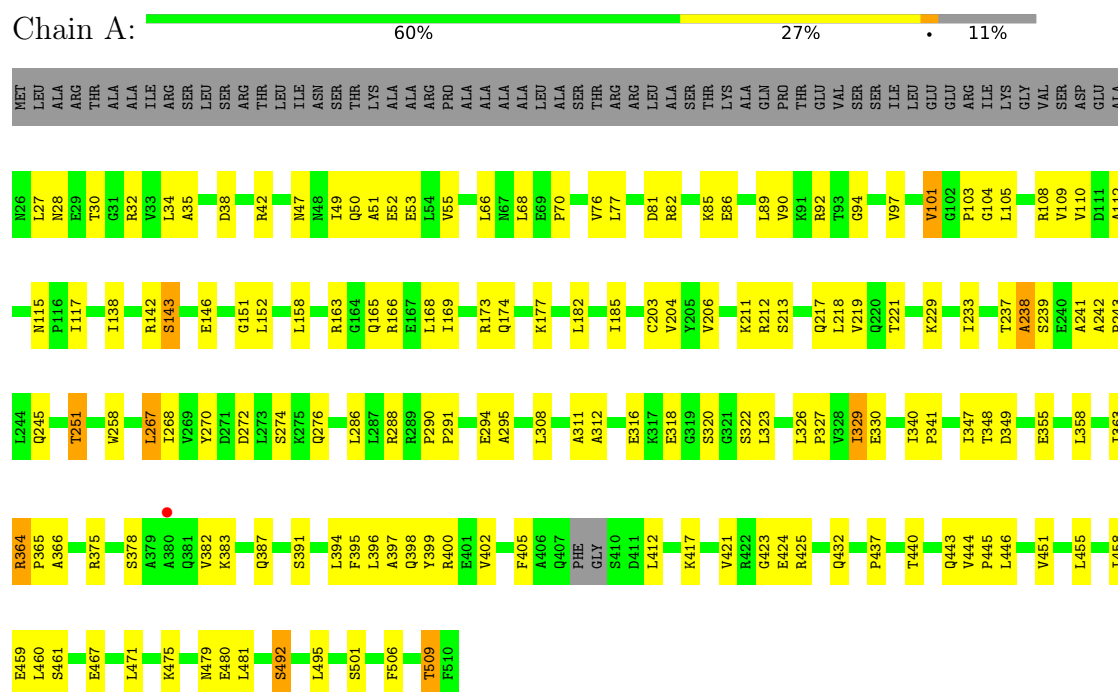
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 8   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 8   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 8   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 8   | F     | 1        | Total Mg<br>1 1 | 0       | 0       |

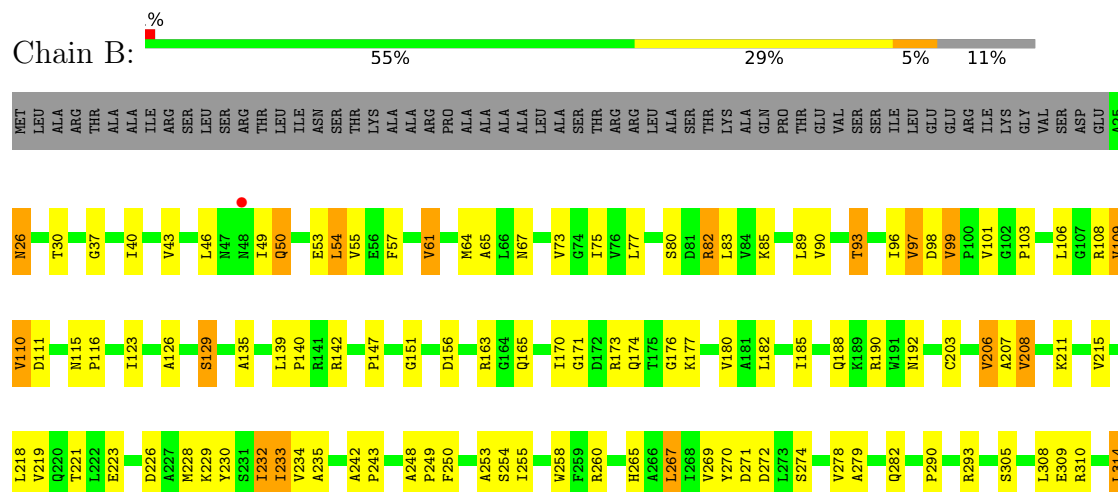
### 3 Residue-property plots

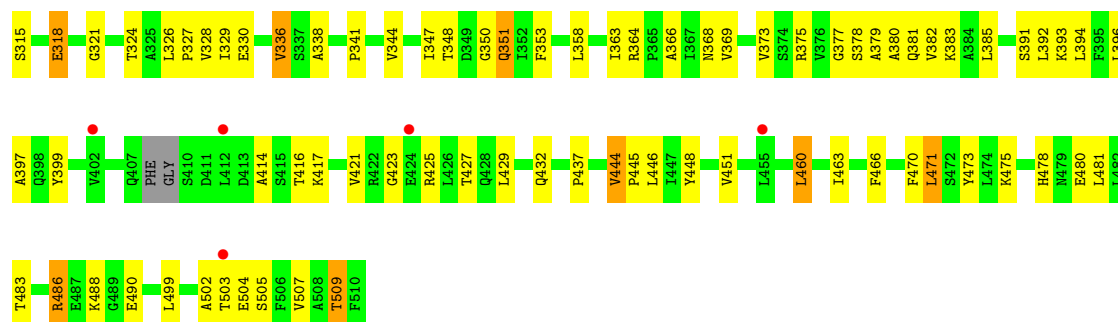
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



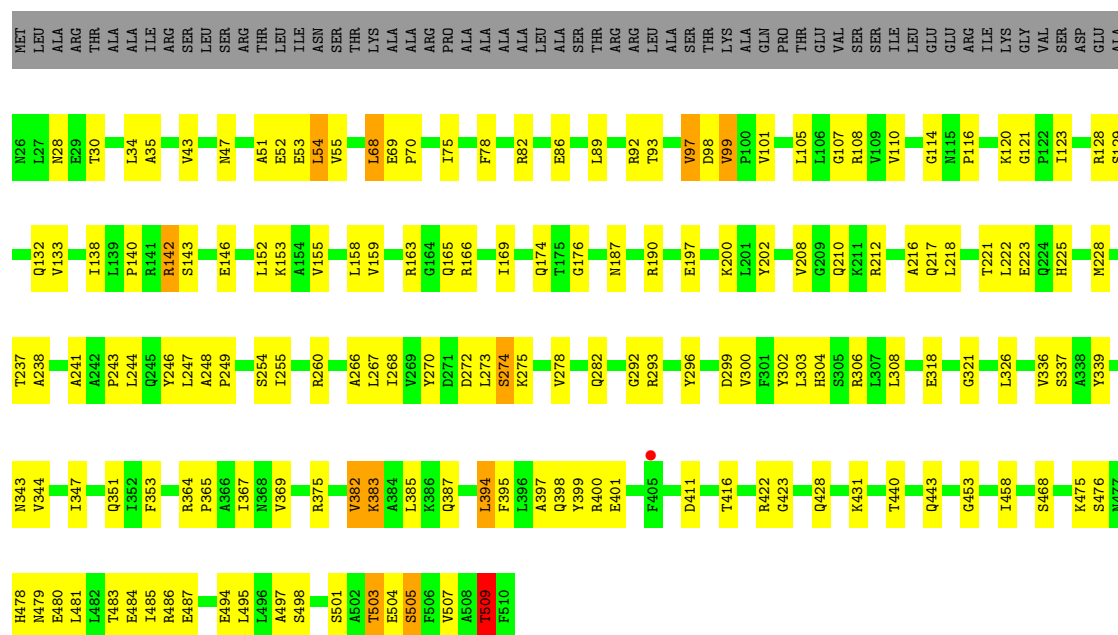
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL





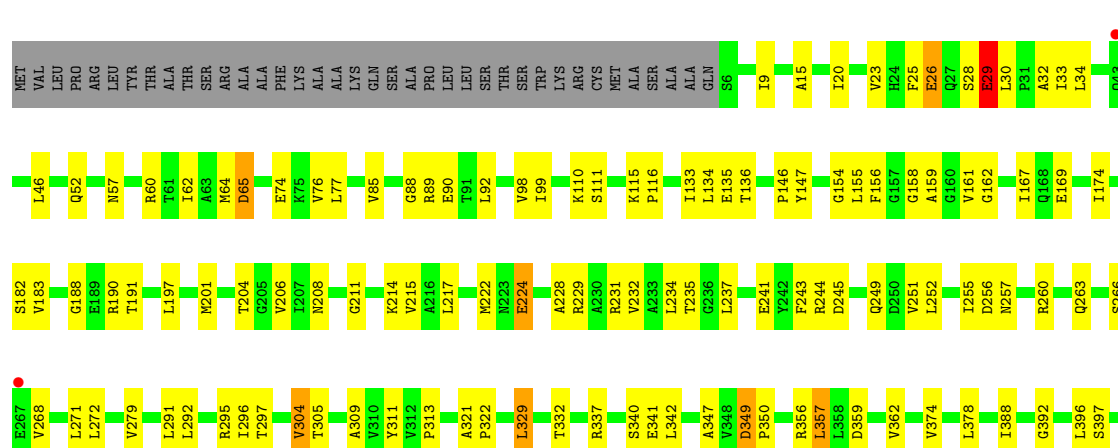
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

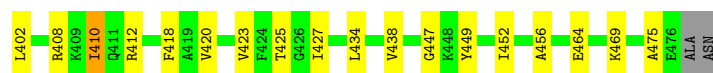
Chain C: 59% 27% 11%



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

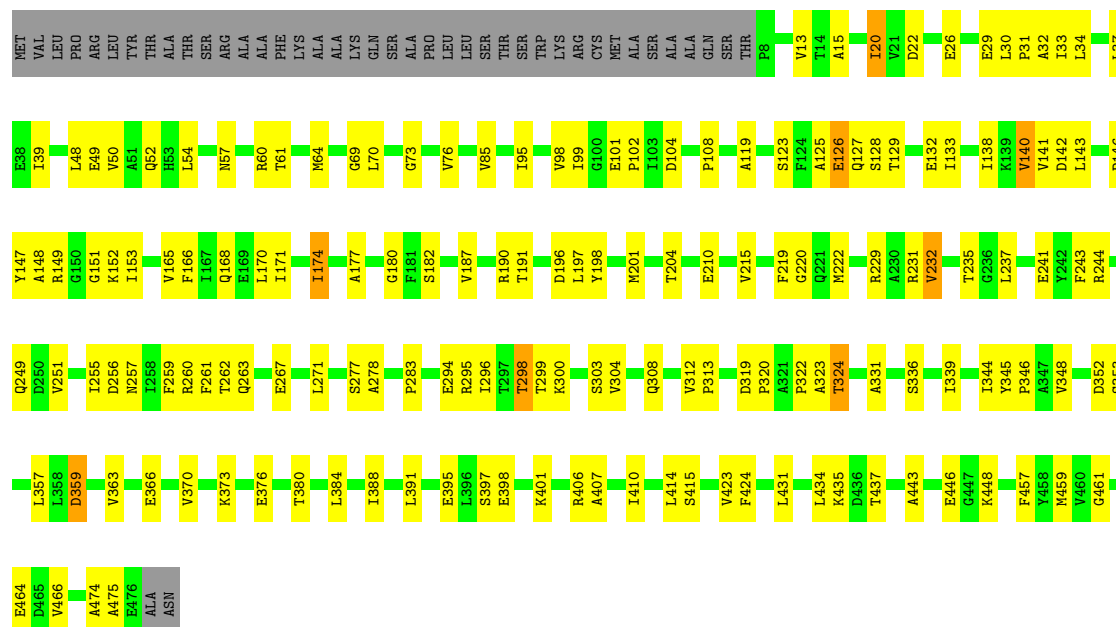
Chain D: 65% 25% 8%





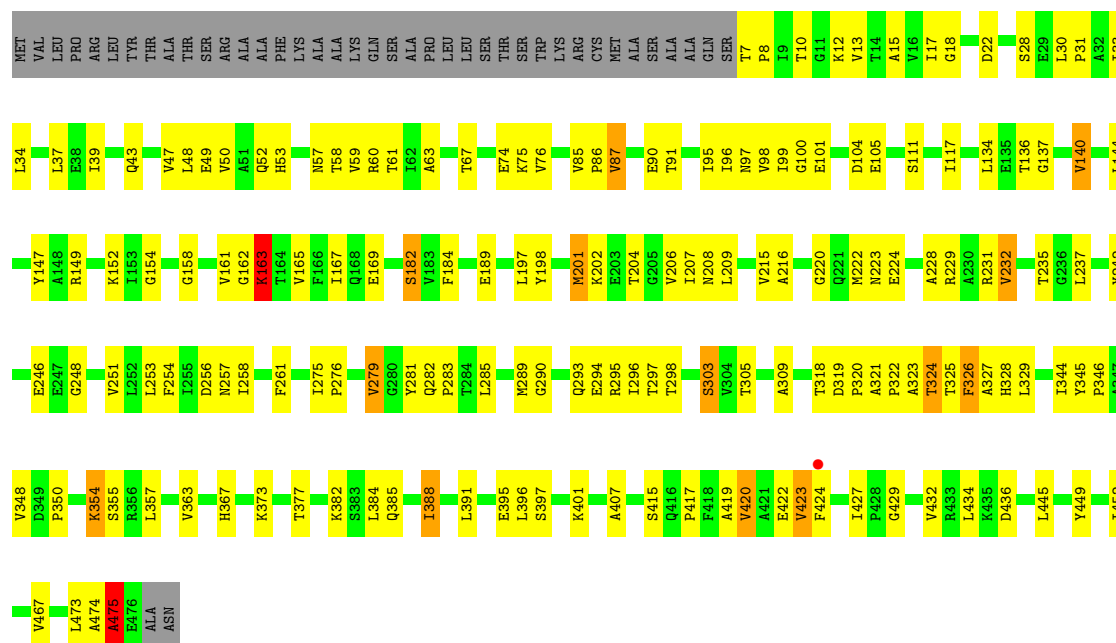
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 60% 30% 8%

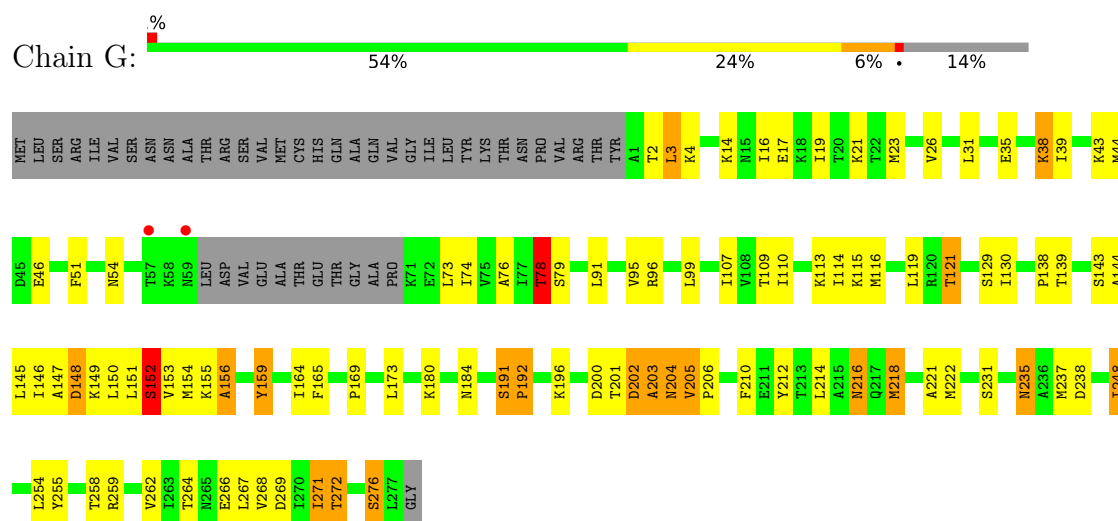


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

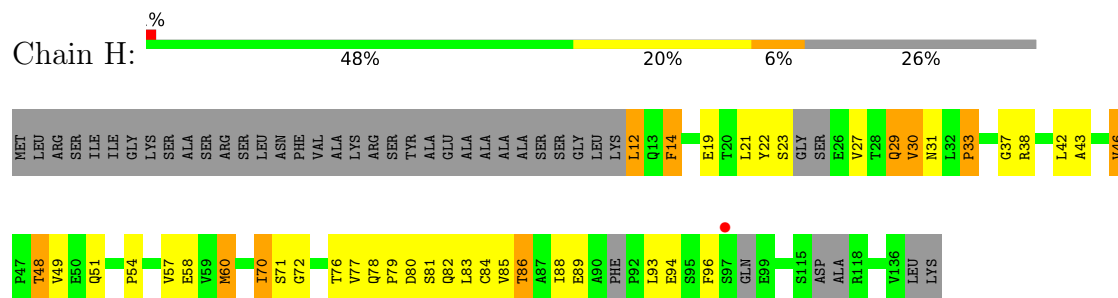
Chain F: 59% 30% 8%



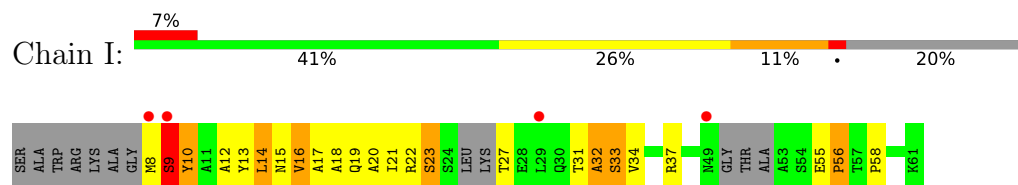
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



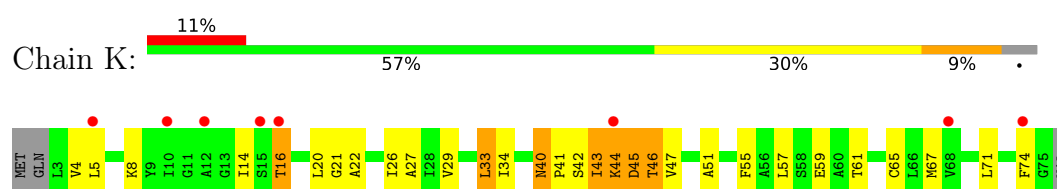
• Molecule 4: ATP SYNTHASE



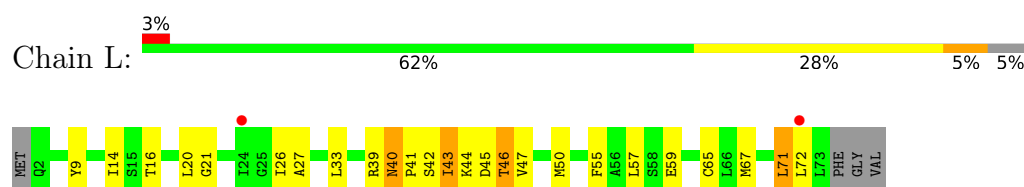
• Molecule 5: ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUBUNIT



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



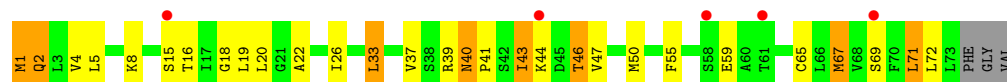
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



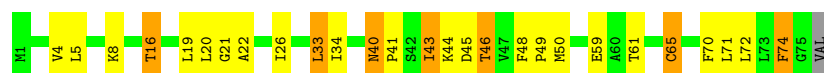
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



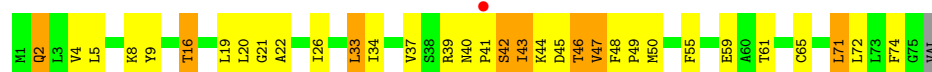
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



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• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



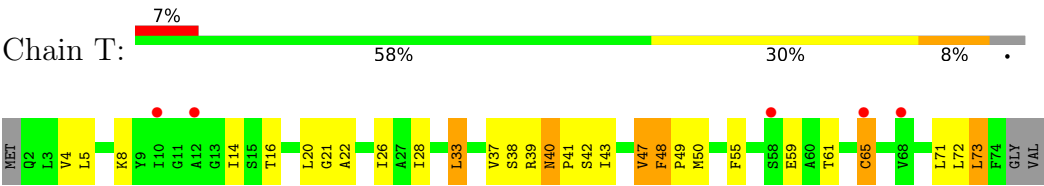
• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



● Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 135.35Å 173.71Å 137.89Å<br>90.00° 91.77° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.01<br>20.00 – 3.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 74.8 (20.00-3.01)<br>74.6 (20.00-3.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.73 (at 3.04Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.210 , 0.253<br>0.217 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 88.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.086                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 89.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.43$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for l,k,-h<br>0.004 for h,-k,-l<br>0.011 for l,-k,h   | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 30113                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 116.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: ANP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.67         | 1/3719 (0.0%)   | 0.98        | 5/5034 (0.1%)   |
| 1   | B     | 0.61         | 1/3724 (0.0%)   | 0.94        | 4/5041 (0.1%)   |
| 1   | C     | 0.72         | 1/3729 (0.0%)   | 1.03        | 3/5049 (0.1%)   |
| 2   | D     | 0.71         | 1/3606 (0.0%)   | 1.03        | 9/4891 (0.2%)   |
| 2   | E     | 0.58         | 1/3593 (0.0%)   | 0.89        | 0/4872          |
| 2   | F     | 0.68         | 2/3600 (0.1%)   | 1.00        | 4/4883 (0.1%)   |
| 3   | G     | 0.58         | 1/2056 (0.0%)   | 0.97        | 5/2768 (0.2%)   |
| 4   | H     | 0.63         | 0/759           | 1.05        | 0/1040          |
| 5   | I     | 0.73         | 1/327 (0.3%)    | 1.21        | 5/447 (1.1%)    |
| 6   | K     | 0.64         | 1/525 (0.2%)    | 0.99        | 1/712 (0.1%)    |
| 6   | L     | 0.65         | 1/514 (0.2%)    | 0.94        | 0/697           |
| 6   | M     | 0.67         | 1/522 (0.2%)    | 1.02        | 0/707           |
| 6   | N     | 0.65         | 1/522 (0.2%)    | 1.00        | 0/707           |
| 6   | O     | 0.64         | 1/530 (0.2%)    | 0.97        | 0/718           |
| 6   | P     | 0.60         | 1/542 (0.2%)    | 0.91        | 0/734           |
| 6   | Q     | 0.63         | 1/542 (0.2%)    | 0.95        | 0/734           |
| 6   | R     | 0.65         | 1/530 (0.2%)    | 1.00        | 0/718           |
| 6   | S     | 0.64         | 1/530 (0.2%)    | 0.97        | 0/718           |
| 6   | T     | 0.64         | 1/522 (0.2%)    | 0.99        | 0/708           |
| All | All   | 0.65         | 19/30392 (0.1%) | 0.98        | 36/41178 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | I     | 0                   | 1                   |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | O     | 73  | LEU  | C-N   | -7.21 | 1.23        | 1.33     |
| 6   | P     | 74  | PHE  | C-N   | -7.02 | 1.23        | 1.33     |
| 6   | T     | 73  | LEU  | C-N   | -7.02 | 1.23        | 1.33     |
| 6   | L     | 72  | LEU  | C-N   | -6.96 | 1.23        | 1.33     |
| 6   | K     | 74  | PHE  | C-N   | -6.96 | 1.23        | 1.33     |
| 2   | F     | 475 | ALA  | C-N   | -6.93 | 1.23        | 1.33     |
| 2   | D     | 475 | ALA  | C-N   | -6.91 | 1.23        | 1.33     |
| 5   | I     | 23  | SER  | C-N   | -6.86 | 1.23        | 1.33     |
| 6   | Q     | 74  | PHE  | C-N   | -6.85 | 1.23        | 1.33     |
| 1   | A     | 509 | THR  | C-N   | -6.84 | 1.23        | 1.33     |
| 6   | R     | 73  | LEU  | C-N   | -6.81 | 1.23        | 1.33     |
| 6   | M     | 72  | LEU  | C-N   | -6.64 | 1.24        | 1.33     |
| 6   | N     | 72  | LEU  | C-N   | -6.57 | 1.24        | 1.33     |
| 6   | S     | 73  | LEU  | C-N   | -6.54 | 1.24        | 1.33     |
| 2   | E     | 475 | ALA  | C-N   | -6.53 | 1.24        | 1.33     |
| 1   | B     | 509 | THR  | C-N   | -6.51 | 1.24        | 1.33     |
| 3   | G     | 276 | SER  | C-N   | -6.42 | 1.24        | 1.33     |
| 1   | C     | 509 | THR  | C-N   | -6.39 | 1.24        | 1.33     |
| 2   | F     | 297 | THR  | CA-CB | 5.77  | 1.63        | 1.53     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 224 | GLU  | CA-C-N  | 10.35 | 127.22      | 119.66   |
| 2   | D     | 224 | GLU  | C-N-CA  | 10.35 | 127.22      | 119.66   |
| 5   | I     | 16  | VAL  | N-CA-C  | -7.70 | 105.66      | 112.12   |
| 5   | I     | 56  | PRO  | N-CA-CB | 7.29  | 110.90      | 103.25   |
| 5   | I     | 20  | ALA  | N-CA-C  | -7.04 | 103.03      | 111.69   |
| 5   | I     | 10  | TYR  | N-CA-C  | -6.88 | 103.53      | 112.68   |
| 5   | I     | 58  | PRO  | N-CA-CB | 6.69  | 110.27      | 103.25   |
| 2   | D     | 349 | ASP  | CA-C-N  | 6.56  | 126.25      | 119.56   |
| 2   | D     | 349 | ASP  | C-N-CA  | 6.56  | 126.25      | 119.56   |
| 2   | D     | 215 | VAL  | N-CA-C  | 6.49  | 116.91      | 108.35   |
| 3   | G     | 191 | SER  | CA-C-N  | 6.44  | 127.89      | 119.84   |
| 3   | G     | 191 | SER  | C-N-CA  | 6.44  | 127.89      | 119.84   |
| 3   | G     | 159 | TYR  | CA-C-N  | 6.09  | 126.54      | 119.47   |
| 3   | G     | 159 | TYR  | C-N-CA  | 6.09  | 126.54      | 119.47   |
| 1   | A     | 312 | ALA  | N-CA-C  | 5.97  | 117.22      | 108.14   |
| 1   | A     | 267 | LEU  | N-CA-C  | -5.84 | 99.13       | 109.06   |
| 2   | F     | 163 | LYS  | N-CA-C  | -5.58 | 104.70      | 112.45   |
| 1   | B     | 98  | ASP  | N-CA-C  | 5.55  | 117.50      | 109.07   |
| 1   | C     | 121 | GLY  | CA-C-N  | 5.44  | 125.75      | 119.93   |
| 1   | C     | 121 | GLY  | C-N-CA  | 5.44  | 125.75      | 119.93   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 110 | VAL  | N-CA-C | 5.37  | 116.58      | 108.96   |
| 1   | C     | 268 | ILE  | N-CA-C | 5.35  | 115.80      | 107.99   |
| 2   | D     | 65  | ASP  | N-CA-C | 5.32  | 115.26      | 108.24   |
| 1   | B     | 208 | VAL  | N-CA-C | 5.29  | 115.97      | 107.98   |
| 2   | F     | 275 | ILE  | N-CA-C | -5.25 | 103.81      | 108.95   |
| 1   | B     | 99  | VAL  | N-CA-C | 5.22  | 114.71      | 108.45   |
| 2   | F     | 282 | GLN  | CA-C-N | 5.21  | 125.29      | 119.87   |
| 2   | F     | 282 | GLN  | C-N-CA | 5.21  | 125.29      | 119.87   |
| 2   | D     | 452 | ILE  | CA-C-N | 5.16  | 125.09      | 119.78   |
| 2   | D     | 452 | ILE  | C-N-CA | 5.16  | 125.09      | 119.78   |
| 6   | K     | 42  | SER  | N-CA-C | 5.15  | 116.98      | 109.71   |
| 1   | A     | 443 | GLN  | CA-C-N | 5.12  | 123.47      | 120.24   |
| 1   | A     | 443 | GLN  | C-N-CA | 5.12  | 123.47      | 120.24   |
| 3   | G     | 156 | ALA  | N-CA-C | 5.10  | 116.53      | 110.97   |
| 1   | A     | 104 | GLY  | N-CA-C | -5.05 | 109.05      | 115.31   |
| 2   | D     | 297 | THR  | N-CA-C | 5.03  | 116.70      | 108.55   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | I     | 9   | SER  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3665  | 0        | 3747     | 93      | 0            |
| 1   | B     | 3670  | 0        | 3752     | 126     | 0            |
| 1   | C     | 3674  | 0        | 3753     | 94      | 0            |
| 2   | D     | 3550  | 0        | 3620     | 77      | 0            |
| 2   | E     | 3537  | 0        | 3610     | 95      | 0            |
| 2   | F     | 3544  | 0        | 3615     | 112     | 0            |
| 3   | G     | 2031  | 0        | 2081     | 56      | 0            |
| 4   | H     | 751   | 0        | 598      | 35      | 0            |
| 5   | I     | 325   | 0        | 249      | 22      | 0            |
| 6   | K     | 517   | 0        | 559      | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | L     | 507   | 0        | 547      | 20      | 0            |
| 6   | M     | 515   | 0        | 559      | 20      | 0            |
| 6   | N     | 515   | 0        | 559      | 23      | 0            |
| 6   | O     | 523   | 0        | 570      | 21      | 0            |
| 6   | P     | 534   | 0        | 579      | 25      | 0            |
| 6   | Q     | 534   | 0        | 579      | 27      | 0            |
| 6   | R     | 523   | 0        | 570      | 24      | 0            |
| 6   | S     | 523   | 0        | 570      | 21      | 0            |
| 6   | T     | 515   | 0        | 558      | 27      | 0            |
| 7   | A     | 31    | 0        | 13       | 1       | 0            |
| 7   | B     | 31    | 0        | 13       | 1       | 0            |
| 7   | C     | 31    | 0        | 13       | 2       | 0            |
| 7   | D     | 31    | 0        | 13       | 3       | 0            |
| 7   | F     | 31    | 0        | 13       | 7       | 0            |
| 8   | A     | 1     | 0        | 0        | 0       | 0            |
| 8   | B     | 1     | 0        | 0        | 0       | 0            |
| 8   | C     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |
| 8   | F     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 30113 | 0        | 30740    | 853     | 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 14.

All (853) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 6:P:40:ASN:HB3  | 6:P:41:PRO:HA    | 1.35                     | 1.09              |
| 6:M:40:ASN:HB3  | 6:M:41:PRO:HA    | 1.40                     | 1.04              |
| 2:F:7:THR:HB    | 2:F:8:PRO:HD2    | 1.41                     | 1.02              |
| 6:S:40:ASN:HB3  | 6:S:41:PRO:HA    | 1.44                     | 0.98              |
| 3:G:23:MET:HB3  | 3:G:237:MET:HG3  | 1.48                     | 0.96              |
| 4:H:89:GLU:HG3  | 5:I:18:ALA:HB1   | 1.47                     | 0.93              |
| 2:D:224:GLU:O   | 2:D:229:ARG:HD3  | 1.69                     | 0.92              |
| 6:M:40:ASN:HB3  | 6:M:41:PRO:CA    | 1.99                     | 0.92              |
| 6:L:40:ASN:HB3  | 6:L:41:PRO:HA    | 1.52                     | 0.91              |
| 5:I:9:SER:H     | 5:I:12:ALA:HB3   | 1.33                     | 0.91              |
| 3:G:96:ARG:HE   | 3:G:121:THR:HG21 | 1.35                     | 0.90              |
| 2:E:148:ALA:HB3 | 2:E:151:GLY:HA3  | 1.51                     | 0.90              |
| 6:Q:50:MET:HE3  | 6:R:34:ILE:HG22  | 1.54                     | 0.90              |
| 6:T:42:SER:O    | 6:T:47:VAL:HB    | 1.71                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:182:SER:HB3  | 2:F:215:VAL:HG23 | 1.52                     | 0.87              |
| 1:C:142:ARG:HG2  | 1:C:143:SER:N    | 1.88                     | 0.86              |
| 5:I:10:TYR:HA    | 5:I:13:TYR:HB2   | 1.58                     | 0.86              |
| 2:D:85:VAL:HG11  | 2:D:235:THR:HG23 | 1.56                     | 0.86              |
| 6:P:40:ASN:HB3   | 6:P:41:PRO:CA    | 2.06                     | 0.85              |
| 2:D:20:ILE:HG13  | 2:D:271:LEU:HB3  | 1.59                     | 0.85              |
| 3:G:44:MET:HE2   | 4:H:86:THR:HG22  | 1.59                     | 0.85              |
| 2:E:142:ASP:HB3  | 2:E:434:LEU:HD13 | 1.59                     | 0.84              |
| 3:G:51:PHE:HA    | 4:H:78:GLN:HE22  | 1.40                     | 0.83              |
| 6:N:40:ASN:HB3   | 6:N:41:PRO:HA    | 1.59                     | 0.83              |
| 1:B:385:LEU:HD23 | 1:B:444:VAL:HG13 | 1.59                     | 0.83              |
| 4:H:89:GLU:CG    | 5:I:18:ALA:HB1   | 2.07                     | 0.83              |
| 4:H:88:ILE:HD12  | 5:I:14:LEU:HB2   | 1.59                     | 0.82              |
| 6:R:50:MET:HE3   | 6:S:34:ILE:HG22  | 1.61                     | 0.82              |
| 6:T:40:ASN:HB3   | 6:T:41:PRO:HA    | 1.60                     | 0.82              |
| 2:F:52:GLN:HE21  | 2:F:60:ARG:HD2   | 1.46                     | 0.81              |
| 1:C:375:ARG:HD3  | 7:D:600:ANP:H5'2 | 1.62                     | 0.80              |
| 6:O:37:VAL:HG21  | 6:O:43:ILE:HD13  | 1.63                     | 0.80              |
| 1:B:444:VAL:HG23 | 1:B:445:PRO:HD3  | 1.64                     | 0.80              |
| 6:P:40:ASN:CB    | 6:P:41:PRO:HA    | 2.08                     | 0.79              |
| 3:G:96:ARG:NE    | 3:G:121:THR:HG21 | 1.96                     | 0.79              |
| 6:L:40:ASN:HB3   | 6:L:41:PRO:CA    | 2.10                     | 0.78              |
| 2:F:158:GLY:O    | 2:F:161:VAL:HG22 | 1.84                     | 0.78              |
| 1:C:142:ARG:HG2  | 1:C:143:SER:H    | 1.45                     | 0.77              |
| 2:F:388:ILE:HD12 | 2:F:396:LEU:HD11 | 1.67                     | 0.77              |
| 6:K:21:GLY:HA3   | 6:L:20:LEU:HA    | 1.66                     | 0.76              |
| 1:B:425:ARG:HD3  | 1:B:460:LEU:HD13 | 1.67                     | 0.76              |
| 1:C:169:ILE:HD11 | 1:C:326:LEU:HD22 | 1.68                     | 0.75              |
| 2:F:189:GLU:O    | 2:F:222:MET:HG2  | 1.86                     | 0.75              |
| 1:B:109:VAL:HG22 | 1:B:233:ILE:HB   | 1.67                     | 0.74              |
| 6:T:40:ASN:CB    | 6:T:41:PRO:HA    | 2.18                     | 0.73              |
| 1:C:282:GLN:HG3  | 2:F:283:PRO:O    | 1.89                     | 0.73              |
| 4:H:31:ASN:HB3   | 4:H:38:ARG:HH21  | 1.55                     | 0.72              |
| 4:H:12:LEU:N     | 4:H:22:TYR:O     | 2.23                     | 0.72              |
| 2:F:7:THR:HB     | 2:F:8:PRO:CD     | 2.17                     | 0.71              |
| 3:G:95:VAL:O     | 3:G:99:LEU:HB2   | 1.90                     | 0.71              |
| 1:A:185:ILE:HG12 | 1:A:203:CYS:SG   | 2.30                     | 0.71              |
| 2:F:289:MET:HE1  | 2:F:324:THR:HB   | 1.73                     | 0.71              |
| 2:F:162:GLY:HA2  | 7:F:600:ANP:O3A  | 1.91                     | 0.70              |
| 2:E:384:LEU:O    | 2:E:388:ILE:HG12 | 1.91                     | 0.70              |
| 6:K:33:LEU:HD23  | 6:K:47:VAL:HG12  | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:76:THR:HG23  | 4:H:84:CYS:HB2   | 1.72                     | 0.70              |
| 1:C:116:PRO:HD3  | 1:C:123:ILE:HG12 | 1.74                     | 0.70              |
| 2:D:29:GLU:O     | 2:D:29:GLU:HG2   | 1.91                     | 0.69              |
| 1:C:365:PRO:HB2  | 1:C:367:ILE:HG13 | 1.75                     | 0.69              |
| 2:F:391:LEU:HD22 | 2:F:395:GLU:HG3  | 1.74                     | 0.69              |
| 6:S:40:ASN:HB3   | 6:S:41:PRO:CA    | 2.22                     | 0.69              |
| 6:Q:65:CYS:SG    | 6:R:16:THR:HG22  | 2.33                     | 0.69              |
| 1:B:375:ARG:HG2  | 7:F:600:ANP:O3'  | 1.93                     | 0.68              |
| 6:K:20:LEU:HA    | 6:T:21:GLY:HA3   | 1.74                     | 0.68              |
| 2:F:97:ASN:HB2   | 2:F:101:GLU:H    | 1.58                     | 0.68              |
| 1:B:272:ASP:HB2  | 1:B:328:VAL:O    | 1.95                     | 0.67              |
| 6:P:65:CYS:SG    | 6:Q:16:THR:HG22  | 2.34                     | 0.67              |
| 2:D:237:LEU:HD13 | 2:D:296:ILE:HG12 | 1.76                     | 0.67              |
| 1:C:69:GLU:HB3   | 1:C:70:PRO:CD    | 2.24                     | 0.67              |
| 2:D:197:LEU:O    | 2:D:201:MET:HG2  | 1.95                     | 0.66              |
| 6:L:47:VAL:HA    | 6:L:50:MET:HE2   | 1.78                     | 0.66              |
| 6:N:37:VAL:HG11  | 6:N:43:ILE:HD13  | 1.76                     | 0.66              |
| 2:E:20:ILE:HD11  | 2:E:271:LEU:HB3  | 1.78                     | 0.66              |
| 4:H:29:GLN:HB3   | 4:H:60:MET:HE2   | 1.78                     | 0.65              |
| 3:G:113:LYS:HA   | 3:G:116:MET:HE3  | 1.76                     | 0.65              |
| 6:P:50:MET:SD    | 6:Q:33:LEU:HD11  | 2.37                     | 0.65              |
| 2:F:197:LEU:O    | 2:F:201:MET:HG2  | 1.95                     | 0.65              |
| 6:N:40:ASN:CB    | 6:N:41:PRO:HA    | 2.27                     | 0.65              |
| 6:T:40:ASN:HB3   | 6:T:41:PRO:CA    | 2.23                     | 0.65              |
| 1:B:171:GLY:H    | 1:B:177:LYS:HD3  | 1.62                     | 0.64              |
| 2:E:49:GLU:HB2   | 2:E:64:MET:HE3   | 1.79                     | 0.64              |
| 1:A:506:PHE:HA   | 1:A:509:THR:HG22 | 1.78                     | 0.64              |
| 6:N:39:ARG:HH22  | 6:O:39:ARG:HG2   | 1.62                     | 0.64              |
| 1:A:168:LEU:HB2  | 1:A:348:THR:HG21 | 1.80                     | 0.64              |
| 1:C:54:LEU:HD13  | 1:C:97:VAL:HG22  | 1.80                     | 0.64              |
| 2:E:102:PRO:HG3  | 2:E:108:PRO:HA   | 1.80                     | 0.64              |
| 2:E:148:ALA:CB   | 2:E:151:GLY:HA3  | 2.28                     | 0.64              |
| 4:H:70:ILE:HG23  | 4:H:72:GLY:H     | 1.63                     | 0.64              |
| 1:C:494:GLU:CD   | 1:C:494:GLU:H    | 2.06                     | 0.64              |
| 4:H:88:ILE:HG22  | 4:H:89:GLU:HG2   | 1.79                     | 0.64              |
| 2:D:222:MET:HA   | 2:D:229:ARG:HD2  | 1.79                     | 0.63              |
| 6:R:47:VAL:HA    | 6:R:50:MET:HE2   | 1.79                     | 0.63              |
| 2:F:53:HIS:CD2   | 2:F:59:VAL:HG12  | 2.33                     | 0.63              |
| 1:C:43:VAL:HG21  | 1:C:75:ILE:HD12  | 1.80                     | 0.63              |
| 2:F:202:LYS:HE3  | 2:F:209:LEU:HD11 | 1.79                     | 0.63              |
| 1:C:274:SER:O    | 1:C:278:VAL:HG23 | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:ARG:HH22 | 1:B:116:PRO:HB3  | 1.63                     | 0.63              |
| 1:A:349:ASP:HA   | 1:A:375:ARG:HD3  | 1.79                     | 0.63              |
| 5:I:9:SER:N      | 5:I:12:ALA:HB3   | 2.08                     | 0.63              |
| 2:F:384:LEU:O    | 2:F:388:ILE:HG12 | 1.99                     | 0.63              |
| 2:D:33:ILE:HG22  | 2:D:34:LEU:HG    | 1.81                     | 0.62              |
| 2:F:33:ILE:O     | 2:F:34:LEU:HB2   | 1.99                     | 0.62              |
| 3:G:35:GLU:O     | 3:G:39:ILE:HG12  | 2.00                     | 0.62              |
| 1:B:329:ILE:HD11 | 1:B:344:VAL:HG21 | 1.82                     | 0.62              |
| 3:G:115:LYS:O    | 3:G:119:LEU:HB2  | 1.99                     | 0.62              |
| 1:A:32:ARG:NH1   | 1:A:89:LEU:HB2   | 2.14                     | 0.62              |
| 1:C:440:THR:HA   | 1:C:443:GLN:HE21 | 1.65                     | 0.62              |
| 1:C:97:VAL:HG11  | 1:C:247:LEU:HD21 | 1.80                     | 0.62              |
| 1:C:28:ASN:HA    | 1:C:47:ASN:HB2   | 1.82                     | 0.62              |
| 6:K:44:LYS:O     | 6:K:45:ASP:HB2   | 2.00                     | 0.62              |
| 1:B:106:LEU:HD23 | 1:B:230:TYR:HA   | 1.80                     | 0.61              |
| 2:F:473:LEU:C    | 2:F:475:ALA:H    | 2.07                     | 0.61              |
| 1:B:211:LYS:O    | 1:B:215:VAL:HG23 | 2.00                     | 0.61              |
| 1:C:375:ARG:NH1  | 7:D:600:ANP:HNB1 | 1.97                     | 0.61              |
| 2:E:15:ALA:HB3   | 2:E:22:ASP:HB2   | 1.82                     | 0.61              |
| 1:A:182:LEU:HD13 | 1:A:218:LEU:HD11 | 1.83                     | 0.61              |
| 4:H:46:VAL:HG22  | 6:Q:39:ARG:HA    | 1.83                     | 0.61              |
| 1:A:316:GLU:HA   | 1:A:320:SER:OG   | 2.01                     | 0.61              |
| 2:D:279:VAL:HG12 | 2:D:279:VAL:O    | 2.00                     | 0.61              |
| 4:H:12:LEU:N     | 4:H:23:SER:HA    | 2.16                     | 0.61              |
| 6:K:16:THR:HG22  | 6:T:65:CYS:SG    | 2.40                     | 0.61              |
| 1:A:272:ASP:OD1  | 1:A:274:SER:HB2  | 2.01                     | 0.61              |
| 1:A:382:VAL:HG11 | 1:A:440:THR:HG21 | 1.83                     | 0.61              |
| 1:C:187:ASN:OD1  | 1:C:190:ARG:NH1  | 2.34                     | 0.61              |
| 1:C:241:ALA:HB3  | 1:C:244:LEU:HD12 | 1.83                     | 0.61              |
| 2:F:322:PRO:O    | 2:F:323:ALA:C    | 2.38                     | 0.61              |
| 4:H:29:GLN:O     | 4:H:60:MET:HB2   | 2.00                     | 0.61              |
| 1:A:77:LEU:CD1   | 1:A:81:ASP:HB3   | 2.31                     | 0.61              |
| 1:A:364:ARG:HA   | 1:A:365:PRO:C    | 2.25                     | 0.61              |
| 1:C:483:THR:HG23 | 1:C:486:ARG:NH2  | 2.16                     | 0.61              |
| 2:D:263:GLN:O    | 2:D:266:SER:HB3  | 2.00                     | 0.61              |
| 3:G:200:ASP:C    | 3:G:202:ASP:H    | 2.07                     | 0.61              |
| 1:A:444:VAL:HG22 | 1:A:445:PRO:HD3  | 1.82                     | 0.61              |
| 2:E:168:GLN:HA   | 2:E:171:ILE:HD12 | 1.81                     | 0.61              |
| 2:F:285:LEU:C    | 2:F:285:LEU:HD23 | 2.26                     | 0.61              |
| 6:P:22:ALA:O     | 6:P:26:ILE:HG12  | 2.01                     | 0.61              |
| 2:E:398:GLU:HA   | 2:E:401:LYS:HE2  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:65:CYS:SG    | 6:M:16:THR:HG22  | 2.41                     | 0.60              |
| 2:F:162:GLY:HA2  | 7:F:600:ANP:PA   | 2.41                     | 0.60              |
| 3:G:144:ALA:HB1  | 5:I:12:ALA:HB2   | 1.82                     | 0.60              |
| 1:A:211:LYS:HE3  | 1:A:213:SER:OG   | 2.01                     | 0.60              |
| 2:D:252:LEU:HD23 | 2:D:305:THR:HB   | 1.83                     | 0.60              |
| 3:G:54:ASN:ND2   | 4:H:78:GLN:HE21  | 1.99                     | 0.60              |
| 6:R:71:LEU:CD2   | 6:S:73:LEU:HD21  | 2.32                     | 0.60              |
| 1:C:272:ASP:OD2  | 1:C:275:LYS:HD2  | 2.02                     | 0.60              |
| 1:B:185:ILE:HG23 | 1:B:203:CYS:SG   | 2.41                     | 0.60              |
| 1:A:212:ARG:HG2  | 1:A:237:THR:HG21 | 1.83                     | 0.60              |
| 1:C:336:VAL:HG11 | 1:C:353:PHE:CE2  | 2.37                     | 0.60              |
| 2:F:345:TYR:HA   | 2:F:346:PRO:C    | 2.26                     | 0.59              |
| 2:D:85:VAL:CG1   | 2:D:235:THR:HG23 | 2.32                     | 0.59              |
| 3:G:3:LEU:CD2    | 3:G:255:TYR:CE1  | 2.85                     | 0.59              |
| 6:S:22:ALA:O     | 6:S:26:ILE:HG12  | 2.02                     | 0.59              |
| 2:E:423:VAL:HG23 | 2:E:424:PHE:HD2  | 1.67                     | 0.59              |
| 1:B:182:LEU:HA   | 1:B:185:ILE:HD12 | 1.84                     | 0.59              |
| 6:S:40:ASN:CB    | 6:S:41:PRO:HA    | 2.26                     | 0.59              |
| 1:A:38:ASP:O     | 1:A:286:LEU:HD13 | 2.03                     | 0.59              |
| 1:C:55:VAL:HG21  | 1:C:75:ILE:HD13  | 1.84                     | 0.59              |
| 2:E:243:PHE:HB2  | 2:E:251:VAL:HG21 | 1.83                     | 0.59              |
| 1:C:222:LEU:HB3  | 1:C:228:MET:HG2  | 1.84                     | 0.59              |
| 2:E:320:PRO:O    | 2:E:324:THR:OG1  | 2.20                     | 0.59              |
| 6:L:26:ILE:HD12  | 6:L:55:PHE:HD1   | 1.67                     | 0.59              |
| 6:M:26:ILE:HD12  | 6:M:55:PHE:HD1   | 1.66                     | 0.59              |
| 2:E:126:GLU:HA   | 2:E:300:LYS:HE3  | 1.84                     | 0.59              |
| 6:T:33:LEU:CD2   | 6:T:47:VAL:HG13  | 2.33                     | 0.58              |
| 1:B:206:VAL:HG23 | 1:B:269:VAL:O    | 2.04                     | 0.58              |
| 2:F:13:VAL:CG2   | 2:F:74:GLU:HB3   | 2.32                     | 0.58              |
| 2:D:26:GLU:OE1   | 2:D:26:GLU:HA    | 2.03                     | 0.58              |
| 1:A:138:ILE:HD13 | 2:E:191:THR:HG23 | 1.85                     | 0.58              |
| 1:C:299:ASP:OD1  | 1:C:299:ASP:N    | 2.28                     | 0.58              |
| 1:A:446:LEU:HD11 | 1:A:467:GLU:HG3  | 1.85                     | 0.58              |
| 2:D:46:LEU:CD1   | 2:D:65:ASP:HB3   | 2.33                     | 0.58              |
| 1:C:174:GLN:HA   | 7:C:600:ANP:HNB1 | 1.67                     | 0.58              |
| 6:R:40:ASN:CB    | 6:R:41:PRO:HA    | 2.34                     | 0.58              |
| 3:G:149:LYS:HA   | 3:G:152:SER:HB2  | 1.86                     | 0.58              |
| 1:A:311:ALA:HA   | 1:A:323:LEU:HD23 | 1.86                     | 0.57              |
| 1:A:475:LYS:O    | 1:A:479:ASN:HB2  | 2.04                     | 0.57              |
| 1:C:146:GLU:HB2  | 1:C:163:ARG:HB2  | 1.85                     | 0.57              |
| 1:A:66:LEU:HD12  | 1:A:76:VAL:HG11  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:50:MET:SD    | 6:O:33:LEU:HD11  | 2.45                     | 0.57              |
| 6:L:40:ASN:CB    | 6:L:41:PRO:HA    | 2.27                     | 0.57              |
| 2:F:201:MET:HA   | 2:F:201:MET:HE2  | 1.85                     | 0.57              |
| 1:B:242:ALA:HB2  | 1:B:282:GLN:NE2  | 2.20                     | 0.57              |
| 1:B:293:ARG:HH21 | 2:F:319:ASP:HB2  | 1.69                     | 0.57              |
| 2:F:321:ALA:HB3  | 2:F:322:PRO:HD3  | 1.86                     | 0.57              |
| 1:B:269:VAL:HG22 | 1:B:326:LEU:HB2  | 1.86                     | 0.57              |
| 2:F:85:VAL:HG11  | 2:F:235:THR:HG23 | 1.87                     | 0.56              |
| 3:G:76:ALA:HB3   | 3:G:109:THR:HG22 | 1.87                     | 0.56              |
| 1:C:344:VAL:HA   | 1:C:347:ILE:HD12 | 1.87                     | 0.56              |
| 2:E:345:TYR:HB2  | 2:E:459:MET:HE1  | 1.86                     | 0.56              |
| 1:A:151:GLY:HA3  | 1:A:437:PRO:HB2  | 1.86                     | 0.56              |
| 1:B:142:ARG:HB2  | 1:B:315:SER:HA   | 1.85                     | 0.56              |
| 1:C:398:GLN:O    | 1:C:401:GLU:HB3  | 2.05                     | 0.56              |
| 2:E:259:PHE:CZ   | 2:E:263:GLN:HG2  | 2.40                     | 0.56              |
| 2:F:152:LYS:NZ   | 2:F:293:GLN:HG3  | 2.21                     | 0.56              |
| 1:A:101:VAL:HG23 | 1:A:258:TRP:CD1  | 2.40                     | 0.56              |
| 2:E:132:GLU:HG3  | 2:E:149:ARG:HB3  | 1.87                     | 0.56              |
| 6:O:40:ASN:CB    | 6:O:41:PRO:HA    | 2.35                     | 0.56              |
| 1:A:347:ILE:HA   | 2:E:222:MET:HE1  | 1.88                     | 0.56              |
| 2:E:229:ARG:HH22 | 2:E:267:GLU:CD   | 2.14                     | 0.56              |
| 5:I:9:SER:HB3    | 5:I:12:ALA:H     | 1.69                     | 0.56              |
| 6:K:40:ASN:CB    | 6:K:41:PRO:HA    | 2.36                     | 0.56              |
| 6:K:14:ILE:HG21  | 6:L:14:ILE:HD13  | 1.86                     | 0.56              |
| 6:R:43:ILE:HG23  | 6:R:44:LYS:H     | 1.70                     | 0.56              |
| 1:B:163:ARG:HH11 | 1:B:265:HIS:CD2  | 2.24                     | 0.56              |
| 2:E:140:VAL:HG13 | 2:E:414:LEU:HD22 | 1.87                     | 0.56              |
| 2:E:182:SER:O    | 2:E:215:VAL:HA   | 2.06                     | 0.56              |
| 2:F:320:PRO:O    | 2:F:324:THR:OG1  | 2.22                     | 0.56              |
| 1:A:212:ARG:CG   | 1:A:237:THR:HG21 | 2.37                     | 0.56              |
| 2:F:258:ILE:HD13 | 2:F:293:GLN:HE22 | 1.71                     | 0.56              |
| 2:F:298:THR:HG23 | 2:F:303:SER:HA   | 1.88                     | 0.56              |
| 1:C:34:LEU:O     | 1:C:86:GLU:HG3   | 2.05                     | 0.55              |
| 2:D:98:VAL:HA    | 2:D:232:VAL:HG23 | 1.89                     | 0.55              |
| 2:D:244:ARG:HD3  | 2:D:304:VAL:CG2  | 2.35                     | 0.55              |
| 1:B:248:ALA:HB3  | 1:B:249:PRO:HD3  | 1.88                     | 0.55              |
| 1:B:338:ALA:HB3  | 1:B:341:PRO:HG2  | 1.88                     | 0.55              |
| 2:D:20:ILE:CG1   | 2:D:271:LEU:HB3  | 2.34                     | 0.55              |
| 2:E:391:LEU:HB3  | 2:E:395:GLU:HG3  | 1.87                     | 0.55              |
| 1:B:135:ALA:HB3  | 2:F:223:ASN:HD22 | 1.72                     | 0.55              |
| 1:B:429:LEU:HD11 | 1:B:446:LEU:HB3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:78:GLN:HG3   | 4:H:79:PRO:HD2   | 1.89                     | 0.55              |
| 6:K:33:LEU:HG    | 6:K:51:ALA:HB2   | 1.89                     | 0.55              |
| 1:B:414:ALA:HA   | 1:B:417:LYS:HB3  | 1.87                     | 0.55              |
| 1:C:260:ARG:O    | 1:C:321:GLY:HA3  | 2.05                     | 0.55              |
| 6:L:50:MET:HE3   | 6:M:34:ILE:HG22  | 1.88                     | 0.55              |
| 6:O:46:THR:HG23  | 6:P:43:ILE:HD13  | 1.87                     | 0.55              |
| 1:A:51:ALA:O     | 1:A:52:GLU:HB2   | 2.07                     | 0.55              |
| 2:E:220:GLY:HA3  | 2:E:232:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:35:ALA:HB3   | 1:A:42:ARG:NH1   | 2.22                     | 0.55              |
| 1:B:101:VAL:HG12 | 1:B:255:ILE:HA   | 1.89                     | 0.55              |
| 6:T:61:THR:O     | 6:T:65:CYS:HB2   | 2.06                     | 0.55              |
| 2:F:50:VAL:HA    | 2:F:61:THR:HG22  | 1.88                     | 0.55              |
| 6:K:14:ILE:HD13  | 6:T:14:ILE:HG21  | 1.87                     | 0.55              |
| 6:O:43:ILE:HG23  | 6:O:44:LYS:H     | 1.70                     | 0.55              |
| 1:A:165:GLN:HG2  | 1:A:166:ARG:N    | 2.22                     | 0.55              |
| 1:C:397:ALA:HA   | 1:C:400:ARG:NH2  | 2.22                     | 0.55              |
| 2:F:325:THR:O    | 2:F:326:PHE:C    | 2.50                     | 0.55              |
| 6:Q:47:VAL:HA    | 6:Q:50:MET:HE2   | 1.88                     | 0.55              |
| 6:N:1:MET:HG3    | 6:N:4:VAL:HB     | 1.88                     | 0.55              |
| 2:E:133:ILE:HD12 | 2:E:146:PRO:HB2  | 1.89                     | 0.55              |
| 2:E:153:ILE:HD12 | 2:E:153:ILE:N    | 2.22                     | 0.54              |
| 2:F:53:HIS:HD2   | 2:F:59:VAL:HG12  | 1.71                     | 0.54              |
| 2:F:95:ILE:HD11  | 2:F:198:TYR:CD1  | 2.42                     | 0.54              |
| 2:F:242:TYR:CE1  | 2:F:246:GLU:HG3  | 2.43                     | 0.54              |
| 3:G:14:LYS:HA    | 3:G:248:ILE:HD11 | 1.89                     | 0.54              |
| 6:Q:43:ILE:HG23  | 6:Q:44:LYS:H     | 1.72                     | 0.54              |
| 6:N:26:ILE:HD12  | 6:N:55:PHE:HD1   | 1.72                     | 0.54              |
| 2:D:434:LEU:O    | 2:D:438:VAL:HG23 | 2.08                     | 0.54              |
| 2:E:166:PHE:HE2  | 2:E:170:LEU:HD11 | 1.72                     | 0.54              |
| 3:G:23:MET:CB    | 3:G:237:MET:HG3  | 2.30                     | 0.54              |
| 2:E:85:VAL:HG11  | 2:E:235:THR:HG23 | 1.89                     | 0.54              |
| 6:O:22:ALA:O     | 6:O:26:ILE:HG12  | 2.07                     | 0.54              |
| 6:O:50:MET:SD    | 6:P:33:LEU:HD11  | 2.47                     | 0.54              |
| 1:A:112:ALA:O    | 1:A:251:THR:HG21 | 2.07                     | 0.54              |
| 1:B:293:ARG:NH2  | 2:F:319:ASP:HB2  | 2.22                     | 0.54              |
| 1:B:385:LEU:HD23 | 1:B:444:VAL:CG1  | 2.35                     | 0.54              |
| 2:F:137:GLY:HA2  | 2:F:432:VAL:O    | 2.07                     | 0.54              |
| 2:F:363:VAL:HB   | 2:F:367:HIS:ND1  | 2.23                     | 0.54              |
| 1:B:171:GLY:N    | 1:B:177:LYS:HD3  | 2.21                     | 0.54              |
| 1:B:110:VAL:CG1  | 1:B:123:ILE:HD11 | 2.38                     | 0.54              |
| 2:F:48:LEU:HD23  | 2:F:63:ALA:HA    | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:268:VAL:O    | 3:G:272:THR:HG23 | 2.07                     | 0.54              |
| 6:P:8:LYS:HG2    | 6:P:72:LEU:O     | 2.08                     | 0.54              |
| 1:C:494:GLU:CD   | 1:C:494:GLU:N    | 2.66                     | 0.54              |
| 2:E:259:PHE:O    | 2:E:262:THR:HB   | 2.08                     | 0.54              |
| 1:A:103:PRO:HD3  | 1:A:258:TRP:CZ2  | 2.43                     | 0.53              |
| 1:B:55:VAL:HG21  | 1:B:75:ILE:HD13  | 1.90                     | 0.53              |
| 1:C:267:LEU:HD11 | 1:C:326:LEU:HD12 | 1.89                     | 0.53              |
| 2:D:98:VAL:HG13  | 2:D:99:ILE:HG23  | 1.89                     | 0.53              |
| 2:E:98:VAL:HG13  | 2:E:99:ILE:HG23  | 1.89                     | 0.53              |
| 6:P:50:MET:HE3   | 6:Q:34:ILE:HG22  | 1.91                     | 0.53              |
| 1:A:174:GLN:HA   | 7:A:600:ANP:HNB1 | 1.73                     | 0.53              |
| 1:B:46:LEU:HD13  | 1:B:49:ILE:HD12  | 1.91                     | 0.53              |
| 1:A:103:PRO:C    | 1:A:105:LEU:H    | 2.15                     | 0.53              |
| 6:P:43:ILE:HG13  | 6:P:44:LYS:N     | 2.24                     | 0.53              |
| 1:B:250:PHE:O    | 1:B:253:ALA:HB3  | 2.09                     | 0.53              |
| 1:C:174:GLN:HB3  | 2:F:354:LYS:HD2  | 1.89                     | 0.53              |
| 2:D:156:PHE:N    | 2:D:156:PHE:CD2  | 2.77                     | 0.53              |
| 6:M:4:VAL:HG23   | 6:N:2:GLN:HG2    | 1.90                     | 0.53              |
| 1:A:50:GLN:HB3   | 2:E:69:GLY:HA2   | 1.91                     | 0.53              |
| 1:B:50:GLN:OE1   | 1:B:96:ILE:HD11  | 2.08                     | 0.53              |
| 1:C:69:GLU:HB3   | 1:C:70:PRO:HD3   | 1.91                     | 0.53              |
| 6:S:46:THR:HG23  | 6:T:43:ILE:HD13  | 1.91                     | 0.53              |
| 1:B:30:THR:HA    | 1:B:90:VAL:O     | 2.09                     | 0.52              |
| 1:B:267:LEU:HD12 | 1:B:324:THR:HB   | 1.91                     | 0.52              |
| 2:E:50:VAL:HA    | 2:E:61:THR:HG22  | 1.90                     | 0.52              |
| 3:G:31:LEU:O     | 3:G:35:GLU:HG2   | 2.09                     | 0.52              |
| 1:C:51:ALA:O     | 1:C:52:GLU:HB2   | 2.07                     | 0.52              |
| 4:H:78:GLN:HB2   | 4:H:82:GLN:O     | 2.09                     | 0.52              |
| 6:N:37:VAL:C     | 6:N:39:ARG:H     | 2.16                     | 0.52              |
| 1:A:32:ARG:HH12  | 1:A:89:LEU:HB2   | 1.74                     | 0.52              |
| 1:A:425:ARG:HG3  | 1:A:460:LEU:HD12 | 1.90                     | 0.52              |
| 1:B:478:HIS:CE1  | 1:B:502:ALA:HB2  | 2.44                     | 0.52              |
| 2:D:26:GLU:OE1   | 2:D:26:GLU:CA    | 2.58                     | 0.52              |
| 2:E:359:ASP:O    | 2:E:363:VAL:HG22 | 2.10                     | 0.52              |
| 2:F:377:THR:HG22 | 2:F:407:ALA:HB2  | 1.91                     | 0.52              |
| 3:G:3:LEU:HD21   | 3:G:255:TYR:CE1  | 2.45                     | 0.52              |
| 6:L:26:ILE:HD12  | 6:L:55:PHE:CD1   | 2.43                     | 0.52              |
| 6:M:40:ASN:HB3   | 6:M:41:PRO:C     | 2.33                     | 0.52              |
| 6:Q:46:THR:HG23  | 6:R:43:ILE:HD13  | 1.91                     | 0.52              |
| 5:I:8:MET:N      | 5:I:12:ALA:O     | 2.42                     | 0.52              |
| 1:B:471:LEU:O    | 1:B:475:LYS:HG3  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:42:SER:HB2   | 6:L:46:THR:HB    | 1.92                     | 0.52              |
| 1:B:151:GLY:O    | 1:B:432:GLN:NE2  | 2.40                     | 0.52              |
| 2:E:30:LEU:HD21  | 2:E:57:ASN:HA    | 1.91                     | 0.52              |
| 1:A:417:LYS:O    | 1:A:421:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:505:SER:O    | 1:B:509:THR:HG22 | 2.10                     | 0.52              |
| 1:C:132:GLN:OE1  | 1:C:306:ARG:NH1  | 2.43                     | 0.52              |
| 2:E:177:ALA:HB2  | 2:E:431:LEU:HD11 | 1.92                     | 0.52              |
| 6:M:21:GLY:HA3   | 6:N:20:LEU:HA    | 1.92                     | 0.52              |
| 1:B:26:ASN:N     | 1:B:26:ASN:HD22  | 2.08                     | 0.51              |
| 1:C:155:VAL:HG23 | 1:C:367:ILE:HD11 | 1.92                     | 0.51              |
| 2:E:201:MET:HA   | 2:E:204:THR:HG22 | 1.92                     | 0.51              |
| 2:E:255:ILE:HB   | 2:E:308:GLN:HG2  | 1.92                     | 0.51              |
| 6:K:40:ASN:HB3   | 6:K:41:PRO:HA    | 1.92                     | 0.51              |
| 6:L:57:LEU:HD22  | 6:M:55:PHE:CZ    | 2.45                     | 0.51              |
| 6:R:71:LEU:HD23  | 6:S:73:LEU:HD11  | 1.92                     | 0.51              |
| 2:E:166:PHE:CE2  | 2:E:170:LEU:HD11 | 2.45                     | 0.51              |
| 2:E:241:GLU:OE2  | 2:E:295:ARG:HB3  | 2.10                     | 0.51              |
| 3:G:73:LEU:CD1   | 3:G:154:MET:HE2  | 2.41                     | 0.51              |
| 3:G:262:VAL:O    | 3:G:266:GLU:HG3  | 2.10                     | 0.51              |
| 1:A:152:LEU:HD23 | 1:A:432:GLN:NE2  | 2.26                     | 0.51              |
| 1:B:377:GLY:C    | 1:B:379:ALA:H    | 2.16                     | 0.51              |
| 1:C:82:ARG:HA    | 2:F:33:ILE:HB    | 1.92                     | 0.51              |
| 2:E:26:GLU:HB2   | 2:E:29:GLU:OE1   | 2.09                     | 0.51              |
| 2:F:154:GLY:HA3  | 2:F:329:LEU:HD13 | 1.93                     | 0.51              |
| 6:T:22:ALA:O     | 6:T:26:ILE:HG12  | 2.10                     | 0.51              |
| 1:A:105:LEU:O    | 1:A:108:ARG:HB2  | 2.10                     | 0.51              |
| 1:A:444:VAL:CG2  | 1:A:445:PRO:HD3  | 2.40                     | 0.51              |
| 2:F:281:TYR:CE2  | 2:F:320:PRO:HD2  | 2.45                     | 0.51              |
| 2:E:277:SER:HB2  | 2:E:283:PRO:HA   | 1.93                     | 0.51              |
| 2:E:319:ASP:O    | 2:E:322:PRO:HD2  | 2.10                     | 0.51              |
| 2:F:134:LEU:HB2  | 2:F:149:ARG:HG2  | 1.93                     | 0.51              |
| 1:A:77:LEU:HD13  | 1:A:81:ASP:HB3   | 1.92                     | 0.51              |
| 1:A:270:TYR:HB2  | 1:A:327:PRO:HA   | 1.93                     | 0.51              |
| 4:H:14:PHE:CD1   | 4:H:85:VAL:HG23  | 2.46                     | 0.51              |
| 6:Q:71:LEU:HD23  | 6:R:73:LEU:HD11  | 1.92                     | 0.51              |
| 3:G:184:ASN:HA   | 3:G:210:PHE:CD1  | 2.46                     | 0.51              |
| 6:K:27:ALA:HB1   | 6:T:28:ILE:HB    | 1.92                     | 0.51              |
| 6:T:8:LYS:HG2    | 6:T:72:LEU:O     | 2.10                     | 0.51              |
| 1:B:43:VAL:HG21  | 1:B:75:ILE:HD12  | 1.93                     | 0.51              |
| 2:D:425:THR:C    | 2:D:427:ILE:H    | 2.19                     | 0.51              |
| 6:M:37:VAL:C     | 6:M:39:ARG:H     | 2.17                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:421:VAL:O    | 1:A:425:ARG:NH1  | 2.39                     | 0.51              |
| 1:C:395:PHE:C    | 1:C:395:PHE:CD2  | 2.89                     | 0.51              |
| 2:F:397:SER:O    | 2:F:401:LYS:HB2  | 2.11                     | 0.51              |
| 2:F:15:ALA:HB3   | 2:F:22:ASP:HB2   | 1.93                     | 0.50              |
| 6:K:22:ALA:O     | 6:K:26:ILE:HG12  | 2.10                     | 0.50              |
| 1:A:424:GLU:HB3  | 1:A:460:LEU:HD21 | 1.94                     | 0.50              |
| 1:C:197:GLU:HA   | 1:C:200:LYS:HD2  | 1.93                     | 0.50              |
| 2:F:39:ILE:HG13  | 2:F:76:VAL:HG13  | 1.93                     | 0.50              |
| 2:F:382:LYS:HA   | 2:F:385:GLN:HG2  | 1.93                     | 0.50              |
| 1:C:101:VAL:HG12 | 1:C:255:ILE:HA   | 1.91                     | 0.50              |
| 2:E:345:TYR:HA   | 2:E:346:PRO:C    | 2.36                     | 0.50              |
| 2:F:348:VAL:O    | 2:F:350:PRO:HD3  | 2.10                     | 0.50              |
| 6:N:43:ILE:HG23  | 6:N:44:LYS:H     | 1.75                     | 0.50              |
| 2:D:378:LEU:HD21 | 2:D:410:ILE:HG22 | 1.93                     | 0.50              |
| 2:F:90:GLU:HG3   | 2:F:111:SER:HA   | 1.94                     | 0.50              |
| 1:B:111:ASP:OD2  | 1:B:115:ASN:HB2  | 2.12                     | 0.50              |
| 1:C:273:LEU:HD13 | 1:C:304:HIS:CD2  | 2.47                     | 0.50              |
| 2:D:133:ILE:HD11 | 2:D:146:PRO:HB2  | 1.92                     | 0.50              |
| 2:D:447:GLY:C    | 2:D:449:TYR:H    | 2.19                     | 0.50              |
| 4:H:29:GLN:HG2   | 4:H:60:MET:HG3   | 1.94                     | 0.50              |
| 1:C:336:VAL:HG11 | 1:C:353:PHE:HE2  | 1.75                     | 0.50              |
| 1:B:108:ARG:NH1  | 1:B:123:ILE:HD13 | 2.27                     | 0.50              |
| 3:G:258:THR:O    | 3:G:259:ARG:C    | 2.55                     | 0.50              |
| 1:A:166:ARG:HD3  | 1:A:308:LEU:O    | 2.12                     | 0.49              |
| 1:A:383:LYS:O    | 1:A:387:GLN:HG3  | 2.12                     | 0.49              |
| 1:B:26:ASN:N     | 1:B:26:ASN:ND2   | 2.58                     | 0.49              |
| 1:B:129:SER:HB3  | 1:B:254:SER:HB3  | 1.94                     | 0.49              |
| 1:B:163:ARG:HH11 | 1:B:265:HIS:HD2  | 1.59                     | 0.49              |
| 1:C:140:PRO:HB2  | 1:C:318:GLU:HG3  | 1.92                     | 0.49              |
| 2:F:242:TYR:CD1  | 2:F:246:GLU:HG3  | 2.47                     | 0.49              |
| 6:R:65:CYS:SG    | 6:S:16:THR:HG22  | 2.52                     | 0.49              |
| 1:B:82:ARG:NH1   | 2:E:33:ILE:O     | 2.45                     | 0.49              |
| 2:E:85:VAL:CG1   | 2:E:235:THR:HG23 | 2.42                     | 0.49              |
| 2:E:257:ASN:OD1  | 2:E:259:PHE:HB3  | 2.12                     | 0.49              |
| 2:F:96:ILE:HG22  | 2:F:97:ASN:N     | 2.28                     | 0.49              |
| 1:B:208:VAL:HG21 | 1:B:249:PRO:HG3  | 1.94                     | 0.49              |
| 1:C:216:ALA:C    | 1:C:218:LEU:N    | 2.70                     | 0.49              |
| 1:C:422:ARG:HH12 | 1:C:453:GLY:CA   | 2.25                     | 0.49              |
| 2:D:208:ASN:ND2  | 2:D:211:GLY:HA3  | 2.27                     | 0.49              |
| 2:F:290:GLY:O    | 2:F:294:GLU:HB2  | 2.11                     | 0.49              |
| 2:F:152:LYS:HZ1  | 2:F:293:GLN:HG3  | 1.75                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:220:GLY:N    | 2:F:232:VAL:HG21 | 2.27                     | 0.49              |
| 5:I:12:ALA:O     | 5:I:15:ASN:N     | 2.33                     | 0.49              |
| 2:F:204:THR:OG1  | 2:F:206:VAL:HG23 | 2.12                     | 0.49              |
| 1:B:358:LEU:HB2  | 1:B:366:ALA:HB1  | 1.94                     | 0.49              |
| 2:D:190:ARG:O    | 2:D:191:THR:C    | 2.55                     | 0.49              |
| 3:G:205:VAL:HA   | 4:H:51:GLN:NE2   | 2.28                     | 0.49              |
| 1:A:103:PRO:HD3  | 1:A:258:TRP:CH2  | 2.48                     | 0.49              |
| 1:B:77:LEU:O     | 1:B:243:PRO:HG2  | 2.13                     | 0.49              |
| 1:C:155:VAL:HG23 | 1:C:367:ILE:CD1  | 2.43                     | 0.49              |
| 2:D:135:GLU:HG3  | 2:D:434:LEU:HB2  | 1.94                     | 0.49              |
| 2:D:408:ARG:O    | 2:D:412:ARG:HD2  | 2.13                     | 0.49              |
| 2:F:237:LEU:HD13 | 2:F:296:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:391:SER:OG   | 1:A:451:VAL:HG11 | 2.13                     | 0.49              |
| 4:H:80:ASP:O     | 4:H:81:SER:HB3   | 2.12                     | 0.49              |
| 6:O:21:GLY:HA3   | 6:P:20:LEU:HA    | 1.94                     | 0.49              |
| 1:B:478:HIS:HB3  | 1:B:481:LEU:HG   | 1.94                     | 0.49              |
| 6:K:26:ILE:HD12  | 6:K:55:PHE:CD1   | 2.48                     | 0.49              |
| 6:P:21:GLY:HA3   | 6:Q:20:LEU:HA    | 1.94                     | 0.49              |
| 6:R:22:ALA:O     | 6:R:26:ILE:HG12  | 2.13                     | 0.49              |
| 1:A:492:SER:HB2  | 1:A:495:LEU:H    | 1.77                     | 0.48              |
| 6:N:15:SER:HB2   | 6:N:69:SER:HB3   | 1.95                     | 0.48              |
| 6:R:47:VAL:HG13  | 6:S:34:ILE:HB    | 1.93                     | 0.48              |
| 6:T:37:VAL:C     | 6:T:39:ARG:H     | 2.21                     | 0.48              |
| 1:A:459:GLU:OE1  | 1:A:461:SER:OG   | 2.30                     | 0.48              |
| 1:B:43:VAL:CG2   | 1:B:75:ILE:HD12  | 2.43                     | 0.48              |
| 1:B:139:LEU:HD23 | 2:F:105:GLU:HG3  | 1.95                     | 0.48              |
| 1:B:173:ARG:HG2  | 1:B:174:GLN:HG2  | 1.96                     | 0.48              |
| 1:B:290:PRO:HB3  | 2:F:276:PRO:HG3  | 1.95                     | 0.48              |
| 2:D:89:ARG:HG2   | 2:D:92:LEU:HD12  | 1.95                     | 0.48              |
| 2:F:49:GLU:CD    | 2:F:231:ARG:HE   | 2.21                     | 0.48              |
| 2:F:140:VAL:O    | 2:F:144:LEU:HB2  | 2.13                     | 0.48              |
| 6:P:70:PHE:O     | 6:P:74:PHE:HD1   | 1.96                     | 0.48              |
| 6:T:40:ASN:CB    | 6:T:41:PRO:CA    | 2.89                     | 0.48              |
| 1:A:158:LEU:HD11 | 1:A:396:LEU:HD12 | 1.96                     | 0.48              |
| 2:F:432:VAL:HG12 | 2:F:436:ASP:HB3  | 1.95                     | 0.48              |
| 6:L:21:GLY:HA3   | 6:M:20:LEU:HA    | 1.95                     | 0.48              |
| 6:P:46:THR:HG23  | 6:Q:43:ILE:HD13  | 1.94                     | 0.48              |
| 1:C:507:VAL:C    | 1:C:509:THR:H    | 2.22                     | 0.48              |
| 2:D:188:GLY:O    | 2:D:260:ARG:HD2  | 2.12                     | 0.48              |
| 3:G:110:ILE:HD11 | 3:G:146:ILE:HG21 | 1.94                     | 0.48              |
| 5:I:12:ALA:O     | 5:I:13:TYR:C     | 2.57                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:314:LEU:HD22 | 1:B:318:GLU:HB2  | 1.96                     | 0.48              |
| 1:B:473:TYR:HE2  | 1:B:502:ALA:O    | 1.96                     | 0.48              |
| 2:F:281:TYR:HE2  | 2:F:320:PRO:HD2  | 1.78                     | 0.48              |
| 3:G:235:ASN:O    | 3:G:238:ASP:HB3  | 2.14                     | 0.48              |
| 5:I:9:SER:OG     | 5:I:10:TYR:N     | 2.46                     | 0.48              |
| 5:I:19:GLN:HA    | 5:I:22:ARG:CB    | 2.43                     | 0.48              |
| 1:A:394:LEU:HG   | 1:A:398:GLN:NE2  | 2.29                     | 0.48              |
| 1:B:103:PRO:HD2  | 1:B:126:ALA:HB2  | 1.96                     | 0.48              |
| 1:C:54:LEU:HD11  | 1:C:78:PHE:HE2   | 1.78                     | 0.48              |
| 3:G:271:ILE:HD13 | 3:G:271:ILE:N    | 2.29                     | 0.48              |
| 1:A:168:LEU:HD11 | 1:A:329:ILE:HB   | 1.95                     | 0.48              |
| 1:C:399:TYR:CD1  | 1:C:423:GLY:HA3  | 2.48                     | 0.48              |
| 2:D:311:TYR:CE2  | 2:D:313:PRO:HA   | 2.49                     | 0.48              |
| 2:D:388:ILE:HA   | 2:D:392:GLY:O    | 2.14                     | 0.48              |
| 2:E:197:LEU:HD23 | 2:E:219:PHE:HZ   | 1.79                     | 0.48              |
| 2:E:423:VAL:HG23 | 2:E:424:PHE:CD2  | 2.49                     | 0.48              |
| 6:R:40:ASN:HB3   | 6:R:41:PRO:HA    | 1.95                     | 0.48              |
| 1:C:218:LEU:C    | 1:C:218:LEU:HD23 | 2.39                     | 0.47              |
| 2:E:168:GLN:HE21 | 2:E:201:MET:HG3  | 1.79                     | 0.47              |
| 2:F:253:LEU:HD23 | 2:F:296:ILE:HG23 | 1.95                     | 0.47              |
| 6:M:52:ILE:HA    | 6:M:55:PHE:HB3   | 1.96                     | 0.47              |
| 1:C:216:ALA:O    | 1:C:217:GLN:C    | 2.55                     | 0.47              |
| 2:F:344:ILE:HG23 | 2:F:415:SER:HB3  | 1.96                     | 0.47              |
| 2:F:384:LEU:HB3  | 2:F:388:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:399:TYR:CE1  | 1:B:423:GLY:HA3  | 2.49                     | 0.47              |
| 6:S:21:GLY:HA3   | 6:T:20:LEU:HA    | 1.96                     | 0.47              |
| 3:G:180:LYS:HE2  | 3:G:221:ALA:HB2  | 1.96                     | 0.47              |
| 6:M:4:VAL:O      | 6:M:8:LYS:HB2    | 2.14                     | 0.47              |
| 6:O:40:ASN:CG    | 6:O:41:PRO:HA    | 2.39                     | 0.47              |
| 1:A:446:LEU:CD1  | 1:A:467:GLU:HG3  | 2.43                     | 0.47              |
| 1:B:85:LYS:HE2   | 2:E:32:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:174:GLN:HA   | 7:B:600:ANP:HNB1 | 1.79                     | 0.47              |
| 1:B:305:SER:O    | 1:B:309:GLU:HG2  | 2.13                     | 0.47              |
| 1:B:466:PHE:CZ   | 1:B:470:PHE:HB2  | 2.49                     | 0.47              |
| 1:C:383:LYS:O    | 1:C:387:GLN:HG3  | 2.13                     | 0.47              |
| 6:N:40:ASN:HB3   | 6:N:41:PRO:CA    | 2.31                     | 0.47              |
| 1:B:344:VAL:HA   | 1:B:347:ILE:HD12 | 1.97                     | 0.47              |
| 6:Q:41:PRO:C     | 6:Q:43:ILE:H     | 2.22                     | 0.47              |
| 6:T:33:LEU:HD21  | 6:T:47:VAL:HG13  | 1.95                     | 0.47              |
| 1:B:226:ASP:O    | 1:B:229:LYS:HG2  | 2.15                     | 0.47              |
| 1:B:499:LEU:HD12 | 1:B:502:ALA:HB3  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:216:ALA:O    | 1:C:218:LEU:N    | 2.48                     | 0.47              |
| 2:D:23:VAL:CG1   | 2:D:76:VAL:HG21  | 2.44                     | 0.47              |
| 3:G:74:ILE:O     | 3:G:107:ILE:HA   | 2.15                     | 0.47              |
| 1:A:92:ARG:HH21  | 1:A:94:GLY:HA2   | 1.80                     | 0.47              |
| 2:D:23:VAL:HG13  | 2:D:76:VAL:HG21  | 1.97                     | 0.47              |
| 2:D:62:ILE:HD11  | 2:D:272:LEU:HD11 | 1.96                     | 0.47              |
| 2:D:340:SER:HB3  | 2:D:347:ALA:HB2  | 1.97                     | 0.47              |
| 6:L:67:MET:O     | 6:L:71:LEU:HB2   | 2.15                     | 0.47              |
| 1:A:85:LYS:HE2   | 2:D:32:ALA:HB2   | 1.96                     | 0.47              |
| 1:C:478:HIS:HB3  | 1:C:481:LEU:HG   | 1.97                     | 0.47              |
| 2:E:174:ILE:HD13 | 2:E:174:ILE:HA   | 1.78                     | 0.47              |
| 2:F:37:LEU:HB2   | 2:F:48:LEU:HB2   | 1.96                     | 0.47              |
| 6:M:26:ILE:HD12  | 6:M:55:PHE:CD1   | 2.48                     | 0.47              |
| 6:Q:21:GLY:HA3   | 6:R:20:LEU:HA    | 1.96                     | 0.47              |
| 1:B:188:GLN:HB3  | 1:B:192:ASN:ND2  | 2.29                     | 0.47              |
| 2:D:425:THR:C    | 2:D:427:ILE:N    | 2.73                     | 0.47              |
| 2:F:13:VAL:HG23  | 2:F:74:GLU:HB3   | 1.97                     | 0.47              |
| 6:P:4:VAL:O      | 6:P:8:LYS:HB2    | 2.15                     | 0.47              |
| 6:T:26:ILE:HD12  | 6:T:55:PHE:HD1   | 1.80                     | 0.47              |
| 1:B:53:GLU:HA    | 1:B:96:ILE:HA    | 1.96                     | 0.46              |
| 1:B:377:GLY:HA2  | 1:B:380:ALA:HB3  | 1.96                     | 0.46              |
| 1:C:382:VAL:HG11 | 1:C:440:THR:HG21 | 1.97                     | 0.46              |
| 1:C:503:THR:O    | 1:C:507:VAL:HG23 | 2.15                     | 0.46              |
| 2:F:30:LEU:HD11  | 2:F:57:ASN:HA    | 1.97                     | 0.46              |
| 3:G:191:SER:HA   | 3:G:192:PRO:HD2  | 1.73                     | 0.46              |
| 2:D:90:GLU:OE1   | 2:D:90:GLU:HA    | 2.14                     | 0.46              |
| 2:E:322:PRO:O    | 2:E:323:ALA:C    | 2.58                     | 0.46              |
| 6:O:61:THR:HG23  | 6:P:19:LEU:HB3   | 1.97                     | 0.46              |
| 1:B:67:ASN:HB2   | 2:F:17:ILE:HG12  | 1.97                     | 0.46              |
| 1:C:248:ALA:HB3  | 1:C:249:PRO:HD3  | 1.96                     | 0.46              |
| 1:C:484:GLU:O    | 1:C:485:ILE:C    | 2.58                     | 0.46              |
| 2:E:39:ILE:HG12  | 2:E:76:VAL:HG22  | 1.97                     | 0.46              |
| 3:G:200:ASP:C    | 3:G:202:ASP:N    | 2.72                     | 0.46              |
| 1:A:109:VAL:HG12 | 1:A:117:ILE:CG1  | 2.45                     | 0.46              |
| 1:B:260:ARG:HG2  | 1:B:314:LEU:HD12 | 1.97                     | 0.46              |
| 1:B:396:LEU:HA   | 1:B:399:TYR:HB3  | 1.98                     | 0.46              |
| 6:P:61:THR:HG23  | 6:Q:19:LEU:HB3   | 1.98                     | 0.46              |
| 6:P:61:THR:O     | 6:P:65:CYS:HB2   | 2.16                     | 0.46              |
| 1:C:35:ALA:HB1   | 2:F:53:HIS:O     | 2.16                     | 0.46              |
| 2:F:162:GLY:CA   | 7:F:600:ANP:O3A  | 2.61                     | 0.46              |
| 2:E:457:PHE:CE1  | 2:E:466:VAL:HG11 | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:201:MET:HA   | 2:F:201:MET:CE   | 2.46                     | 0.46              |
| 6:K:4:VAL:O      | 6:K:8:LYS:HB2    | 2.16                     | 0.46              |
| 6:M:43:ILE:HG13  | 6:M:44:LYS:N     | 2.30                     | 0.46              |
| 6:Q:22:ALA:O     | 6:Q:26:ILE:HG12  | 2.15                     | 0.46              |
| 6:T:37:VAL:HG22  | 6:T:47:VAL:HG21  | 1.97                     | 0.46              |
| 1:A:169:ILE:HD11 | 1:A:326:LEU:HD13 | 1.97                     | 0.46              |
| 1:A:399:TYR:CD1  | 1:A:423:GLY:HA3  | 2.51                     | 0.46              |
| 4:H:70:ILE:HG23  | 4:H:71:SER:N     | 2.31                     | 0.46              |
| 6:P:44:LYS:O     | 6:P:45:ASP:HB3   | 2.15                     | 0.46              |
| 1:A:177:LYS:HB2  | 1:A:177:LYS:HE2  | 1.81                     | 0.46              |
| 1:B:73:VAL:HG12  | 1:B:75:ILE:HG13  | 1.98                     | 0.46              |
| 1:B:363:ILE:C    | 1:B:364:ARG:HG2  | 2.41                     | 0.46              |
| 3:G:205:VAL:HB   | 4:H:51:GLN:HE22  | 1.81                     | 0.46              |
| 6:N:4:VAL:O      | 6:N:8:LYS:HB2    | 2.16                     | 0.46              |
| 6:P:8:LYS:HG3    | 6:Q:9:TYR:HD1    | 1.81                     | 0.46              |
| 1:B:176:GLY:O    | 1:B:180:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:158:LEU:CD1  | 1:C:369:VAL:HG22 | 2.46                     | 0.46              |
| 3:G:44:MET:CE    | 4:H:86:THR:HG22  | 2.39                     | 0.46              |
| 6:O:44:LYS:O     | 6:O:45:ASP:CB    | 2.63                     | 0.46              |
| 6:K:57:LEU:HD22  | 6:L:55:PHE:CZ    | 2.51                     | 0.46              |
| 1:C:98:ASP:HB2   | 1:C:129:SER:O    | 2.17                     | 0.45              |
| 2:D:237:LEU:HD22 | 2:D:292:LEU:HD12 | 1.97                     | 0.45              |
| 6:N:67:MET:O     | 6:N:71:LEU:HB2   | 2.16                     | 0.45              |
| 6:T:4:VAL:O      | 6:T:8:LYS:HB2    | 2.15                     | 0.45              |
| 1:A:53:GLU:OE2   | 1:A:92:ARG:NE    | 2.44                     | 0.45              |
| 1:A:340:ILE:HB   | 1:A:341:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:109:VAL:HG23 | 1:B:228:MET:HE1  | 1.97                     | 0.45              |
| 2:E:277:SER:OG   | 2:E:278:ALA:N    | 2.47                     | 0.45              |
| 6:M:37:VAL:HG13  | 6:M:43:ILE:HG22  | 1.98                     | 0.45              |
| 1:A:391:SER:O    | 1:A:394:LEU:HB3  | 2.16                     | 0.45              |
| 1:B:165:GLN:O    | 1:B:324:THR:HG23 | 2.17                     | 0.45              |
| 1:B:173:ARG:O    | 1:B:174:GLN:HB2  | 2.16                     | 0.45              |
| 1:B:444:VAL:CG2  | 1:B:445:PRO:HD3  | 2.42                     | 0.45              |
| 2:E:180:GLY:HA2  | 2:E:249:GLN:OE1  | 2.17                     | 0.45              |
| 4:H:57:VAL:HG12  | 4:H:58:GLU:N     | 2.32                     | 0.45              |
| 2:D:136:THR:HG21 | 2:D:147:TYR:CD2  | 2.51                     | 0.45              |
| 6:N:22:ALA:O     | 6:N:26:ILE:HG12  | 2.16                     | 0.45              |
| 6:P:48:PHE:N     | 6:P:49:PRO:CD    | 2.79                     | 0.45              |
| 1:A:70:PRO:HD3   | 2:E:15:ALA:HB2   | 1.99                     | 0.45              |
| 1:B:139:LEU:N    | 1:B:140:PRO:CD   | 2.80                     | 0.45              |
| 6:Q:42:SER:HB2   | 6:Q:46:THR:HB    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:S:67:MET:O     | 6:S:71:LEU:HB2   | 2.16                     | 0.45              |
| 2:E:407:ALA:HA   | 2:E:410:ILE:HD12 | 1.98                     | 0.45              |
| 6:N:26:ILE:HD12  | 6:N:55:PHE:CD1   | 2.50                     | 0.45              |
| 1:A:103:PRO:C    | 1:A:105:LEU:N    | 2.74                     | 0.45              |
| 1:A:363:ILE:O    | 1:A:366:ALA:HA   | 2.16                     | 0.45              |
| 1:B:156:ASP:O    | 1:B:381:GLN:NE2  | 2.49                     | 0.45              |
| 2:E:31:PRO:HG3   | 2:E:37:LEU:HD21  | 1.98                     | 0.45              |
| 1:B:110:VAL:O    | 1:B:234:VAL:HA   | 2.16                     | 0.45              |
| 1:B:391:SER:O    | 1:B:393:LYS:N    | 2.49                     | 0.45              |
| 3:G:205:VAL:HG13 | 3:G:206:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:147:PRO:HG3  | 1:B:380:ALA:O    | 2.17                     | 0.45              |
| 1:C:152:LEU:O    | 1:C:153:LYS:C    | 2.59                     | 0.45              |
| 1:C:241:ALA:HB1  | 1:C:243:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:504:GLU:O    | 1:C:505:SER:C    | 2.60                     | 0.45              |
| 2:E:336:SER:HB3  | 2:E:339:ILE:HG12 | 1.99                     | 0.45              |
| 2:E:391:LEU:CB   | 2:E:395:GLU:HG3  | 2.47                     | 0.45              |
| 3:G:78:THR:HB    | 3:G:79:SER:H     | 1.52                     | 0.45              |
| 6:K:43:ILE:HG13  | 6:K:44:LYS:N     | 2.32                     | 0.45              |
| 6:N:33:LEU:HD23  | 6:N:47:VAL:HG12  | 1.99                     | 0.45              |
| 6:R:52:ILE:HA    | 6:R:55:PHE:HB3   | 1.98                     | 0.45              |
| 6:S:43:ILE:HG13  | 6:S:44:LYS:N     | 2.31                     | 0.45              |
| 6:S:47:VAL:HA    | 6:S:50:MET:HE2   | 1.98                     | 0.45              |
| 1:B:270:TYR:O    | 1:B:272:ASP:HA   | 2.17                     | 0.45              |
| 2:E:143:LEU:HB2  | 2:E:437:THR:HG22 | 1.99                     | 0.45              |
| 2:E:152:LYS:HE3  | 2:E:296:ILE:O    | 2.17                     | 0.45              |
| 2:E:346:PRO:HB2  | 2:E:348:VAL:HG23 | 1.98                     | 0.45              |
| 2:F:12:LYS:HA    | 2:F:74:GLU:O     | 2.17                     | 0.45              |
| 6:S:4:VAL:O      | 6:S:8:LYS:HB2    | 2.16                     | 0.45              |
| 2:D:244:ARG:NE   | 2:D:245:ASP:OD1  | 2.40                     | 0.44              |
| 1:A:146:GLU:HB2  | 1:A:163:ARG:HD2  | 1.99                     | 0.44              |
| 1:A:241:ALA:HB1  | 1:A:243:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:446:LEU:HD21 | 1:A:467:GLU:HA   | 1.99                     | 0.44              |
| 1:B:488:LYS:HD3  | 1:B:490:GLU:HB2  | 1.99                     | 0.44              |
| 2:E:33:ILE:O     | 2:E:34:LEU:HB2   | 2.17                     | 0.44              |
| 2:F:256:ASP:HA   | 2:F:257:ASN:HA   | 1.73                     | 0.44              |
| 4:H:72:GLY:C     | 5:I:14:LEU:HD22  | 2.43                     | 0.44              |
| 6:Q:4:VAL:O      | 6:Q:8:LYS:HB2    | 2.16                     | 0.44              |
| 1:C:108:ARG:NH2  | 1:C:120:LYS:HB2  | 2.32                     | 0.44              |
| 2:D:162:GLY:HA2  | 7:D:600:ANP:H8   | 1.99                     | 0.44              |
| 1:A:242:ALA:N    | 1:A:243:PRO:CD   | 2.81                     | 0.44              |
| 1:A:272:ASP:OD1  | 1:A:274:SER:CB   | 2.65                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:ALA:O    | 1:B:282:GLN:HB3  | 2.18                     | 0.44              |
| 2:F:163:LYS:H    | 7:F:600:ANP:PB   | 2.40                     | 0.44              |
| 2:F:201:MET:CB   | 2:F:207:ILE:HD12 | 2.47                     | 0.44              |
| 3:G:214:LEU:O    | 3:G:218:MET:HB2  | 2.17                     | 0.44              |
| 6:S:8:LYS:HG2    | 6:S:72:LEU:O     | 2.17                     | 0.44              |
| 2:E:344:ILE:HG23 | 2:E:415:SER:HB3  | 2.00                     | 0.44              |
| 2:F:134:LEU:HB2  | 2:F:149:ARG:CG   | 2.47                     | 0.44              |
| 3:G:139:THR:HG21 | 5:I:37:ARG:HA    | 1.99                     | 0.44              |
| 6:K:14:ILE:HG21  | 6:L:14:ILE:CD1   | 2.47                     | 0.44              |
| 6:O:48:PHE:N     | 6:O:49:PRO:CD    | 2.80                     | 0.44              |
| 1:B:37:GLY:HA3   | 2:E:52:GLN:HG2   | 2.00                     | 0.44              |
| 2:D:52:GLN:OE1   | 2:D:60:ARG:HD2   | 2.17                     | 0.44              |
| 2:F:201:MET:HB2  | 2:F:207:ILE:HD12 | 2.00                     | 0.44              |
| 2:F:326:PHE:C    | 2:F:328:HIS:H    | 2.26                     | 0.44              |
| 3:G:148:ASP:HA   | 3:G:151:LEU:HD12 | 2.00                     | 0.44              |
| 6:K:26:ILE:HD12  | 6:K:55:PHE:HD1   | 1.82                     | 0.44              |
| 1:C:343:ASN:O    | 1:C:347:ILE:HG13 | 2.16                     | 0.44              |
| 2:D:30:LEU:HD11  | 2:D:57:ASN:HA    | 2.00                     | 0.44              |
| 2:E:138:ILE:HG22 | 2:E:140:VAL:HG23 | 2.00                     | 0.44              |
| 2:F:96:ILE:CG2   | 2:F:97:ASN:N     | 2.81                     | 0.44              |
| 3:G:154:MET:O    | 3:G:159:TYR:HE2  | 2.00                     | 0.44              |
| 6:Q:46:THR:O     | 6:Q:50:MET:HG3   | 2.18                     | 0.44              |
| 1:A:152:LEU:HA   | 1:A:432:GLN:HE22 | 1.83                     | 0.44              |
| 1:B:270:TYR:HB2  | 1:B:327:PRO:HA   | 1.99                     | 0.44              |
| 1:C:364:ARG:HA   | 1:C:365:PRO:C    | 2.43                     | 0.44              |
| 2:E:95:ILE:HB    | 2:E:104:ASP:HB3  | 1.99                     | 0.44              |
| 2:E:125:ALA:C    | 2:E:127:GLN:H    | 2.26                     | 0.44              |
| 2:F:237:LEU:HD21 | 2:F:295:ARG:HB2  | 2.00                     | 0.44              |
| 6:K:8:LYS:HG3    | 6:L:9:TYR:HD1    | 1.83                     | 0.44              |
| 6:O:61:THR:O     | 6:O:65:CYS:HB2   | 2.18                     | 0.44              |
| 6:R:46:THR:O     | 6:R:50:MET:HE2   | 2.18                     | 0.44              |
| 1:B:106:LEU:HA   | 1:B:232:ILE:HG12 | 1.99                     | 0.44              |
| 1:B:394:LEU:HA   | 1:B:397:ALA:HB3  | 2.00                     | 0.44              |
| 2:D:134:LEU:HD11 | 2:D:174:ILE:HD12 | 2.00                     | 0.44              |
| 2:D:456:ALA:HA   | 2:D:469:LYS:HD3  | 1.99                     | 0.44              |
| 2:F:473:LEU:C    | 2:F:475:ALA:N    | 2.74                     | 0.44              |
| 4:H:33:PRO:HD3   | 4:H:57:VAL:HG22  | 1.99                     | 0.44              |
| 5:I:13:TYR:O     | 5:I:16:VAL:HG12  | 2.17                     | 0.44              |
| 6:P:46:THR:O     | 6:P:50:MET:HE2   | 2.18                     | 0.44              |
| 1:A:27:LEU:HA    | 1:A:30:THR:O     | 2.18                     | 0.43              |
| 1:B:488:LYS:HB3  | 1:B:490:GLU:H    | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:169:GLU:HG2  | 2:D:418:PHE:CG   | 2.53                     | 0.43              |
| 1:B:190:ARG:HH12 | 1:B:437:PRO:HB2  | 1.82                     | 0.43              |
| 1:C:99:VAL:O     | 1:C:128:ARG:HA   | 2.17                     | 0.43              |
| 1:C:336:VAL:CG1  | 1:C:353:PHE:HE2  | 2.31                     | 0.43              |
| 2:D:321:ALA:HB3  | 2:D:322:PRO:CD   | 2.48                     | 0.43              |
| 2:E:147:TYR:CZ   | 2:E:153:ILE:HG21 | 2.53                     | 0.43              |
| 2:E:256:ASP:HA   | 2:E:257:ASN:HA   | 1.68                     | 0.43              |
| 3:G:91:LEU:HD23  | 3:G:114:ILE:HD13 | 2.01                     | 0.43              |
| 4:H:48:THR:H     | 4:H:77:VAL:HB    | 1.83                     | 0.43              |
| 6:O:48:PHE:N     | 6:O:49:PRO:HD2   | 2.32                     | 0.43              |
| 6:R:4:VAL:O      | 6:R:8:LYS:HB2    | 2.17                     | 0.43              |
| 1:A:402:VAL:HG13 | 1:A:405:PHE:CD1  | 2.54                     | 0.43              |
| 1:B:139:LEU:HD22 | 2:F:104:ASP:HA   | 2.00                     | 0.43              |
| 1:B:336:VAL:HG13 | 1:B:353:PHE:CE1  | 2.53                     | 0.43              |
| 2:E:166:PHE:C    | 2:E:166:PHE:CD2  | 2.96                     | 0.43              |
| 6:K:34:ILE:HG22  | 6:T:50:MET:HE3   | 2.00                     | 0.43              |
| 6:O:4:VAL:O      | 6:O:8:LYS:HB2    | 2.18                     | 0.43              |
| 1:A:217:GLN:HG2  | 2:D:356:ARG:NH2  | 2.34                     | 0.43              |
| 1:B:421:VAL:O    | 1:B:425:ARG:HG2  | 2.18                     | 0.43              |
| 6:Q:43:ILE:O     | 6:Q:48:PHE:HB2   | 2.18                     | 0.43              |
| 1:A:34:LEU:O     | 1:A:86:GLU:HG3   | 2.19                     | 0.43              |
| 1:C:176:GLY:N    | 7:C:600:ANP:O3A  | 2.51                     | 0.43              |
| 2:F:10:THR:HG21  | 2:F:75:LYS:HD3   | 2.00                     | 0.43              |
| 2:F:449:TYR:HD1  | 2:F:452:ILE:HD12 | 1.84                     | 0.43              |
| 3:G:152:SER:HB3  | 3:G:153:VAL:H    | 1.70                     | 0.43              |
| 5:I:32:ALA:O     | 5:I:33:SER:C     | 2.61                     | 0.43              |
| 6:Q:42:SER:O     | 6:Q:47:VAL:HG23  | 2.19                     | 0.43              |
| 1:B:188:GLN:HB3  | 1:B:192:ASN:HD22 | 1.83                     | 0.43              |
| 1:B:271:ASP:HA   | 1:B:272:ASP:HA   | 1.69                     | 0.43              |
| 2:F:136:THR:HG21 | 2:F:147:TYR:CD2  | 2.53                     | 0.43              |
| 3:G:73:LEU:HD11  | 3:G:154:MET:HE2  | 1.99                     | 0.43              |
| 6:K:61:THR:O     | 6:K:65:CYS:HB2   | 2.18                     | 0.43              |
| 1:A:68:LEU:O     | 2:E:15:ALA:HA    | 2.18                     | 0.43              |
| 3:G:78:THR:OG1   | 3:G:114:ILE:HB   | 2.19                     | 0.43              |
| 1:B:108:ARG:NH2  | 1:B:116:PRO:HB3  | 2.32                     | 0.43              |
| 2:F:18:GLY:O     | 2:F:67:THR:OG1   | 2.29                     | 0.43              |
| 6:L:39:ARG:NH2   | 6:M:39:ARG:NH1   | 2.66                     | 0.43              |
| 6:O:50:MET:HE3   | 6:P:34:ILE:HG22  | 2.01                     | 0.43              |
| 1:A:397:ALA:HA   | 1:A:400:ARG:NH2  | 2.34                     | 0.43              |
| 1:B:103:PRO:HD3  | 1:B:258:TRP:CZ2  | 2.54                     | 0.43              |
| 1:B:140:PRO:O    | 1:B:314:LEU:HD23 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:153:ILE:HA   | 2:E:331:ALA:O    | 2.19                     | 0.43              |
| 2:E:244:ARG:HD3  | 2:E:304:VAL:HG23 | 2.01                     | 0.43              |
| 2:F:87:VAL:HG21  | 2:F:242:TYR:CD1  | 2.54                     | 0.43              |
| 3:G:147:ALA:O    | 3:G:151:LEU:HG   | 2.19                     | 0.43              |
| 5:I:14:LEU:H     | 5:I:14:LEU:HG    | 1.36                     | 0.43              |
| 6:K:14:ILE:CD1   | 6:T:14:ILE:HG21  | 2.49                     | 0.43              |
| 6:N:33:LEU:O     | 6:N:37:VAL:HG23  | 2.19                     | 0.43              |
| 6:T:26:ILE:HD12  | 6:T:55:PHE:CD1   | 2.54                     | 0.43              |
| 1:B:57:PHE:HD1   | 1:B:61:VAL:O     | 2.02                     | 0.43              |
| 1:B:368:ASN:OD1  | 1:B:368:ASN:C    | 2.62                     | 0.43              |
| 1:C:107:GLY:HA2  | 1:C:228:MET:O    | 2.19                     | 0.43              |
| 3:G:150:LEU:HD22 | 3:G:218:MET:HE2  | 2.01                     | 0.43              |
| 6:R:46:THR:HG23  | 6:S:43:ILE:HD13  | 2.00                     | 0.43              |
| 1:A:237:THR:O    | 1:A:238:ALA:C    | 2.62                     | 0.42              |
| 1:B:54:LEU:HB3   | 1:B:93:THR:OG1   | 2.19                     | 0.42              |
| 1:C:166:ARG:HD3  | 1:C:308:LEU:O    | 2.19                     | 0.42              |
| 1:C:166:ARG:NH1  | 1:C:347:ILE:O    | 2.52                     | 0.42              |
| 2:D:26:GLU:HB2   | 2:D:29:GLU:OE1   | 2.18                     | 0.42              |
| 2:D:182:SER:OG   | 2:D:252:LEU:HB2  | 2.18                     | 0.42              |
| 2:E:244:ARG:HG3  | 2:E:303:SER:N    | 2.33                     | 0.42              |
| 2:E:260:ARG:HA   | 2:E:263:GLN:HB2  | 2.01                     | 0.42              |
| 2:F:373:LYS:HB3  | 2:F:445:LEU:HD13 | 2.00                     | 0.42              |
| 6:K:40:ASN:HB3   | 6:K:41:PRO:CA    | 2.49                     | 0.42              |
| 1:C:208:VAL:O    | 1:C:275:LYS:HD3  | 2.19                     | 0.42              |
| 2:F:422:GLU:C    | 2:F:424:PHE:H    | 2.28                     | 0.42              |
| 3:G:74:ILE:HG23  | 3:G:165:PHE:HD1  | 1.85                     | 0.42              |
| 4:H:29:GLN:HB3   | 4:H:60:MET:CE    | 2.49                     | 0.42              |
| 4:H:94:GLU:C     | 4:H:96:PHE:H     | 2.27                     | 0.42              |
| 1:A:294:GLU:O    | 1:A:295:ALA:HB3  | 2.18                     | 0.42              |
| 1:A:382:VAL:O    | 1:A:383:LYS:C    | 2.62                     | 0.42              |
| 1:B:139:LEU:N    | 1:B:140:PRO:HD2  | 2.33                     | 0.42              |
| 2:D:88:GLY:O     | 2:D:243:PHE:CZ   | 2.72                     | 0.42              |
| 2:D:90:GLU:HB2   | 2:D:111:SER:HB3  | 2.01                     | 0.42              |
| 3:G:216:ASN:HD22 | 3:G:216:ASN:HA   | 1.60                     | 0.42              |
| 4:H:30:VAL:HG21  | 4:H:83:LEU:HD23  | 2.00                     | 0.42              |
| 6:K:20:LEU:HD11  | 6:T:20:LEU:HD22  | 2.01                     | 0.42              |
| 2:D:64:MET:HE1   | 2:D:231:ARG:HB2  | 2.01                     | 0.42              |
| 2:E:443:ALA:O    | 2:E:448:LYS:HB2  | 2.19                     | 0.42              |
| 2:D:256:ASP:HA   | 2:D:257:ASN:HA   | 1.68                     | 0.42              |
| 2:E:39:ILE:HD11  | 2:E:48:LEU:HD11  | 2.01                     | 0.42              |
| 6:O:65:CYS:SG    | 6:P:16:THR:HG22  | 2.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:260:ARG:O    | 1:B:321:GLY:HA3  | 2.19                     | 0.42              |
| 1:C:394:LEU:O    | 1:C:398:GLN:HG3  | 2.19                     | 0.42              |
| 2:E:99:ILE:HG13  | 2:E:101:GLU:HG3  | 2.02                     | 0.42              |
| 3:G:115:LYS:HD3  | 3:G:129:SER:OG   | 2.20                     | 0.42              |
| 1:A:49:ILE:HD11  | 1:A:55:VAL:CG1   | 2.49                     | 0.42              |
| 1:B:483:THR:HA   | 1:B:486:ARG:NH2  | 2.35                     | 0.42              |
| 1:B:425:ARG:HD2  | 1:B:463:ILE:HD11 | 2.02                     | 0.42              |
| 1:C:53:GLU:CD    | 1:C:92:ARG:HH21  | 2.28                     | 0.42              |
| 2:D:201:MET:HE3  | 2:D:217:LEU:HD21 | 2.01                     | 0.42              |
| 2:F:417:PRO:HB2  | 2:F:429:GLY:HA2  | 2.02                     | 0.42              |
| 3:G:138:PRO:HB3  | 3:G:222:MET:HE2  | 2.02                     | 0.42              |
| 6:K:29:VAL:HG23  | 6:L:27:ALA:HA    | 2.02                     | 0.42              |
| 2:D:158:GLY:O    | 2:D:161:VAL:HG22 | 2.20                     | 0.42              |
| 2:D:342:LEU:HD23 | 2:D:342:LEU:HA   | 1.77                     | 0.42              |
| 2:F:13:VAL:HG21  | 2:F:74:GLU:HB3   | 2.00                     | 0.42              |
| 3:G:38:LYS:HD2   | 3:G:169:PRO:HG2  | 2.01                     | 0.42              |
| 3:G:150:LEU:O    | 3:G:156:ALA:HB2  | 2.20                     | 0.42              |
| 5:I:17:ALA:O     | 5:I:21:ILE:CB    | 2.67                     | 0.42              |
| 6:M:61:THR:HG23  | 6:N:19:LEU:HB3   | 2.02                     | 0.42              |
| 6:Q:37:VAL:C     | 6:Q:39:ARG:H     | 2.26                     | 0.42              |
| 1:B:170:ILE:HD11 | 1:B:341:PRO:HB3  | 2.02                     | 0.42              |
| 1:C:302:TYR:CE1  | 1:C:306:ARG:HD3  | 2.54                     | 0.42              |
| 3:G:212:TYR:OH   | 4:H:86:THR:HB    | 2.19                     | 0.42              |
| 1:A:142:ARG:HG2  | 1:A:143:SER:H    | 1.85                     | 0.41              |
| 1:B:177:LYS:NZ   | 1:B:330:GLU:HG3  | 2.36                     | 0.41              |
| 1:B:350:GLY:C    | 1:B:351:GLN:HG3  | 2.45                     | 0.41              |
| 1:C:292:GLY:N    | 1:C:296:TYR:O    | 2.36                     | 0.41              |
| 2:D:349:ASP:HA   | 2:D:350:PRO:HD2  | 1.83                     | 0.41              |
| 2:F:30:LEU:HA    | 2:F:31:PRO:HD2   | 1.86                     | 0.41              |
| 6:N:37:VAL:C     | 6:N:39:ARG:N     | 2.78                     | 0.41              |
| 1:A:109:VAL:HG22 | 1:A:233:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:329:ILE:HD13 | 1:A:329:ILE:HA   | 1.98                     | 0.41              |
| 2:D:25:PHE:O     | 2:D:57:ASN:HB3   | 2.20                     | 0.41              |
| 2:D:33:ILE:O     | 2:D:34:LEU:HB2   | 2.20                     | 0.41              |
| 2:D:64:MET:HE3   | 2:D:228:ALA:HA   | 2.02                     | 0.41              |
| 2:E:54:LEU:HD11  | 2:E:60:ARG:HB2   | 2.01                     | 0.41              |
| 2:F:47:VAL:HG21  | 2:F:99:ILE:HG21  | 2.01                     | 0.41              |
| 2:F:184:PHE:CD1  | 2:F:254:PHE:HB2  | 2.55                     | 0.41              |
| 2:F:388:ILE:CD1  | 2:F:396:LEU:HD11 | 2.45                     | 0.41              |
| 5:I:8:MET:N      | 5:I:16:VAL:HB    | 2.35                     | 0.41              |
| 1:A:290:PRO:HA   | 1:A:291:PRO:HD3  | 1.95                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:223:GLU:HG3  | 1:B:228:MET:HB2  | 2.01                     | 0.41              |
| 1:B:249:PRO:HB3  | 1:B:270:TYR:CD1  | 2.55                     | 0.41              |
| 1:C:223:GLU:C    | 1:C:225:HIS:N    | 2.78                     | 0.41              |
| 2:E:95:ILE:HD11  | 2:E:198:TYR:CD1  | 2.56                     | 0.41              |
| 2:E:237:LEU:HD21 | 2:E:295:ARG:HB2  | 2.01                     | 0.41              |
| 1:B:110:VAL:HG12 | 1:B:116:PRO:HA   | 2.01                     | 0.41              |
| 1:B:381:GLN:HG2  | 1:B:382:VAL:N    | 2.36                     | 0.41              |
| 1:C:54:LEU:O     | 1:C:93:THR:HB    | 2.20                     | 0.41              |
| 1:C:494:GLU:O    | 1:C:497:ALA:HB3  | 2.21                     | 0.41              |
| 2:D:154:GLY:HA3  | 2:D:329:LEU:HD13 | 2.02                     | 0.41              |
| 2:D:222:MET:C    | 2:D:224:GLU:H    | 2.28                     | 0.41              |
| 6:Q:8:LYS:HG2    | 6:Q:72:LEU:O     | 2.20                     | 0.41              |
| 1:B:207:ALA:HB3  | 1:B:235:ALA:CB   | 2.51                     | 0.41              |
| 1:B:308:LEU:C    | 1:B:310:ARG:H    | 2.27                     | 0.41              |
| 2:D:155:LEU:HB2  | 2:D:309:ALA:HA   | 2.03                     | 0.41              |
| 2:E:49:GLU:CD    | 2:E:231:ARG:HE   | 2.28                     | 0.41              |
| 6:T:48:PHE:N     | 6:T:49:PRO:CD    | 2.84                     | 0.41              |
| 1:A:455:LEU:HD22 | 1:A:458:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:57:PHE:HB2   | 1:B:61:VAL:HG13  | 2.03                     | 0.41              |
| 1:B:242:ALA:HB3  | 1:B:243:PRO:HD3  | 2.03                     | 0.41              |
| 2:F:224:GLU:HB2  | 2:F:229:ARG:HG3  | 2.02                     | 0.41              |
| 6:N:8:LYS:HG3    | 6:O:9:TYR:HD1    | 1.84                     | 0.41              |
| 6:N:18:GLY:HA3   | 6:N:65:CYS:SG    | 2.61                     | 0.41              |
| 6:R:67:MET:O     | 6:R:71:LEU:HB2   | 2.21                     | 0.41              |
| 1:A:471:LEU:HD23 | 1:A:471:LEU:HA   | 1.90                     | 0.41              |
| 1:B:308:LEU:HD12 | 1:B:347:ILE:HG21 | 2.01                     | 0.41              |
| 1:C:202:TYR:O    | 1:C:267:LEU:N    | 2.53                     | 0.41              |
| 1:C:270:TYR:O    | 1:C:272:ASP:HA   | 2.21                     | 0.41              |
| 1:C:300:VAL:O    | 1:C:303:LEU:HB3  | 2.21                     | 0.41              |
| 2:D:357:LEU:HD13 | 2:D:362:VAL:HG11 | 2.03                     | 0.41              |
| 2:E:13:VAL:O     | 2:E:73:GLY:N     | 2.46                     | 0.41              |
| 2:E:298:THR:HG23 | 2:E:303:SER:HB3  | 2.01                     | 0.41              |
| 2:F:256:ASP:HA   | 2:F:309:ALA:HB3  | 2.03                     | 0.41              |
| 3:G:43:LYS:O     | 3:G:46:GLU:HB2   | 2.20                     | 0.41              |
| 6:K:67:MET:O     | 6:K:71:LEU:HB2   | 2.20                     | 0.41              |
| 6:Q:26:ILE:HD12  | 6:Q:55:PHE:HD1   | 1.86                     | 0.41              |
| 6:R:61:THR:O     | 6:R:65:CYS:HB2   | 2.21                     | 0.41              |
| 1:A:82:ARG:HG3   | 2:D:33:ILE:O     | 2.21                     | 0.41              |
| 1:A:204:VAL:HB   | 1:A:268:ILE:HG13 | 2.03                     | 0.41              |
| 1:B:383:LYS:HD2  | 1:B:490:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:428:GLN:NE2  | 1:C:431:LYS:HD2  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:70:LEU:HD23  | 2:E:70:LEU:HA    | 1.92                     | 0.41              |
| 2:E:187:VAL:HG11 | 2:E:261:PHE:HB2  | 2.03                     | 0.41              |
| 2:E:196:ASP:O    | 2:E:197:LEU:C    | 2.63                     | 0.41              |
| 2:E:237:LEU:HD21 | 2:E:295:ARG:HD3  | 2.03                     | 0.41              |
| 2:E:366:GLU:O    | 2:E:370:VAL:HG23 | 2.20                     | 0.41              |
| 2:F:85:VAL:HG12  | 2:F:100:GLY:HA3  | 2.03                     | 0.41              |
| 2:F:86:PRO:O     | 2:F:91:THR:HG21  | 2.21                     | 0.41              |
| 2:F:345:TYR:CD1  | 7:F:600:ANP:C5   | 3.03                     | 0.41              |
| 2:F:382:LYS:O    | 2:F:385:GLN:HG2  | 2.21                     | 0.41              |
| 4:H:37:GLY:HA3   | 6:S:39:ARG:HG2   | 2.03                     | 0.41              |
| 1:A:110:VAL:HA   | 1:A:115:ASN:O    | 2.21                     | 0.41              |
| 1:A:391:SER:O    | 1:A:395:PHE:HD2  | 2.03                     | 0.41              |
| 1:B:503:THR:O    | 1:B:507:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:68:LEU:O     | 2:D:15:ALA:HA    | 2.20                     | 0.41              |
| 1:C:202:TYR:O    | 1:C:266:ALA:HA   | 2.21                     | 0.41              |
| 2:F:117:ILE:HG22 | 2:F:235:THR:HA   | 2.03                     | 0.41              |
| 2:F:162:GLY:HA3  | 7:F:600:ANP:H8   | 2.02                     | 0.41              |
| 2:F:169:GLU:OE1  | 2:F:420:VAL:HB   | 2.20                     | 0.41              |
| 6:M:37:VAL:C     | 6:M:39:ARG:N     | 2.78                     | 0.41              |
| 6:R:40:ASN:OD1   | 6:R:41:PRO:HA    | 2.20                     | 0.41              |
| 6:S:52:ILE:HA    | 6:S:55:PHE:HB3   | 2.03                     | 0.41              |
| 6:T:47:VAL:HG12  | 6:T:48:PHE:N     | 2.36                     | 0.41              |
| 1:B:64:MET:HG2   | 1:B:65:ALA:N     | 2.36                     | 0.40              |
| 1:C:110:VAL:HB   | 1:C:114:GLY:HA2  | 2.03                     | 0.40              |
| 2:D:159:ALA:O    | 2:D:337:ARG:NH2  | 2.41                     | 0.40              |
| 2:F:419:ALA:O    | 2:F:422:GLU:HB2  | 2.21                     | 0.40              |
| 5:I:10:TYR:C     | 5:I:12:ALA:N     | 2.78                     | 0.40              |
| 6:O:47:VAL:HA    | 6:O:50:MET:HE2   | 2.03                     | 0.40              |
| 6:Q:65:CYS:SG    | 6:R:16:THR:CG2   | 3.07                     | 0.40              |
| 1:A:108:ARG:HD2  | 1:A:108:ARG:HA   | 1.86                     | 0.40              |
| 1:C:411:ASP:N    | 1:C:411:ASP:OD1  | 2.54                     | 0.40              |
| 2:D:115:LYS:HA   | 2:D:116:PRO:HD3  | 1.96                     | 0.40              |
| 2:D:241:GLU:OE2  | 2:D:295:ARG:HB3  | 2.21                     | 0.40              |
| 3:G:54:ASN:CG    | 4:H:78:GLN:HE21  | 2.28                     | 0.40              |
| 3:G:203:ALA:O    | 3:G:204:ASN:C    | 2.64                     | 0.40              |
| 5:I:33:SER:HB3   | 5:I:37:ARG:NH2   | 2.35                     | 0.40              |
| 1:B:96:ILE:O     | 1:B:97:VAL:C     | 2.64                     | 0.40              |
| 1:B:377:GLY:C    | 1:B:380:ALA:H    | 2.29                     | 0.40              |
| 1:C:222:LEU:CB   | 1:C:228:MET:HG2  | 2.49                     | 0.40              |
| 2:D:89:ARG:HG2   | 2:D:92:LEU:CD1   | 2.50                     | 0.40              |
| 2:D:90:GLU:HG3   | 2:D:110:LYS:O    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:119:ALA:HB3  | 2:E:295:ARG:HH21 | 1.86                     | 0.40              |
| 6:M:48:PHE:HA    | 6:M:51:ALA:HB3   | 2.04                     | 0.40              |
| 6:Q:61:THR:O     | 6:Q:65:CYS:HB2   | 2.22                     | 0.40              |
| 6:S:48:PHE:N     | 6:S:49:PRO:CD    | 2.83                     | 0.40              |
| 1:A:355:GLU:HB2  | 1:A:358:LEU:HD12 | 2.04                     | 0.40              |
| 1:C:212:ARG:HG3  | 1:C:237:THR:HG21 | 2.03                     | 0.40              |
| 2:E:397:SER:O    | 2:E:401:LYS:HG2  | 2.22                     | 0.40              |
| 2:F:215:VAL:HG22 | 2:F:216:ALA:H    | 1.86                     | 0.40              |
| 2:F:224:GLU:HB3  | 2:F:228:ALA:HB3  | 2.02                     | 0.40              |
| 6:O:52:ILE:HA    | 6:O:55:PHE:HB3   | 2.03                     | 0.40              |
| 1:A:28:ASN:OD1   | 1:A:47:ASN:HB2   | 2.21                     | 0.40              |
| 1:C:475:LYS:O    | 1:C:479:ASN:HB2  | 2.22                     | 0.40              |
| 2:D:98:VAL:HG23  | 2:D:232:VAL:HA   | 2.04                     | 0.40              |
| 2:D:356:ARG:CG   | 2:D:357:LEU:HD23 | 2.51                     | 0.40              |
| 2:E:312:VAL:HA   | 2:E:313:PRO:HD3  | 1.93                     | 0.40              |
| 4:H:70:ILE:HG23  | 4:H:72:GLY:N     | 2.34                     | 0.40              |
| 6:K:43:ILE:HD13  | 6:T:50:MET:SD    | 2.61                     | 0.40              |
| 6:L:43:ILE:HG23  | 6:L:44:LYS:H     | 1.85                     | 0.40              |
| 6:R:71:LEU:HD23  | 6:S:73:LEU:HD21  | 2.04                     | 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     | 479/545 (88%) | 427 (89%) | 50 (10%) | 2 (0%)   | 30 63       |
| 1   | B     | 480/545 (88%) | 434 (90%) | 44 (9%)  | 2 (0%)   | 30 63       |
| 1   | C     | 483/545 (89%) | 443 (92%) | 36 (8%)  | 4 (1%)   | 16 48       |
| 2   | D     | 469/511 (92%) | 430 (92%) | 37 (8%)  | 2 (0%)   | 30 63       |
| 2   | E     | 467/511 (91%) | 424 (91%) | 37 (8%)  | 6 (1%)   | 9 36        |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | F     | 468/511 (92%)   | 417 (89%)  | 42 (9%)  | 9 (2%)   | 6           | 28 |
| 3   | G     | 262/311 (84%)   | 231 (88%)  | 24 (9%)  | 7 (3%)   | 4           | 20 |
| 4   | H     | 109/160 (68%)   | 89 (82%)   | 15 (14%) | 5 (5%)   | 2           | 11 |
| 5   | I     | 43/61 (70%)     | 27 (63%)   | 10 (23%) | 6 (14%)  | 0           | 1  |
| 6   | K     | 71/76 (93%)     | 66 (93%)   | 2 (3%)   | 3 (4%)   | 2           | 12 |
| 6   | L     | 70/76 (92%)     | 67 (96%)   | 0        | 3 (4%)   | 2           | 11 |
| 6   | M     | 71/76 (93%)     | 67 (94%)   | 3 (4%)   | 1 (1%)   | 9           | 34 |
| 6   | N     | 71/76 (93%)     | 61 (86%)   | 7 (10%)  | 3 (4%)   | 2           | 12 |
| 6   | O     | 72/76 (95%)     | 65 (90%)   | 5 (7%)   | 2 (3%)   | 4           | 19 |
| 6   | P     | 73/76 (96%)     | 68 (93%)   | 2 (3%)   | 3 (4%)   | 2           | 12 |
| 6   | Q     | 73/76 (96%)     | 64 (88%)   | 3 (4%)   | 6 (8%)   | 0           | 3  |
| 6   | R     | 72/76 (95%)     | 65 (90%)   | 5 (7%)   | 2 (3%)   | 4           | 19 |
| 6   | S     | 72/76 (95%)     | 66 (92%)   | 4 (6%)   | 2 (3%)   | 4           | 19 |
| 6   | T     | 71/76 (93%)     | 65 (92%)   | 5 (7%)   | 1 (1%)   | 9           | 34 |
| All | All   | 3976/4460 (89%) | 3576 (90%) | 331 (8%) | 69 (2%)  | 7           | 30 |

All (69) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 29  | GLU  |
| 2   | F     | 28  | SER  |
| 3   | G     | 152 | SER  |
| 3   | G     | 202 | ASP  |
| 3   | G     | 204 | ASN  |
| 5   | I     | 9   | SER  |
| 5   | I     | 23  | SER  |
| 5   | I     | 33  | SER  |
| 5   | I     | 55  | GLU  |
| 5   | I     | 56  | PRO  |
| 6   | P     | 43  | ILE  |
| 6   | S     | 43  | ILE  |
| 1   | C     | 238 | ALA  |
| 1   | C     | 509 | THR  |
| 2   | E     | 123 | SER  |
| 2   | E     | 474 | ALA  |
| 2   | F     | 43  | GLN  |
| 2   | F     | 423 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 203 | ALA  |
| 4   | H     | 14  | PHE  |
| 5   | I     | 32  | ALA  |
| 6   | L     | 40  | ASN  |
| 6   | M     | 40  | ASN  |
| 6   | N     | 43  | ILE  |
| 6   | O     | 43  | ILE  |
| 6   | P     | 40  | ASN  |
| 6   | Q     | 43  | ILE  |
| 6   | T     | 40  | ASN  |
| 1   | B     | 392 | LEU  |
| 2   | D     | 28  | SER  |
| 2   | E     | 353 | SER  |
| 2   | F     | 327 | ALA  |
| 4   | H     | 43  | ALA  |
| 4   | H     | 93  | LEU  |
| 6   | K     | 45  | ASP  |
| 6   | Q     | 46  | THR  |
| 1   | A     | 238 | ALA  |
| 2   | E     | 126 | GLU  |
| 3   | G     | 192 | PRO  |
| 3   | G     | 201 | THR  |
| 6   | K     | 40  | ASN  |
| 6   | K     | 46  | THR  |
| 6   | L     | 46  | THR  |
| 6   | N     | 40  | ASN  |
| 6   | Q     | 2   | GLN  |
| 6   | Q     | 45  | ASP  |
| 6   | R     | 43  | ILE  |
| 6   | S     | 40  | ASN  |
| 1   | A     | 229 | LYS  |
| 1   | B     | 448 | TYR  |
| 1   | C     | 505 | SER  |
| 2   | F     | 279 | VAL  |
| 2   | F     | 326 | PHE  |
| 2   | F     | 474 | ALA  |
| 2   | F     | 475 | ALA  |
| 3   | G     | 78  | THR  |
| 6   | O     | 40  | ASN  |
| 6   | P     | 46  | THR  |
| 6   | R     | 40  | ASN  |
| 1   | C     | 339 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 33  | PRO  |
| 6   | L     | 45  | ASP  |
| 6   | N     | 46  | THR  |
| 6   | Q     | 40  | ASN  |
| 6   | Q     | 49  | PRO  |
| 2   | E     | 461 | GLY  |
| 2   | E     | 141 | VAL  |
| 2   | F     | 248 | GLY  |
| 4   | H     | 54  | 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     | 388/437 (89%) | 363 (94%) | 25 (6%)  | 16          | 46 |
| 1   | B     | 388/437 (89%) | 348 (90%) | 40 (10%) | 7           | 27 |
| 1   | C     | 388/437 (89%) | 353 (91%) | 35 (9%)  | 9           | 32 |
| 2   | D     | 380/411 (92%) | 350 (92%) | 30 (8%)  | 11          | 37 |
| 2   | E     | 378/411 (92%) | 355 (94%) | 23 (6%)  | 17          | 47 |
| 2   | F     | 379/411 (92%) | 352 (93%) | 27 (7%)  | 13          | 42 |
| 3   | G     | 218/266 (82%) | 185 (85%) | 33 (15%) | 3           | 13 |
| 4   | H     | 54/131 (41%)  | 41 (76%)  | 13 (24%) | 1           | 4  |
| 5   | I     | 23/48 (48%)   | 19 (83%)  | 4 (17%)  | 2           | 10 |
| 6   | K     | 53/56 (95%)   | 46 (87%)  | 7 (13%)  | 4           | 17 |
| 6   | L     | 52/56 (93%)   | 47 (90%)  | 5 (10%)  | 8           | 29 |
| 6   | M     | 53/56 (95%)   | 42 (79%)  | 11 (21%) | 1           | 6  |
| 6   | N     | 53/56 (95%)   | 44 (83%)  | 9 (17%)  | 2           | 10 |
| 6   | O     | 54/56 (96%)   | 46 (85%)  | 8 (15%)  | 3           | 14 |
| 6   | P     | 55/56 (98%)   | 49 (89%)  | 6 (11%)  | 6           | 24 |
| 6   | Q     | 55/56 (98%)   | 47 (86%)  | 8 (14%)  | 3           | 14 |
| 6   | R     | 54/56 (96%)   | 43 (80%)  | 11 (20%) | 1           | 6  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |
|-----|-------|-----------------|------------|-----------|-------------|
| 6   | S     | 54/56 (96%)     | 47 (87%)   | 7 (13%)   | 4 18        |
| 6   | T     | 53/56 (95%)     | 43 (81%)   | 10 (19%)  | 1 8         |
| All | All   | 3132/3549 (88%) | 2820 (90%) | 312 (10%) | 7 28        |

All (312) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 90  | VAL  |
| 1   | A     | 97  | VAL  |
| 1   | A     | 101 | VAL  |
| 1   | A     | 143 | SER  |
| 1   | A     | 173 | ARG  |
| 1   | A     | 206 | VAL  |
| 1   | A     | 219 | VAL  |
| 1   | A     | 221 | THR  |
| 1   | A     | 239 | SER  |
| 1   | A     | 245 | GLN  |
| 1   | A     | 251 | THR  |
| 1   | A     | 267 | LEU  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 288 | ARG  |
| 1   | A     | 318 | GLU  |
| 1   | A     | 322 | SER  |
| 1   | A     | 329 | ILE  |
| 1   | A     | 330 | GLU  |
| 1   | A     | 364 | ARG  |
| 1   | A     | 378 | SER  |
| 1   | A     | 412 | LEU  |
| 1   | A     | 480 | GLU  |
| 1   | A     | 481 | LEU  |
| 1   | A     | 492 | SER  |
| 1   | A     | 501 | SER  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 40  | ILE  |
| 1   | B     | 50  | GLN  |
| 1   | B     | 54  | LEU  |
| 1   | B     | 61  | VAL  |
| 1   | B     | 80  | SER  |
| 1   | B     | 82  | ARG  |
| 1   | B     | 83  | LEU  |
| 1   | B     | 89  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 93  | THR  |
| 1   | B     | 97  | VAL  |
| 1   | B     | 99  | VAL  |
| 1   | B     | 109 | VAL  |
| 1   | B     | 129 | SER  |
| 1   | B     | 206 | VAL  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 219 | VAL  |
| 1   | B     | 221 | THR  |
| 1   | B     | 232 | ILE  |
| 1   | B     | 233 | ILE  |
| 1   | B     | 267 | LEU  |
| 1   | B     | 274 | SER  |
| 1   | B     | 278 | VAL  |
| 1   | B     | 314 | LEU  |
| 1   | B     | 318 | GLU  |
| 1   | B     | 336 | VAL  |
| 1   | B     | 348 | THR  |
| 1   | B     | 351 | GLN  |
| 1   | B     | 369 | VAL  |
| 1   | B     | 373 | VAL  |
| 1   | B     | 378 | SER  |
| 1   | B     | 416 | THR  |
| 1   | B     | 427 | THR  |
| 1   | B     | 444 | VAL  |
| 1   | B     | 451 | VAL  |
| 1   | B     | 460 | LEU  |
| 1   | B     | 471 | LEU  |
| 1   | B     | 480 | GLU  |
| 1   | B     | 486 | ARG  |
| 1   | B     | 504 | GLU  |
| 1   | C     | 30  | THR  |
| 1   | C     | 54  | LEU  |
| 1   | C     | 68  | LEU  |
| 1   | C     | 89  | LEU  |
| 1   | C     | 97  | VAL  |
| 1   | C     | 99  | VAL  |
| 1   | C     | 105 | LEU  |
| 1   | C     | 133 | VAL  |
| 1   | C     | 138 | ILE  |
| 1   | C     | 142 | ARG  |
| 1   | C     | 159 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 165 | GLN  |
| 1   | C     | 210 | GLN  |
| 1   | C     | 221 | THR  |
| 1   | C     | 246 | TYR  |
| 1   | C     | 254 | SER  |
| 1   | C     | 274 | SER  |
| 1   | C     | 293 | ARG  |
| 1   | C     | 337 | SER  |
| 1   | C     | 351 | GLN  |
| 1   | C     | 382 | VAL  |
| 1   | C     | 383 | LYS  |
| 1   | C     | 385 | LEU  |
| 1   | C     | 394 | LEU  |
| 1   | C     | 416 | THR  |
| 1   | C     | 458 | ILE  |
| 1   | C     | 468 | SER  |
| 1   | C     | 476 | SER  |
| 1   | C     | 480 | GLU  |
| 1   | C     | 487 | GLU  |
| 1   | C     | 495 | LEU  |
| 1   | C     | 498 | SER  |
| 1   | C     | 501 | SER  |
| 1   | C     | 503 | THR  |
| 1   | C     | 509 | THR  |
| 2   | D     | 9   | ILE  |
| 2   | D     | 26  | GLU  |
| 2   | D     | 29  | GLU  |
| 2   | D     | 74  | GLU  |
| 2   | D     | 77  | LEU  |
| 2   | D     | 167 | ILE  |
| 2   | D     | 183 | VAL  |
| 2   | D     | 204 | THR  |
| 2   | D     | 206 | VAL  |
| 2   | D     | 214 | LYS  |
| 2   | D     | 234 | LEU  |
| 2   | D     | 249 | GLN  |
| 2   | D     | 251 | VAL  |
| 2   | D     | 255 | ILE  |
| 2   | D     | 268 | VAL  |
| 2   | D     | 291 | LEU  |
| 2   | D     | 304 | VAL  |
| 2   | D     | 329 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 332 | THR  |
| 2   | D     | 341 | GLU  |
| 2   | D     | 357 | LEU  |
| 2   | D     | 359 | ASP  |
| 2   | D     | 374 | VAL  |
| 2   | D     | 396 | LEU  |
| 2   | D     | 397 | SER  |
| 2   | D     | 402 | LEU  |
| 2   | D     | 410 | ILE  |
| 2   | D     | 420 | VAL  |
| 2   | D     | 423 | VAL  |
| 2   | D     | 464 | GLU  |
| 2   | E     | 20  | ILE  |
| 2   | E     | 128 | SER  |
| 2   | E     | 129 | THR  |
| 2   | E     | 140 | VAL  |
| 2   | E     | 165 | VAL  |
| 2   | E     | 174 | ILE  |
| 2   | E     | 190 | ARG  |
| 2   | E     | 210 | GLU  |
| 2   | E     | 232 | VAL  |
| 2   | E     | 294 | GLU  |
| 2   | E     | 298 | THR  |
| 2   | E     | 299 | THR  |
| 2   | E     | 324 | THR  |
| 2   | E     | 352 | ASP  |
| 2   | E     | 357 | LEU  |
| 2   | E     | 359 | ASP  |
| 2   | E     | 373 | LYS  |
| 2   | E     | 376 | GLU  |
| 2   | E     | 380 | THR  |
| 2   | E     | 406 | ARG  |
| 2   | E     | 435 | LYS  |
| 2   | E     | 446 | GLU  |
| 2   | E     | 464 | GLU  |
| 2   | F     | 58  | THR  |
| 2   | F     | 87  | VAL  |
| 2   | F     | 98  | VAL  |
| 2   | F     | 140 | VAL  |
| 2   | F     | 163 | LYS  |
| 2   | F     | 165 | VAL  |
| 2   | F     | 167 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 182 | SER  |
| 2   | F     | 201 | MET  |
| 2   | F     | 208 | ASN  |
| 2   | F     | 232 | VAL  |
| 2   | F     | 251 | VAL  |
| 2   | F     | 261 | PHE  |
| 2   | F     | 279 | VAL  |
| 2   | F     | 303 | SER  |
| 2   | F     | 305 | THR  |
| 2   | F     | 318 | THR  |
| 2   | F     | 324 | THR  |
| 2   | F     | 354 | LYS  |
| 2   | F     | 355 | SER  |
| 2   | F     | 357 | LEU  |
| 2   | F     | 388 | ILE  |
| 2   | F     | 420 | VAL  |
| 2   | F     | 423 | VAL  |
| 2   | F     | 427 | ILE  |
| 2   | F     | 434 | LEU  |
| 2   | F     | 467 | VAL  |
| 3   | G     | 2   | THR  |
| 3   | G     | 3   | LEU  |
| 3   | G     | 4   | LYS  |
| 3   | G     | 16  | ILE  |
| 3   | G     | 17  | GLU  |
| 3   | G     | 19  | ILE  |
| 3   | G     | 21  | LYS  |
| 3   | G     | 26  | VAL  |
| 3   | G     | 38  | LYS  |
| 3   | G     | 78  | THR  |
| 3   | G     | 121 | THR  |
| 3   | G     | 130 | ILE  |
| 3   | G     | 143 | SER  |
| 3   | G     | 145 | LEU  |
| 3   | G     | 148 | ASP  |
| 3   | G     | 152 | SER  |
| 3   | G     | 155 | LYS  |
| 3   | G     | 164 | ILE  |
| 3   | G     | 173 | LEU  |
| 3   | G     | 196 | LYS  |
| 3   | G     | 205 | VAL  |
| 3   | G     | 216 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 218 | MET  |
| 3   | G     | 231 | SER  |
| 3   | G     | 235 | ASN  |
| 3   | G     | 248 | ILE  |
| 3   | G     | 254 | LEU  |
| 3   | G     | 264 | THR  |
| 3   | G     | 267 | LEU  |
| 3   | G     | 269 | ASP  |
| 3   | G     | 271 | ILE  |
| 3   | G     | 272 | THR  |
| 3   | G     | 276 | SER  |
| 4   | H     | 12  | LEU  |
| 4   | H     | 19  | GLU  |
| 4   | H     | 21  | LEU  |
| 4   | H     | 27  | VAL  |
| 4   | H     | 29  | GLN  |
| 4   | H     | 30  | VAL  |
| 4   | H     | 42  | LEU  |
| 4   | H     | 46  | VAL  |
| 4   | H     | 48  | THR  |
| 4   | H     | 49  | VAL  |
| 4   | H     | 60  | MET  |
| 4   | H     | 70  | ILE  |
| 4   | H     | 86  | THR  |
| 5   | I     | 14  | LEU  |
| 5   | I     | 27  | THR  |
| 5   | I     | 31  | THR  |
| 5   | I     | 34  | VAL  |
| 6   | K     | 5   | LEU  |
| 6   | K     | 16  | THR  |
| 6   | K     | 33  | LEU  |
| 6   | K     | 43  | ILE  |
| 6   | K     | 44  | LYS  |
| 6   | K     | 46  | THR  |
| 6   | K     | 59  | GLU  |
| 6   | L     | 16  | THR  |
| 6   | L     | 33  | LEU  |
| 6   | L     | 43  | ILE  |
| 6   | L     | 59  | GLU  |
| 6   | L     | 71  | LEU  |
| 6   | M     | 5   | LEU  |
| 6   | M     | 16  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | M     | 33  | LEU  |
| 6   | M     | 39  | ARG  |
| 6   | M     | 43  | ILE  |
| 6   | M     | 46  | THR  |
| 6   | M     | 47  | VAL  |
| 6   | M     | 48  | PHE  |
| 6   | M     | 52  | ILE  |
| 6   | M     | 59  | GLU  |
| 6   | M     | 71  | LEU  |
| 6   | N     | 1   | MET  |
| 6   | N     | 2   | GLN  |
| 6   | N     | 5   | LEU  |
| 6   | N     | 16  | THR  |
| 6   | N     | 33  | LEU  |
| 6   | N     | 46  | THR  |
| 6   | N     | 59  | GLU  |
| 6   | N     | 67  | MET  |
| 6   | N     | 71  | LEU  |
| 6   | O     | 5   | LEU  |
| 6   | O     | 16  | THR  |
| 6   | O     | 33  | LEU  |
| 6   | O     | 47  | VAL  |
| 6   | O     | 48  | PHE  |
| 6   | O     | 52  | ILE  |
| 6   | O     | 59  | GLU  |
| 6   | O     | 71  | LEU  |
| 6   | P     | 5   | LEU  |
| 6   | P     | 16  | THR  |
| 6   | P     | 33  | LEU  |
| 6   | P     | 59  | GLU  |
| 6   | P     | 65  | CYS  |
| 6   | P     | 71  | LEU  |
| 6   | Q     | 2   | GLN  |
| 6   | Q     | 5   | LEU  |
| 6   | Q     | 16  | THR  |
| 6   | Q     | 33  | LEU  |
| 6   | Q     | 42  | SER  |
| 6   | Q     | 47  | VAL  |
| 6   | Q     | 59  | GLU  |
| 6   | Q     | 71  | LEU  |
| 6   | R     | 1   | MET  |
| 6   | R     | 2   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | R     | 5   | LEU  |
| 6   | R     | 16  | THR  |
| 6   | R     | 33  | LEU  |
| 6   | R     | 43  | ILE  |
| 6   | R     | 44  | LYS  |
| 6   | R     | 45  | ASP  |
| 6   | R     | 59  | GLU  |
| 6   | R     | 71  | LEU  |
| 6   | R     | 73  | LEU  |
| 6   | S     | 5   | LEU  |
| 6   | S     | 16  | THR  |
| 6   | S     | 17  | ILE  |
| 6   | S     | 33  | LEU  |
| 6   | S     | 43  | ILE  |
| 6   | S     | 59  | GLU  |
| 6   | S     | 71  | LEU  |
| 6   | T     | 5   | LEU  |
| 6   | T     | 16  | THR  |
| 6   | T     | 33  | LEU  |
| 6   | T     | 38  | SER  |
| 6   | T     | 47  | VAL  |
| 6   | T     | 48  | PHE  |
| 6   | T     | 59  | GLU  |
| 6   | T     | 65  | CYS  |
| 6   | T     | 71  | LEU  |
| 6   | T     | 73  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | HIS  |
| 1   | A     | 398 | GLN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 454 | HIS  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 47  | ASN  |
| 1   | B     | 67  | ASN  |
| 1   | B     | 149 | GLN  |
| 1   | B     | 192 | ASN  |
| 1   | B     | 265 | HIS  |
| 1   | B     | 282 | GLN  |
| 1   | B     | 398 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 428 | GLN  |
| 1   | B     | 454 | HIS  |
| 1   | B     | 477 | ASN  |
| 1   | C     | 210 | GLN  |
| 1   | C     | 217 | GLN  |
| 1   | C     | 304 | HIS  |
| 2   | D     | 365 | GLN  |
| 2   | E     | 43  | GLN  |
| 2   | E     | 52  | GLN  |
| 2   | E     | 168 | GLN  |
| 2   | E     | 221 | GLN  |
| 2   | E     | 328 | HIS  |
| 2   | E     | 379 | GLN  |
| 2   | E     | 385 | GLN  |
| 2   | F     | 24  | HIS  |
| 2   | F     | 52  | GLN  |
| 2   | F     | 127 | GLN  |
| 2   | F     | 208 | ASN  |
| 2   | F     | 308 | GLN  |
| 2   | F     | 328 | HIS  |
| 3   | G     | 54  | ASN  |
| 3   | G     | 124 | ASN  |
| 3   | G     | 216 | ASN  |
| 3   | G     | 224 | GLN  |
| 4   | H     | 78  | GLN  |
| 5   | I     | 30  | GLN  |
| 6   | L     | 40  | ASN  |
| 6   | M     | 2   | GLN  |
| 6   | M     | 40  | ASN  |
| 6   | N     | 2   | GLN  |
| 6   | N     | 40  | ASN  |
| 6   | O     | 2   | GLN  |
| 6   | P     | 2   | GLN  |
| 6   | T     | 2   | GLN  |

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | ANP  | F     | 600 | 8    | 33,33,33     | 2.89 | 12 (36%) | 45,52,52    | 2.10 | 15 (33%) |
| 7   | ANP  | B     | 600 | 8    | 33,33,33     | 2.90 | 10 (30%) | 45,52,52    | 1.86 | 11 (24%) |
| 7   | ANP  | C     | 600 | 8    | 33,33,33     | 2.74 | 12 (36%) | 45,52,52    | 2.15 | 14 (31%) |
| 7   | ANP  | D     | 600 | 8    | 33,33,33     | 3.03 | 11 (33%) | 45,52,52    | 2.10 | 15 (33%) |
| 7   | ANP  | A     | 600 | 8    | 33,33,33     | 2.82 | 11 (33%) | 45,52,52    | 1.92 | 13 (28%) |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 7   | ANP  | F     | 600 | 8    | -       | 1/18/38/38 | 0/3/3/3 |
| 7   | ANP  | B     | 600 | 8    | -       | 3/18/38/38 | 0/3/3/3 |
| 7   | ANP  | C     | 600 | 8    | -       | 3/18/38/38 | 0/3/3/3 |
| 7   | ANP  | D     | 600 | 8    | -       | 2/18/38/38 | 0/3/3/3 |
| 7   | ANP  | A     | 600 | 8    | -       | 2/18/38/38 | 0/3/3/3 |

All (56) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | D     | 600 | ANP  | PG-O1G | 10.06 | 1.61        | 1.46     |
| 7   | A     | 600 | ANP  | PG-O1G | 9.19  | 1.60        | 1.46     |
| 7   | F     | 600 | ANP  | PG-O1G | 9.07  | 1.59        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | B     | 600 | ANP  | PG-O1G | 9.06  | 1.59        | 1.46     |
| 7   | D     | 600 | ANP  | PB-O1B | 8.57  | 1.59        | 1.46     |
| 7   | B     | 600 | ANP  | PB-O1B | 8.48  | 1.59        | 1.46     |
| 7   | C     | 600 | ANP  | PG-O1G | 8.45  | 1.59        | 1.46     |
| 7   | A     | 600 | ANP  | PB-O1B | 7.90  | 1.58        | 1.46     |
| 7   | F     | 600 | ANP  | PB-O1B | 7.70  | 1.57        | 1.46     |
| 7   | C     | 600 | ANP  | PB-O1B | 7.65  | 1.57        | 1.46     |
| 7   | F     | 600 | ANP  | C4-N3  | 5.91  | 1.45        | 1.34     |
| 7   | B     | 600 | ANP  | C4-N3  | 5.82  | 1.45        | 1.34     |
| 7   | D     | 600 | ANP  | C4-N3  | 5.73  | 1.45        | 1.34     |
| 7   | C     | 600 | ANP  | C4-N3  | 4.82  | 1.43        | 1.34     |
| 7   | A     | 600 | ANP  | C4-N3  | 4.72  | 1.43        | 1.34     |
| 7   | D     | 600 | ANP  | PG-N3B | 4.22  | 1.74        | 1.63     |
| 7   | F     | 600 | ANP  | PB-N3B | 4.21  | 1.74        | 1.63     |
| 7   | F     | 600 | ANP  | PG-N3B | 4.05  | 1.74        | 1.63     |
| 7   | B     | 600 | ANP  | PG-N3B | 4.03  | 1.73        | 1.63     |
| 7   | B     | 600 | ANP  | C5-C4  | 3.96  | 1.46        | 1.39     |
| 7   | D     | 600 | ANP  | C5-C4  | 3.94  | 1.46        | 1.39     |
| 7   | A     | 600 | ANP  | C8-N7  | 3.70  | 1.38        | 1.31     |
| 7   | B     | 600 | ANP  | PB-N3B | 3.69  | 1.73        | 1.63     |
| 7   | C     | 600 | ANP  | PG-N3B | 3.63  | 1.72        | 1.63     |
| 7   | C     | 600 | ANP  | C8-N7  | 3.63  | 1.38        | 1.31     |
| 7   | D     | 600 | ANP  | C8-N7  | 3.61  | 1.38        | 1.31     |
| 7   | A     | 600 | ANP  | PB-N3B | 3.51  | 1.72        | 1.63     |
| 7   | C     | 600 | ANP  | PB-N3B | 3.46  | 1.72        | 1.63     |
| 7   | F     | 600 | ANP  | C5-C4  | 3.46  | 1.45        | 1.39     |
| 7   | A     | 600 | ANP  | PG-N3B | 3.40  | 1.72        | 1.63     |
| 7   | B     | 600 | ANP  | C8-N7  | 3.36  | 1.38        | 1.31     |
| 7   | C     | 600 | ANP  | C4-N9  | -3.20 | 1.31        | 1.37     |
| 7   | D     | 600 | ANP  | PB-N3B | 3.17  | 1.71        | 1.63     |
| 7   | A     | 600 | ANP  | C5-C4  | 3.14  | 1.44        | 1.39     |
| 7   | F     | 600 | ANP  | C8-N7  | 3.14  | 1.37        | 1.31     |
| 7   | D     | 600 | ANP  | C5-C6  | 3.09  | 1.49        | 1.41     |
| 7   | C     | 600 | ANP  | C5-C4  | 2.98  | 1.44        | 1.39     |
| 7   | B     | 600 | ANP  | C5-C6  | 2.97  | 1.49        | 1.41     |
| 7   | A     | 600 | ANP  | C5-C6  | 2.93  | 1.49        | 1.41     |
| 7   | F     | 600 | ANP  | PA-O1A | 2.77  | 1.60        | 1.50     |
| 7   | D     | 600 | ANP  | PA-O1A | 2.47  | 1.59        | 1.50     |
| 7   | C     | 600 | ANP  | C5-N7  | -2.46 | 1.34        | 1.39     |
| 7   | A     | 600 | ANP  | PA-O3A | 2.46  | 1.62        | 1.59     |
| 7   | C     | 600 | ANP  | PA-O1A | 2.45  | 1.59        | 1.50     |
| 7   | A     | 600 | ANP  | PA-O1A | 2.45  | 1.59        | 1.50     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | A     | 600 | ANP  | C4-N9  | -2.44 | 1.32        | 1.37     |
| 7   | B     | 600 | ANP  | PA-O1A | 2.36  | 1.59        | 1.50     |
| 7   | F     | 600 | ANP  | PG-O3G | 2.32  | 1.63        | 1.56     |
| 7   | F     | 600 | ANP  | C5-C6  | 2.30  | 1.47        | 1.41     |
| 7   | C     | 600 | ANP  | PB-O3A | 2.27  | 1.61        | 1.59     |
| 7   | F     | 600 | ANP  | C4-N9  | -2.21 | 1.33        | 1.37     |
| 7   | B     | 600 | ANP  | C5-N7  | -2.20 | 1.35        | 1.39     |
| 7   | C     | 600 | ANP  | C5-C6  | 2.16  | 1.47        | 1.41     |
| 7   | D     | 600 | ANP  | C4-N9  | -2.04 | 1.33        | 1.37     |
| 7   | D     | 600 | ANP  | PG-O2G | 2.03  | 1.62        | 1.56     |
| 7   | F     | 600 | ANP  | C5-N7  | -2.02 | 1.35        | 1.39     |

All (68) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | C     | 600 | ANP  | O4'-C1'-N9  | 6.67  | 120.90      | 108.09   |
| 7   | F     | 600 | ANP  | O1B-PB-N3B  | -5.45 | 103.75      | 111.77   |
| 7   | D     | 600 | ANP  | C4-C5-N7    | -4.85 | 105.04      | 110.58   |
| 7   | A     | 600 | ANP  | C4-C5-N7    | -4.43 | 105.52      | 110.58   |
| 7   | B     | 600 | ANP  | C4-C5-N7    | -4.41 | 105.54      | 110.58   |
| 7   | B     | 600 | ANP  | C5-C4-N3    | -4.32 | 120.77      | 126.72   |
| 7   | D     | 600 | ANP  | C6-C5-N7    | 4.30  | 140.39      | 132.09   |
| 7   | A     | 600 | ANP  | C5-C4-N9    | 4.28  | 110.47      | 105.81   |
| 7   | C     | 600 | ANP  | C6-C5-N7    | 4.18  | 140.16      | 132.09   |
| 7   | B     | 600 | ANP  | C5-C4-N9    | 4.18  | 110.36      | 105.81   |
| 7   | C     | 600 | ANP  | C5-C4-N9    | 4.09  | 110.27      | 105.81   |
| 7   | C     | 600 | ANP  | C4-C5-N7    | -4.08 | 105.92      | 110.58   |
| 7   | A     | 600 | ANP  | C6-C5-N7    | 4.07  | 139.94      | 132.09   |
| 7   | A     | 600 | ANP  | C5-C4-N3    | -4.04 | 121.15      | 126.72   |
| 7   | B     | 600 | ANP  | C6-C5-N7    | 3.92  | 139.65      | 132.09   |
| 7   | F     | 600 | ANP  | N3-C2-N1    | -3.92 | 122.65      | 128.58   |
| 7   | D     | 600 | ANP  | C5-C4-N9    | 3.92  | 110.08      | 105.81   |
| 7   | A     | 600 | ANP  | O1G-PG-N3B  | -3.91 | 106.01      | 111.77   |
| 7   | B     | 600 | ANP  | N3-C2-N1    | -3.91 | 122.67      | 128.58   |
| 7   | D     | 600 | ANP  | C2'-C1'-N9  | -3.84 | 103.77      | 113.30   |
| 7   | C     | 600 | ANP  | N3-C2-N1    | -3.72 | 122.96      | 128.58   |
| 7   | D     | 600 | ANP  | C5-C4-N3    | -3.68 | 121.65      | 126.72   |
| 7   | D     | 600 | ANP  | O1G-PG-N3B  | -3.65 | 106.40      | 111.77   |
| 7   | F     | 600 | ANP  | C6-C5-N7    | 3.64  | 139.10      | 132.09   |
| 7   | D     | 600 | ANP  | O2'-C2'-C1' | -3.51 | 98.02       | 110.10   |
| 7   | F     | 600 | ANP  | O3G-PG-O1G  | -3.43 | 104.84      | 113.45   |
| 7   | D     | 600 | ANP  | N3-C2-N1    | -3.34 | 123.53      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | A     | 600 | ANP  | N3-C2-N1    | -3.26 | 123.64      | 128.58   |
| 7   | F     | 600 | ANP  | C2'-C1'-N9  | -3.25 | 105.24      | 113.30   |
| 7   | F     | 600 | ANP  | C5-C6-N6    | -3.13 | 115.55      | 123.29   |
| 7   | F     | 600 | ANP  | O2B-PB-O1B  | 2.95  | 116.21      | 109.87   |
| 7   | D     | 600 | ANP  | C2-N1-C6    | 2.95  | 123.57      | 118.73   |
| 7   | D     | 600 | ANP  | O2B-PB-O3A  | 2.94  | 114.45      | 104.64   |
| 7   | C     | 600 | ANP  | C2-N1-C6    | 2.88  | 123.47      | 118.73   |
| 7   | F     | 600 | ANP  | O2G-PG-O3G  | 2.86  | 115.28      | 107.59   |
| 7   | B     | 600 | ANP  | C2-N3-C4    | 2.85  | 118.79      | 111.83   |
| 7   | B     | 600 | ANP  | C2-N1-C6    | 2.80  | 123.33      | 118.73   |
| 7   | A     | 600 | ANP  | C2-N3-C4    | 2.78  | 118.61      | 111.83   |
| 7   | F     | 600 | ANP  | C6-C5-C4    | -2.75 | 113.42      | 117.18   |
| 7   | C     | 600 | ANP  | C5-C4-N3    | -2.74 | 122.94      | 126.72   |
| 7   | F     | 600 | ANP  | C4-C5-N7    | -2.72 | 107.47      | 110.58   |
| 7   | F     | 600 | ANP  | C5-C4-N3    | -2.70 | 122.99      | 126.72   |
| 7   | D     | 600 | ANP  | O4'-C1'-N9  | 2.68  | 113.23      | 108.09   |
| 7   | B     | 600 | ANP  | O1G-PG-N3B  | -2.67 | 107.83      | 111.77   |
| 7   | F     | 600 | ANP  | O4'-C1'-C2' | 2.58  | 112.13      | 106.62   |
| 7   | F     | 600 | ANP  | C2-N1-C6    | 2.57  | 122.95      | 118.73   |
| 7   | D     | 600 | ANP  | C3'-C2'-C1' | 2.56  | 106.31      | 101.46   |
| 7   | F     | 600 | ANP  | N6-C6-N1    | 2.51  | 123.98      | 118.38   |
| 7   | D     | 600 | ANP  | C5-N7-C8    | 2.39  | 107.20      | 103.45   |
| 7   | C     | 600 | ANP  | C6-C5-C4    | -2.39 | 113.92      | 117.18   |
| 7   | A     | 600 | ANP  | O3'-C3'-C4' | -2.39 | 104.22      | 111.08   |
| 7   | B     | 600 | ANP  | C3'-C2'-C1' | 2.36  | 105.93      | 101.46   |
| 7   | D     | 600 | ANP  | C2-N3-C4    | 2.33  | 117.53      | 111.83   |
| 7   | F     | 600 | ANP  | C2-N3-C4    | 2.32  | 117.50      | 111.83   |
| 7   | C     | 600 | ANP  | C1'-N9-C8   | 2.28  | 132.15      | 127.09   |
| 7   | A     | 600 | ANP  | O2B-PB-O3A  | 2.25  | 112.15      | 104.64   |
| 7   | D     | 600 | ANP  | O3G-PG-O1G  | -2.21 | 107.92      | 113.45   |
| 7   | C     | 600 | ANP  | C2'-C3'-C4' | 2.19  | 106.83      | 102.61   |
| 7   | A     | 600 | ANP  | C2'-C3'-C4' | 2.12  | 106.71      | 102.61   |
| 7   | C     | 600 | ANP  | C2-N3-C4    | 2.12  | 117.01      | 111.83   |
| 7   | B     | 600 | ANP  | C2'-C3'-C4' | 2.12  | 106.70      | 102.61   |
| 7   | C     | 600 | ANP  | O2G-PG-O3G  | 2.11  | 113.26      | 107.59   |
| 7   | B     | 600 | ANP  | C5'-C4'-C3' | -2.09 | 107.67      | 115.21   |
| 7   | C     | 600 | ANP  | C4-N9-C1'   | -2.08 | 121.78      | 126.63   |
| 7   | C     | 600 | ANP  | O1B-PB-N3B  | -2.05 | 108.75      | 111.77   |
| 7   | A     | 600 | ANP  | O3A-PB-N3B  | -2.03 | 100.96      | 106.59   |
| 7   | A     | 600 | ANP  | C3'-C2'-C1' | 2.03  | 105.30      | 101.46   |
| 7   | A     | 600 | ANP  | C5-N7-C8    | 2.01  | 106.61      | 103.45   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

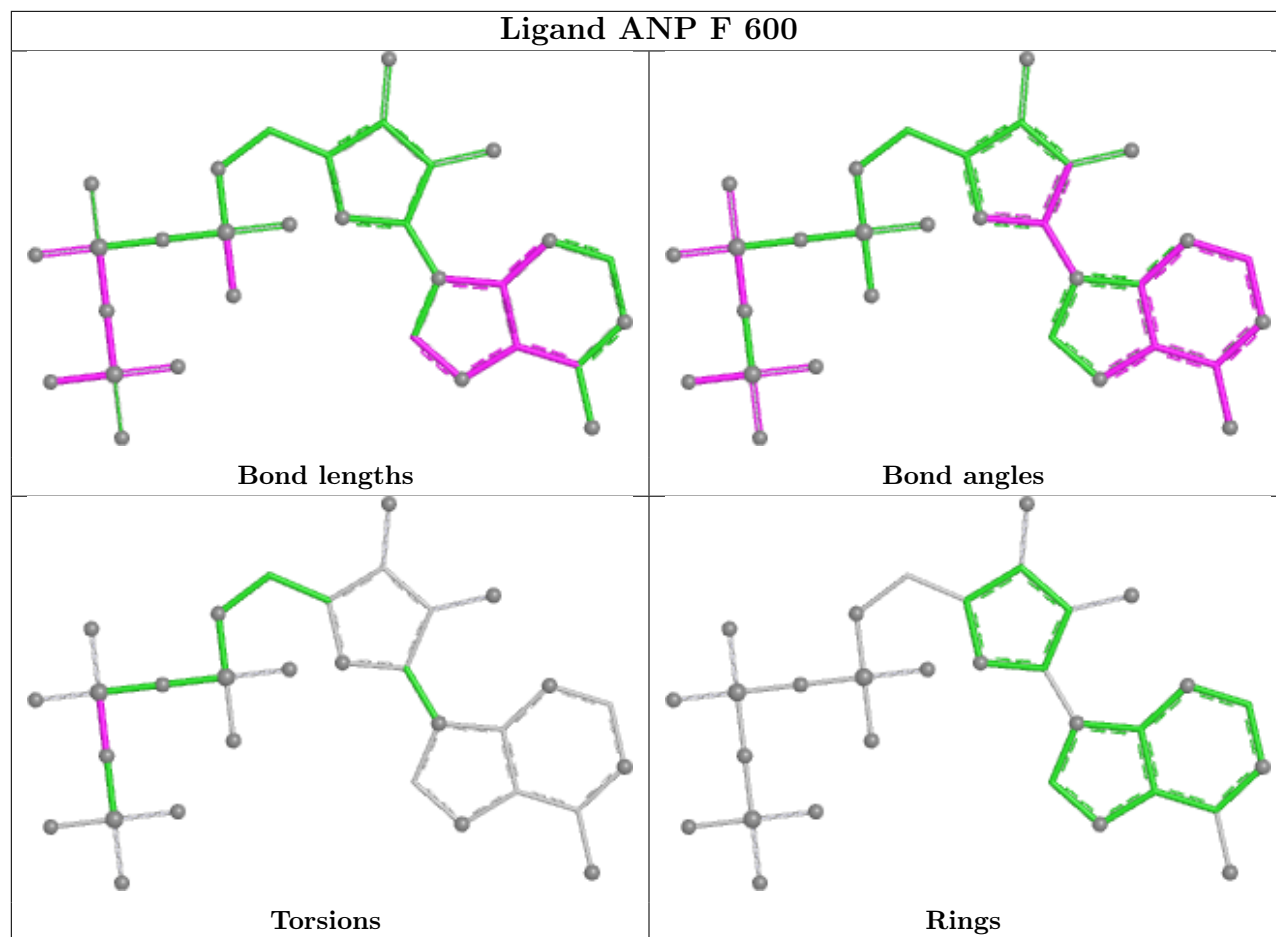
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | A     | 600 | ANP  | PB-N3B-PG-O1G   |
| 7   | A     | 600 | ANP  | PG-N3B-PB-O1B   |
| 7   | B     | 600 | ANP  | PG-N3B-PB-O1B   |
| 7   | C     | 600 | ANP  | PB-N3B-PG-O1G   |
| 7   | C     | 600 | ANP  | PG-N3B-PB-O1B   |
| 7   | D     | 600 | ANP  | PG-N3B-PB-O1B   |
| 7   | D     | 600 | ANP  | PG-N3B-PB-O3A   |
| 7   | F     | 600 | ANP  | PG-N3B-PB-O1B   |
| 7   | B     | 600 | ANP  | O4'-C4'-C5'-O5' |
| 7   | B     | 600 | ANP  | C3'-C4'-C5'-O5' |
| 7   | C     | 600 | ANP  | PB-O3A-PA-O1A   |

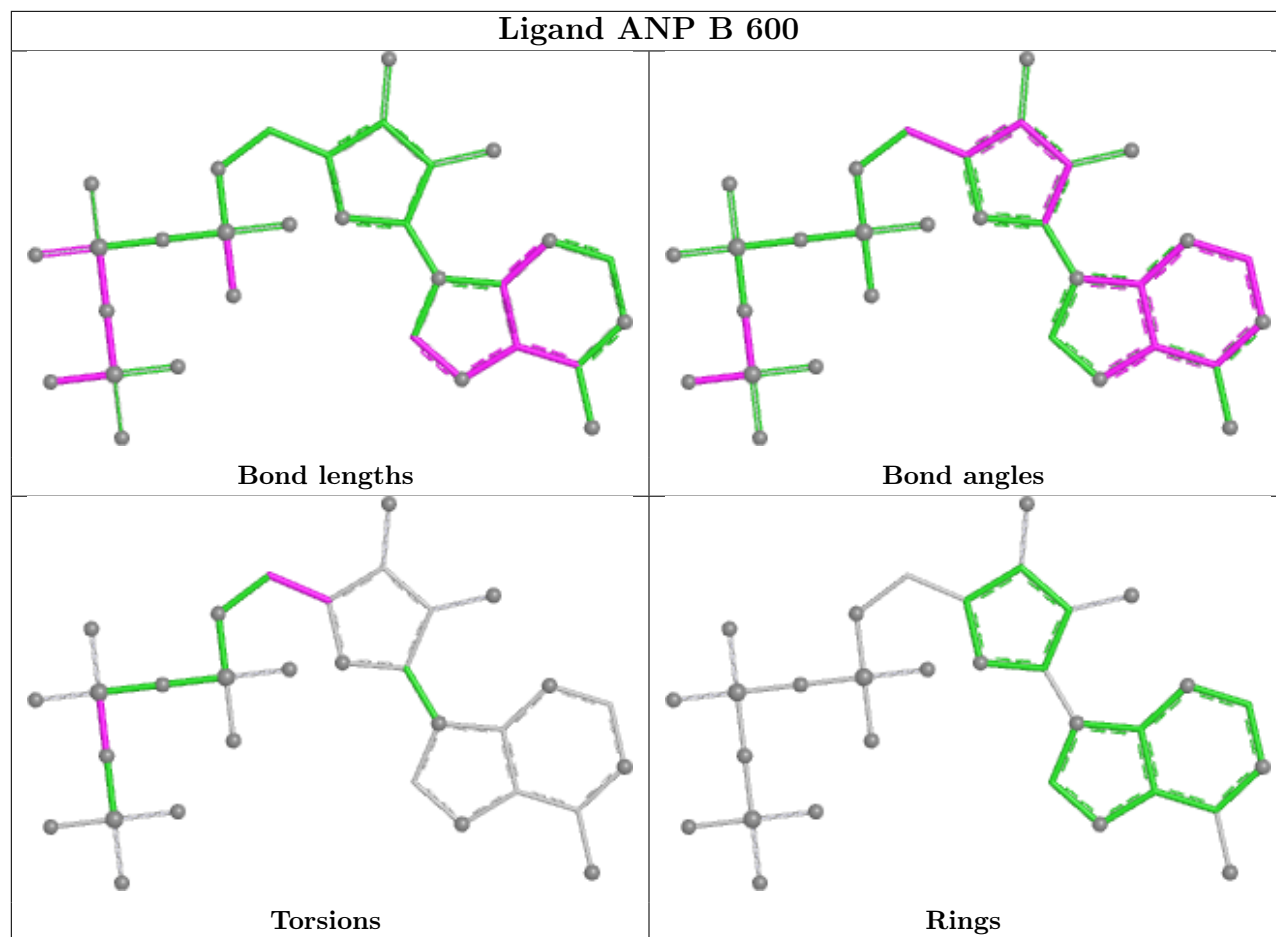
There are no ring outliers.

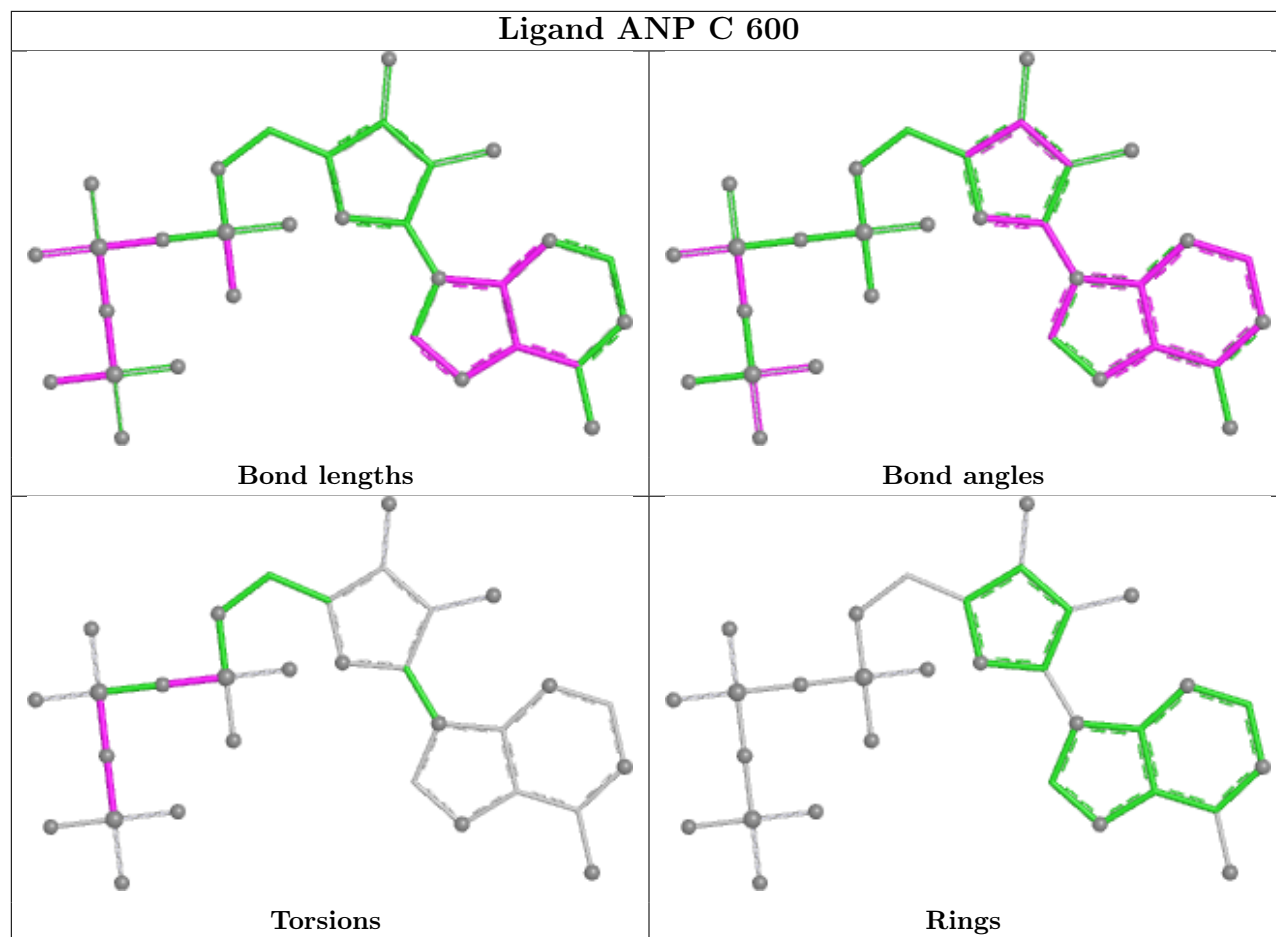
5 monomers are involved in 14 short contacts:

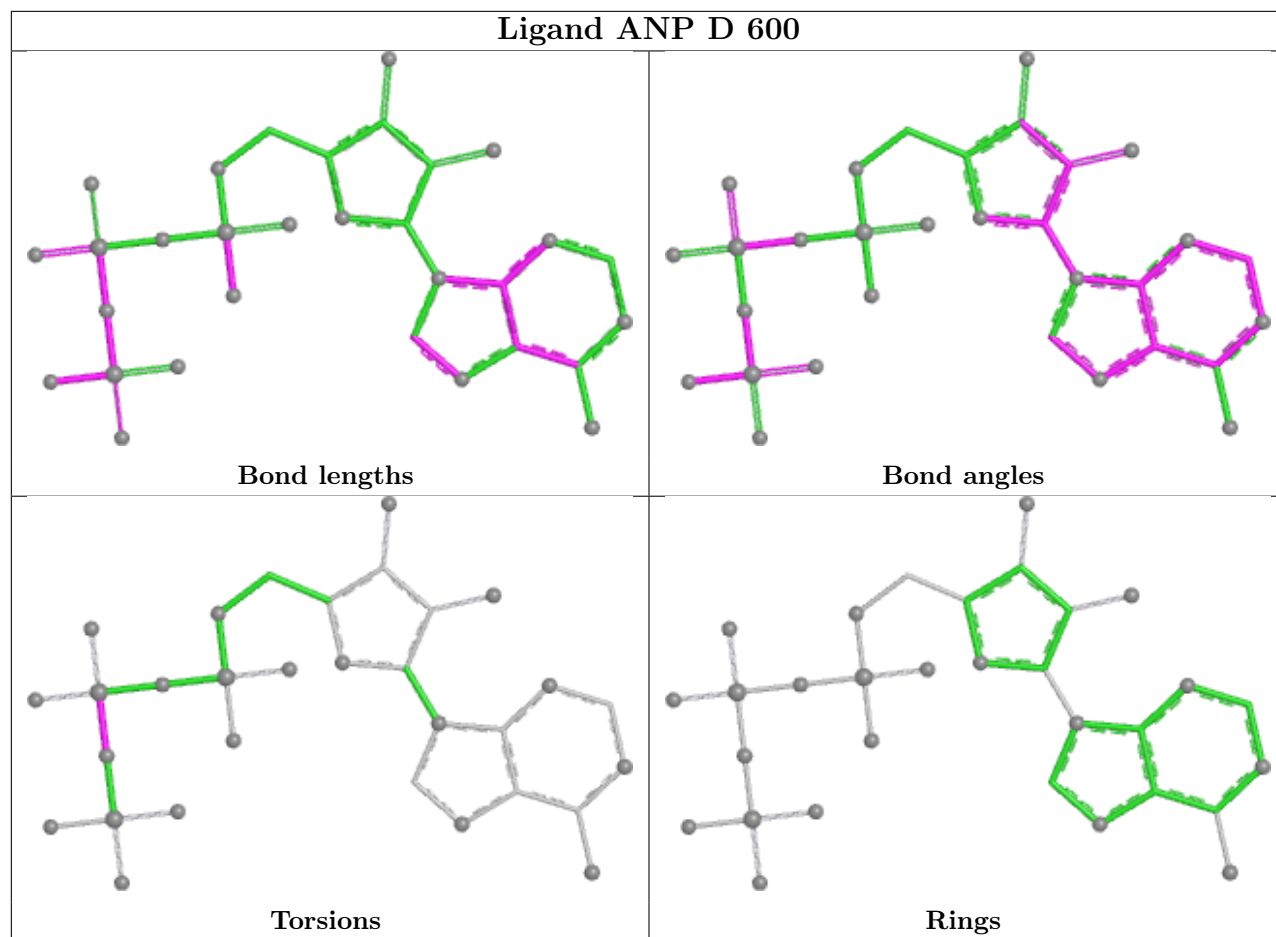
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | F     | 600 | ANP  | 7       | 0            |
| 7   | B     | 600 | ANP  | 1       | 0            |
| 7   | C     | 600 | ANP  | 2       | 0            |
| 7   | D     | 600 | ANP  | 3       | 0            |
| 7   | A     | 600 | ANP  | 1       | 0            |

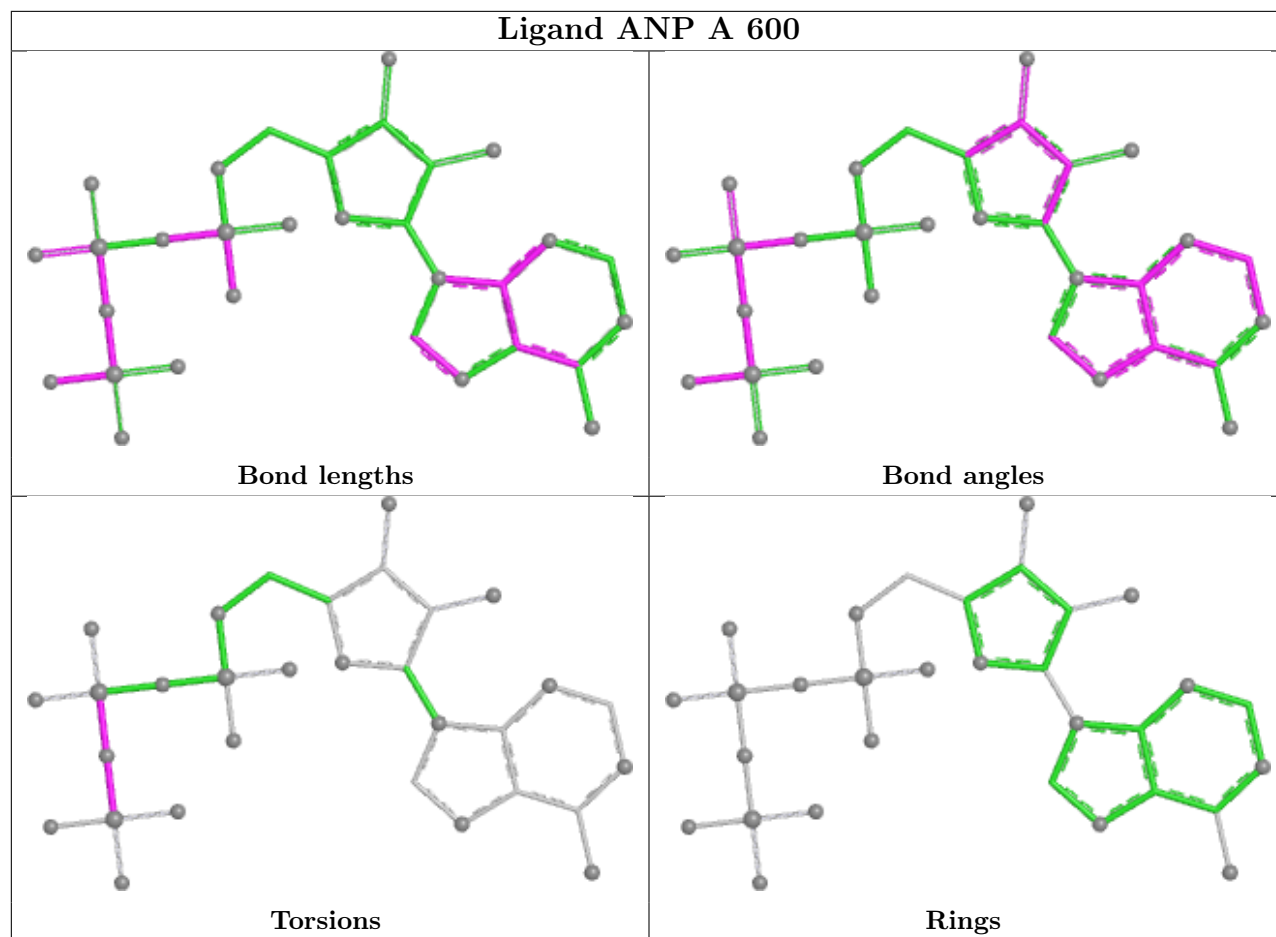
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 483/545 (88%)   | -0.49  | 1 (0%) 91 83  | 61, 89, 128, 145      | 0     |
| 1   | B     | 484/545 (88%)   | -0.24  | 6 (1%) 76 55  | 66, 116, 205, 226     | 0     |
| 1   | C     | 485/545 (88%)   | -0.50  | 1 (0%) 91 83  | 56, 81, 125, 176      | 0     |
| 2   | D     | 471/511 (92%)   | -0.45  | 2 (0%) 88 76  | 64, 85, 123, 160      | 0     |
| 2   | E     | 469/511 (91%)   | -0.36  | 0 100 100     | 71, 114, 176, 213     | 0     |
| 2   | F     | 470/511 (91%)   | -0.48  | 1 (0%) 91 83  | 51, 93, 137, 165      | 0     |
| 3   | G     | 266/311 (85%)   | -0.21  | 2 (0%) 82 64  | 64, 122, 155, 172     | 0     |
| 4   | H     | 119/160 (74%)   | 0.15   | 1 (0%) 82 64  | 102, 146, 195, 216    | 0     |
| 5   | I     | 49/61 (80%)     | 0.48   | 4 (8%) 17 9   | 134, 162, 208, 228    | 0     |
| 6   | K     | 73/76 (96%)     | 0.77   | 8 (10%) 10 6  | 151, 188, 222, 243    | 0     |
| 6   | L     | 72/76 (94%)     | 0.53   | 2 (2%) 55 32  | 149, 188, 213, 217    | 0     |
| 6   | M     | 73/76 (96%)     | 0.63   | 4 (5%) 30 15  | 144, 180, 200, 210    | 0     |
| 6   | N     | 73/76 (96%)     | 0.50   | 5 (6%) 23 12  | 131, 166, 183, 195    | 0     |
| 6   | O     | 74/76 (97%)     | 0.14   | 0 100 100     | 123, 154, 171, 184    | 0     |
| 6   | P     | 75/76 (98%)     | 0.18   | 0 100 100     | 118, 150, 164, 175    | 0     |
| 6   | Q     | 75/76 (98%)     | 0.20   | 1 (1%) 75 53  | 117, 152, 169, 189    | 0     |
| 6   | R     | 74/76 (97%)     | 0.32   | 2 (2%) 56 33  | 125, 164, 183, 196    | 0     |
| 6   | S     | 74/76 (97%)     | 0.44   | 1 (1%) 73 51  | 138, 175, 204, 221    | 0     |
| 6   | T     | 73/76 (96%)     | 0.59   | 5 (6%) 23 12  | 147, 187, 218, 225    | 0     |
| All | All   | 4032/4460 (90%) | -0.22  | 46 (1%) 78 57 | 51, 109, 193, 243     | 0     |

All (46) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | K     | 12  | ALA  | 6.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 43  | GLN  | 3.9  |
| 4   | H     | 97  | SER  | 3.7  |
| 6   | M     | 69  | SER  | 3.5  |
| 6   | T     | 65  | CYS  | 3.2  |
| 6   | M     | 22  | ALA  | 3.2  |
| 5   | I     | 29  | LEU  | 3.1  |
| 5   | I     | 49  | ASN  | 3.0  |
| 5   | I     | 9   | SER  | 2.8  |
| 6   | T     | 12  | ALA  | 2.8  |
| 6   | N     | 61  | THR  | 2.7  |
| 6   | M     | 12  | ALA  | 2.7  |
| 1   | B     | 424 | GLU  | 2.6  |
| 5   | I     | 8   | MET  | 2.6  |
| 6   | T     | 58  | SER  | 2.5  |
| 6   | K     | 68  | VAL  | 2.4  |
| 2   | D     | 267 | GLU  | 2.4  |
| 6   | T     | 10  | ILE  | 2.4  |
| 1   | C     | 405 | PHE  | 2.4  |
| 6   | K     | 15  | SER  | 2.4  |
| 3   | G     | 59  | ASN  | 2.4  |
| 6   | T     | 68  | VAL  | 2.4  |
| 6   | K     | 74  | PHE  | 2.3  |
| 6   | N     | 69  | SER  | 2.3  |
| 6   | K     | 10  | ILE  | 2.3  |
| 6   | N     | 15  | SER  | 2.3  |
| 1   | B     | 48  | ASN  | 2.3  |
| 1   | B     | 412 | LEU  | 2.3  |
| 6   | K     | 5   | LEU  | 2.3  |
| 6   | R     | 65  | CYS  | 2.3  |
| 3   | G     | 57  | THR  | 2.2  |
| 6   | M     | 72  | LEU  | 2.2  |
| 6   | S     | 44  | LYS  | 2.2  |
| 6   | R     | 69  | SER  | 2.2  |
| 6   | L     | 24  | ILE  | 2.2  |
| 1   | A     | 380 | ALA  | 2.2  |
| 6   | N     | 58  | SER  | 2.1  |
| 6   | Q     | 41  | PRO  | 2.1  |
| 1   | B     | 402 | VAL  | 2.1  |
| 1   | B     | 503 | THR  | 2.1  |
| 6   | K     | 44  | LYS  | 2.1  |
| 6   | K     | 16  | THR  | 2.1  |
| 2   | F     | 424 | PHE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | L     | 72  | LEU  | 2.0  |
| 6   | N     | 44  | LYS  | 2.0  |
| 1   | B     | 455 | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

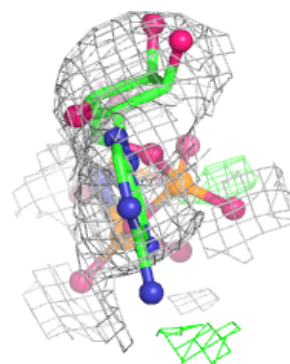
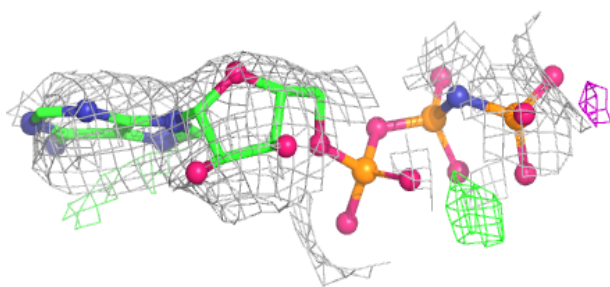
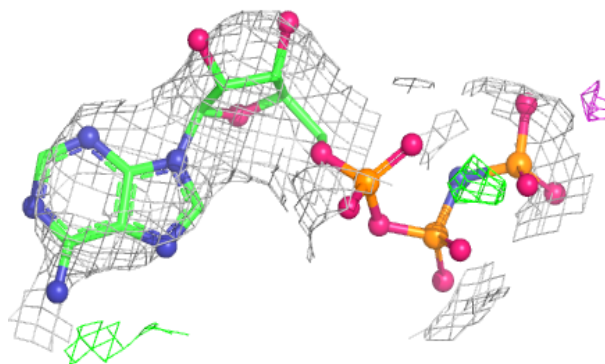
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 8   | MG   | A     | 700 | 1/1   | 0.70 | 0.20 | 66,66,66,66                | 0     |
| 8   | MG   | D     | 700 | 1/1   | 0.91 | 0.16 | 71,71,71,71                | 0     |
| 8   | MG   | C     | 700 | 1/1   | 0.93 | 0.17 | 80,80,80,80                | 0     |
| 7   | ANP  | B     | 600 | 31/31 | 0.95 | 0.08 | 110,134,145,146            | 0     |
| 7   | ANP  | D     | 600 | 31/31 | 0.95 | 0.09 | 66,73,116,122              | 0     |
| 7   | ANP  | F     | 600 | 31/31 | 0.95 | 0.09 | 39,72,95,95                | 0     |
| 8   | MG   | B     | 700 | 1/1   | 0.96 | 0.12 | 86,86,86,86                | 0     |
| 8   | MG   | F     | 700 | 1/1   | 0.96 | 0.10 | 52,52,52,52                | 0     |
| 7   | ANP  | C     | 600 | 31/31 | 0.97 | 0.06 | 51,69,77,83                | 0     |
| 7   | ANP  | A     | 600 | 31/31 | 0.97 | 0.06 | 60,71,80,88                | 0     |

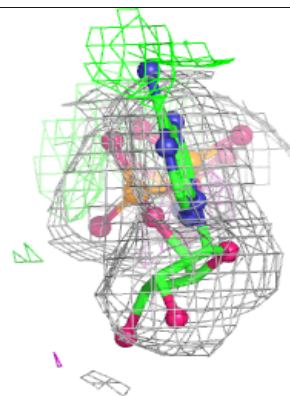
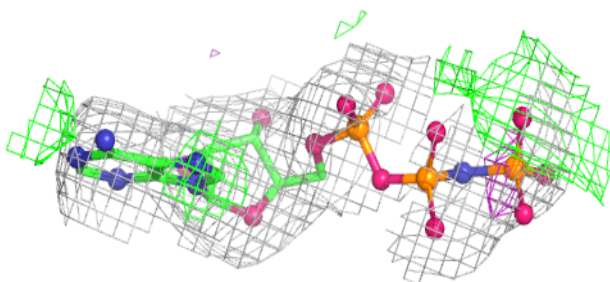
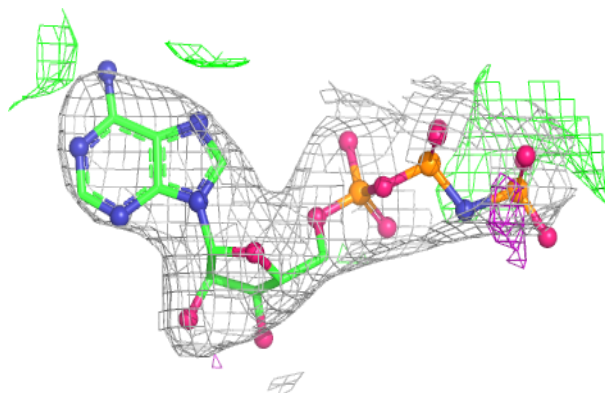
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP B 600:**

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

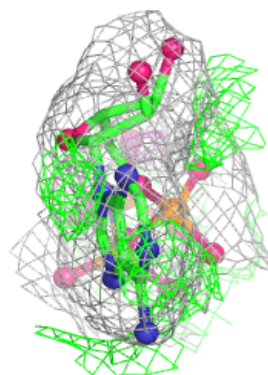
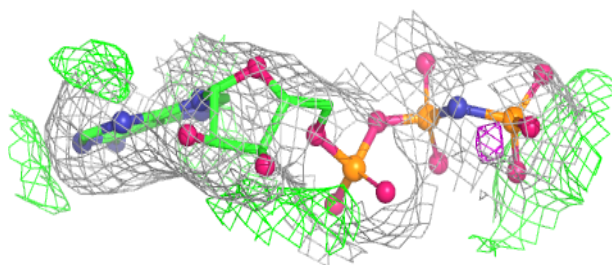
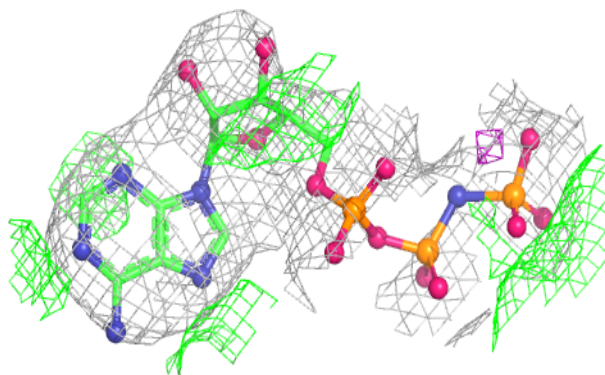
**Electron density around ANP D 600:**

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

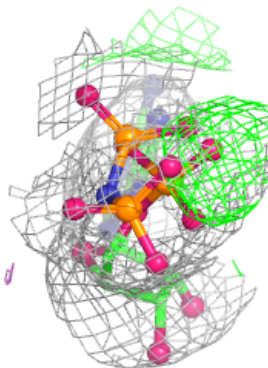
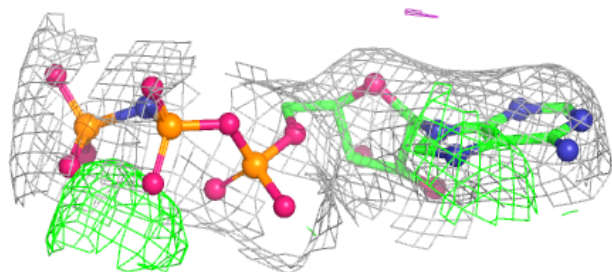
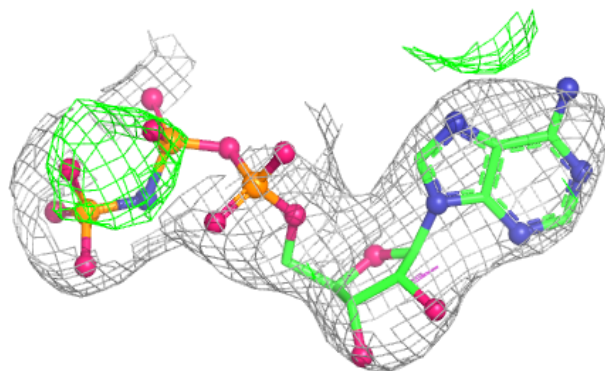


**Electron density around ANP F 600:**

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

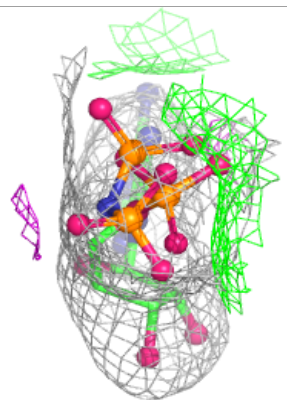
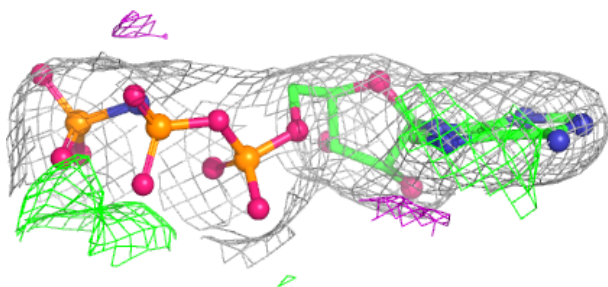
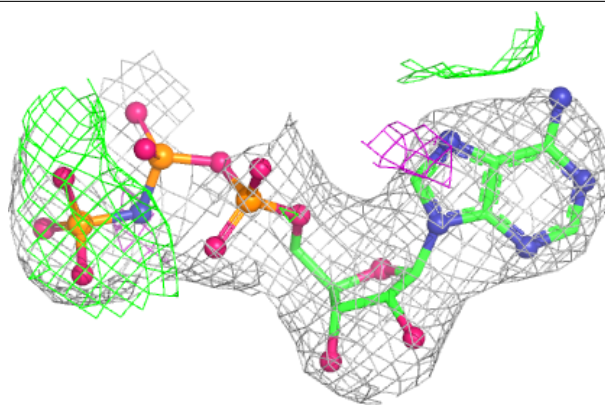
**Electron density around ANP C 600:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.