



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:57 AM UTC

PDB ID : 3KFB / pdb\_00003kfb  
Title : Crystal structure of a group II chaperonin from *Methanococcus maripaludis*  
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.  
Deposited on : 2009-10-27  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

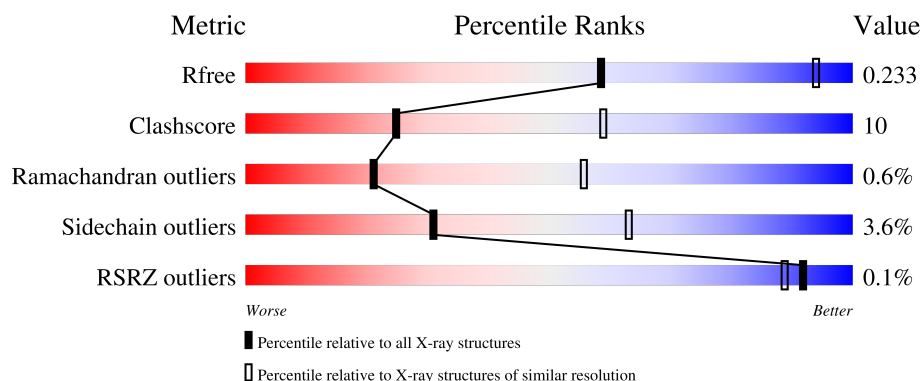
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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     | 543    | <div> <div>72%</div> <div>20%</div> <div>• 6%</div> </div> |
| 1   | B     | 543    | <div> <div>72%</div> <div>20%</div> <div>• 6%</div> </div> |
| 1   | C     | 543    | <div> <div>72%</div> <div>20%</div> <div>• 6%</div> </div> |
| 1   | D     | 543    | <div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div> |
| 1   | E     | 543    | <div> <div>71%</div> <div>21%</div> <div>• 6%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                  |
|-----|-------|--------|-------------------------------------------------------------------|
| 1   | F     | 543    | <div><div></div><div>72%</div><div>20%</div><div>• 6%</div></div> |
| 1   | G     | 543    | <div><div></div><div>74%</div><div>19%</div><div>• 6%</div></div> |
| 1   | H     | 543    | <div><div></div><div>72%</div><div>21%</div><div>• 6%</div></div> |

## 2 Entry composition

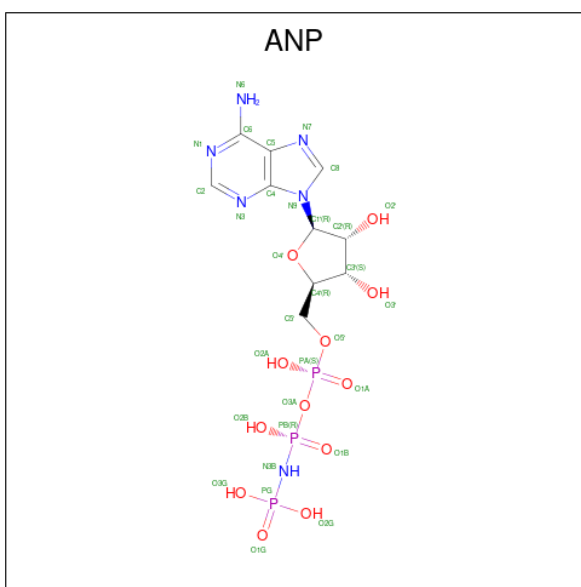
There are 3 unique types of molecules in this entry. The entry contains 30816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chaperonin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | B     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | C     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | D     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | E     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | F     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | G     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |
| 1   | H     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2370 | 660 | 765 | 25 |         |         |       |

- Molecule 2 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 |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 2   | A     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | B     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 2   | H     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |

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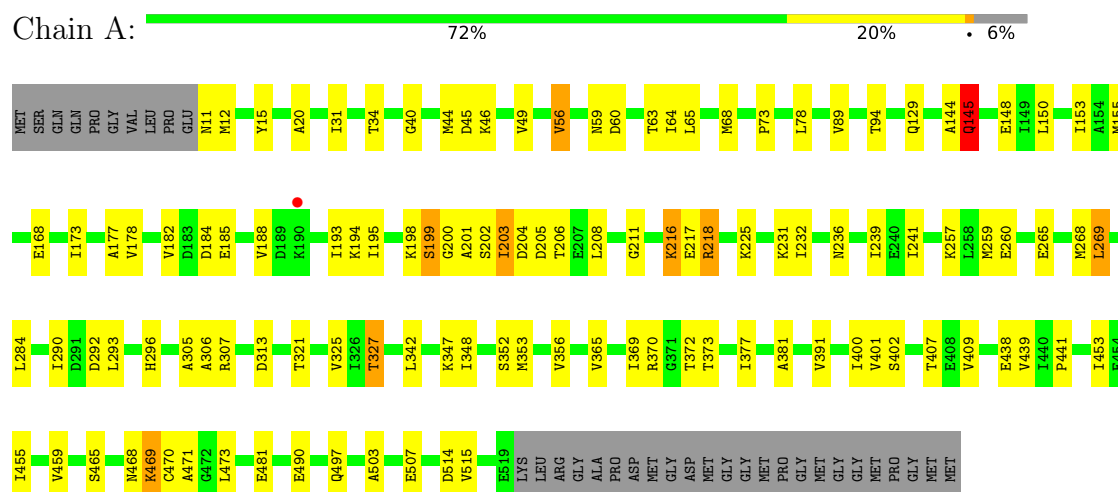
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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | E     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 3   | G     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 3   | H     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

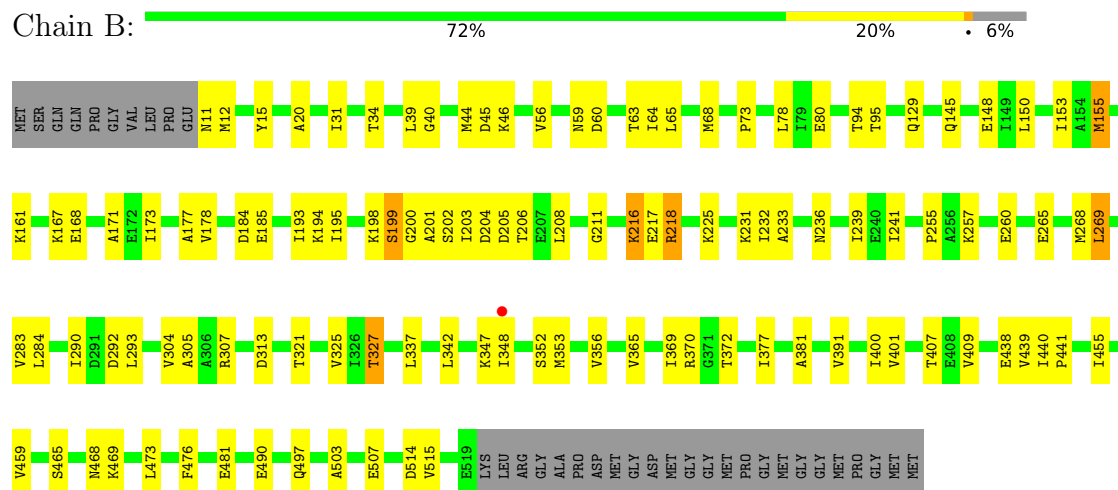
### 3 Residue-property plots

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: Chaperonin



#### • Molecule 1: Chaperonin

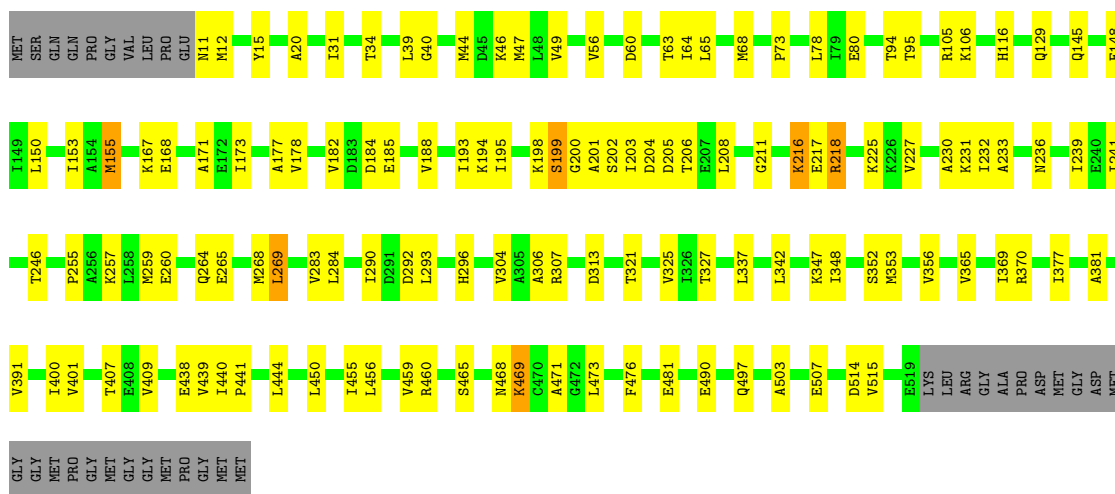


#### • Molecule 1: Chaperonin



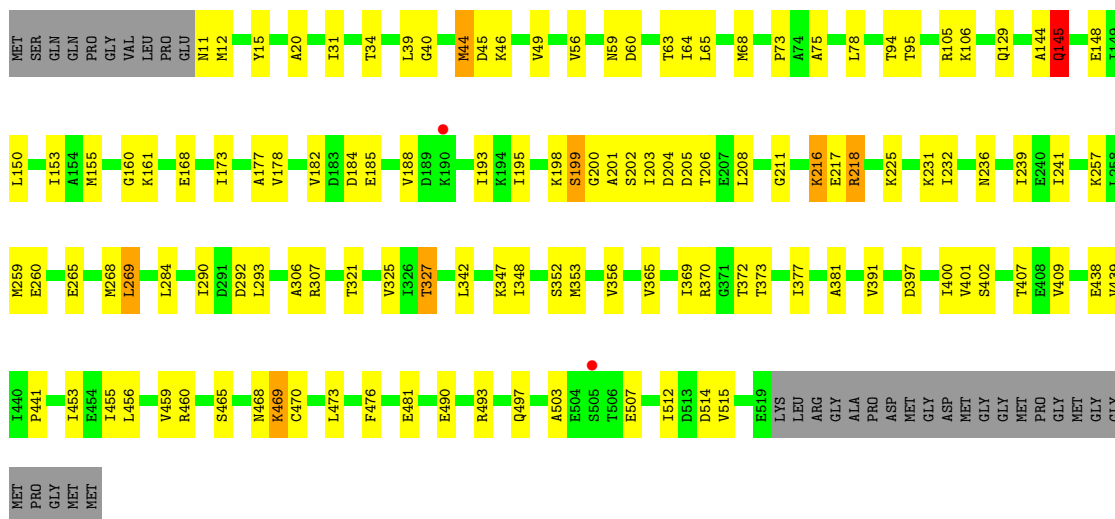
- Molecule 1: Chaperonin

Chain D:  70% 23% 6%



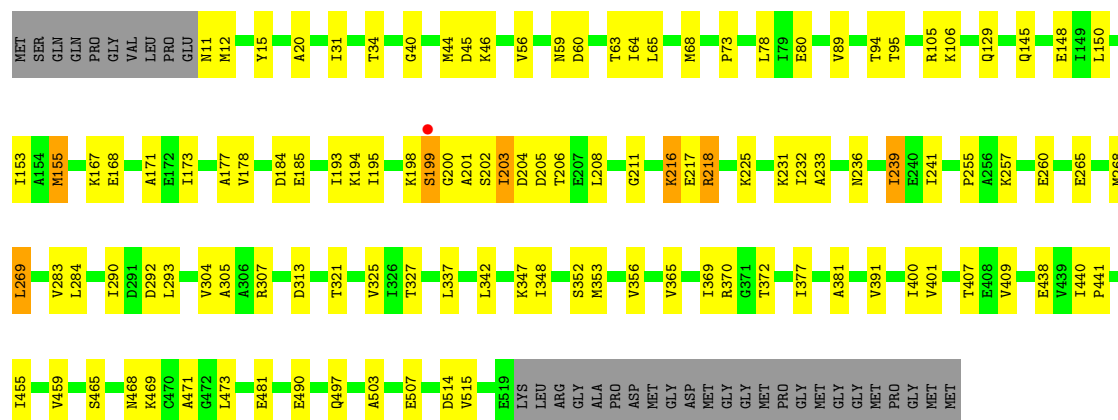
- Molecule 1: Chaperonin

Chain E:  71% 21% • 6%



- Molecule 1: Chaperonin

Chain F:  72% 20% • 6%



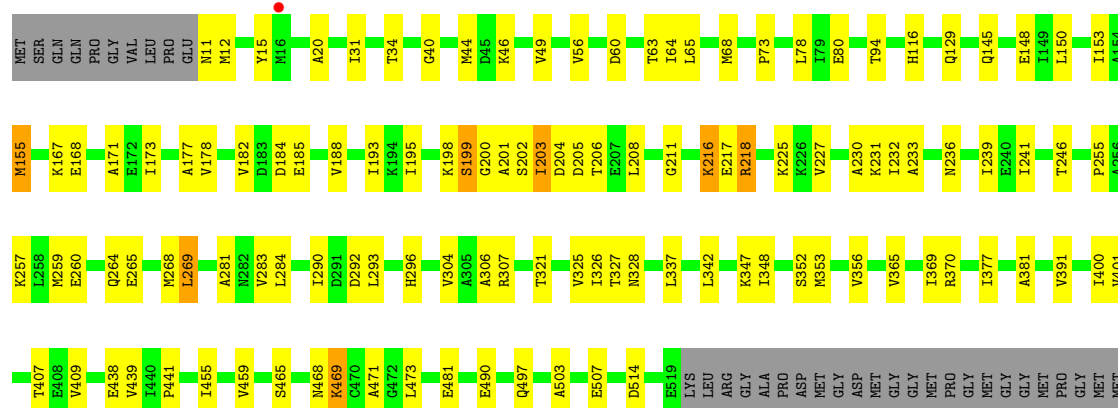
- Molecule 1: Chaperonin

Chain G:  74% 19% • 6%



- Molecule 1: Chaperonin

Chain H:  72% 21% • 6%



## 4 Data and refinement statistics

| Property                                                                | Value                                                                  | Source           |
|-------------------------------------------------------------------------|------------------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                                | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 260.69Å 162.22Å 184.73Å<br>90.00° 135.05° 90.00°                       | Depositor        |
| Resolution (Å)                                                          | 48.84 – 3.20<br>48.84 – 3.20                                           | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.5 (48.84-3.20)<br>93.8 (48.84-3.20)                                 | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.15 (at 3.19Å)                                                        | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.4_162)                                        | Depositor        |
| R, $R_{free}$                                                           | 0.210 , 0.239<br>0.209 , 0.233                                         | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4193 reflections (5.00%)                                               | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.2                                                                   | Xtriage          |
| Anisotropy                                                              | 0.135                                                                  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 81.1                                                            | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$            | Xtriage          |
| Estimated twinning fraction                                             | 0.002 for -h-2*1,k,h+1<br>0.003 for h,-k,-h-l<br>0.387 for h+2*1,-k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                                   | EDS              |
| Total number of atoms                                                   | 30816                                                                  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 92.0                                                                   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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     | 0.65         | 1/3842 (0.0%)  | 0.91        | 7/5169 (0.1%)   |
| 1   | B     | 0.61         | 0/3842         | 0.90        | 5/5169 (0.1%)   |
| 1   | C     | 0.63         | 0/3842         | 0.92        | 5/5169 (0.1%)   |
| 1   | D     | 0.61         | 0/3842         | 0.91        | 5/5169 (0.1%)   |
| 1   | E     | 0.64         | 1/3842 (0.0%)  | 0.92        | 7/5169 (0.1%)   |
| 1   | F     | 0.62         | 0/3842         | 0.90        | 5/5169 (0.1%)   |
| 1   | G     | 0.63         | 0/3842         | 0.91        | 4/5169 (0.1%)   |
| 1   | H     | 0.60         | 0/3842         | 0.90        | 5/5169 (0.1%)   |
| All | All   | 0.62         | 2/30736 (0.0%) | 0.91        | 43/41352 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | E     | 145 | GLN  | CA-CB | 5.61 | 1.60        | 1.53     |
| 1   | A     | 145 | GLN  | CA-CB | 5.38 | 1.60        | 1.53     |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 40  | GLY  | CA-C-N | 8.11 | 127.78      | 119.19   |
| 1   | B     | 40  | GLY  | C-N-CA | 8.11 | 127.78      | 119.19   |
| 1   | H     | 40  | GLY  | CA-C-N | 7.77 | 127.43      | 119.19   |
| 1   | H     | 40  | GLY  | C-N-CA | 7.77 | 127.43      | 119.19   |
| 1   | F     | 40  | GLY  | CA-C-N | 7.70 | 127.35      | 119.19   |
| 1   | F     | 40  | GLY  | C-N-CA | 7.70 | 127.35      | 119.19   |
| 1   | C     | 40  | GLY  | CA-C-N | 7.67 | 127.33      | 119.19   |
| 1   | C     | 40  | GLY  | C-N-CA | 7.67 | 127.33      | 119.19   |
| 1   | E     | 40  | GLY  | CA-C-N | 7.64 | 127.29      | 119.19   |
| 1   | E     | 40  | GLY  | C-N-CA | 7.64 | 127.29      | 119.19   |
| 1   | D     | 40  | GLY  | CA-C-N | 7.57 | 127.22      | 119.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 40  | GLY  | C-N-CA   | 7.57  | 127.22      | 119.19   |
| 1   | G     | 40  | GLY  | CA-C-N   | 7.48  | 127.11      | 119.19   |
| 1   | G     | 40  | GLY  | C-N-CA   | 7.48  | 127.11      | 119.19   |
| 1   | A     | 40  | GLY  | CA-C-N   | 7.41  | 127.04      | 119.19   |
| 1   | A     | 40  | GLY  | C-N-CA   | 7.41  | 127.04      | 119.19   |
| 1   | E     | 145 | GLN  | CB-CA-C  | -6.35 | 101.25      | 111.28   |
| 1   | C     | 372 | THR  | N-CA-C   | 6.23  | 118.15      | 111.36   |
| 1   | H     | 200 | GLY  | CA-C-O   | -6.14 | 117.67      | 122.52   |
| 1   | E     | 200 | GLY  | CA-C-O   | -6.07 | 117.73      | 122.52   |
| 1   | A     | 145 | GLN  | CB-CA-C  | -5.97 | 101.85      | 111.28   |
| 1   | A     | 89  | VAL  | N-CA-C   | 5.78  | 116.19      | 111.62   |
| 1   | B     | 372 | THR  | N-CA-C   | 5.76  | 117.64      | 111.36   |
| 1   | D     | 200 | GLY  | CA-C-O   | -5.75 | 117.98      | 122.52   |
| 1   | E     | 160 | GLY  | N-CA-C   | -5.74 | 107.07      | 113.79   |
| 1   | E     | 372 | THR  | N-CA-C   | 5.64  | 117.51      | 111.36   |
| 1   | H     | 116 | HIS  | CA-C-N   | 5.57  | 125.41      | 119.28   |
| 1   | H     | 116 | HIS  | C-N-CA   | 5.57  | 125.41      | 119.28   |
| 1   | D     | 116 | HIS  | CA-C-N   | 5.51  | 125.34      | 119.28   |
| 1   | D     | 116 | HIS  | C-N-CA   | 5.51  | 125.34      | 119.28   |
| 1   | A     | 372 | THR  | N-CA-C   | 5.45  | 117.30      | 111.36   |
| 1   | C     | 200 | GLY  | CA-C-O   | -5.29 | 118.34      | 122.52   |
| 1   | A     | 200 | GLY  | CA-C-O   | -5.25 | 118.37      | 122.52   |
| 1   | A     | 56  | VAL  | N-CA-C   | 5.22  | 115.49      | 107.77   |
| 1   | C     | 185 | GLU  | CB-CG-CD | 5.20  | 121.44      | 112.60   |
| 1   | F     | 372 | THR  | N-CA-C   | 5.19  | 117.02      | 111.36   |
| 1   | F     | 200 | GLY  | CA-C-O   | -5.16 | 118.44      | 122.52   |
| 1   | B     | 161 | LYS  | N-CA-C   | -5.12 | 107.04      | 113.28   |
| 1   | G     | 185 | GLU  | CB-CG-CD | 5.10  | 121.28      | 112.60   |
| 1   | G     | 89  | VAL  | N-CA-C   | 5.08  | 115.64      | 111.62   |
| 1   | F     | 89  | VAL  | N-CA-C   | 5.06  | 115.62      | 111.62   |
| 1   | E     | 161 | LYS  | N-CA-C   | -5.05 | 107.12      | 113.28   |
| 1   | B     | 200 | GLY  | CA-C-O   | -5.00 | 118.57      | 122.52   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3820  | 0        | 3958     | 81      | 2            |
| 1   | B     | 3820  | 0        | 3958     | 82      | 0            |
| 1   | C     | 3820  | 0        | 3958     | 83      | 2            |
| 1   | D     | 3820  | 0        | 3958     | 89      | 0            |
| 1   | E     | 3820  | 0        | 3958     | 82      | 2            |
| 1   | F     | 3820  | 0        | 3958     | 80      | 0            |
| 1   | G     | 3820  | 0        | 3958     | 83      | 2            |
| 1   | H     | 3820  | 0        | 3958     | 88      | 0            |
| 2   | A     | 31    | 0        | 13       | 2       | 0            |
| 2   | B     | 31    | 0        | 13       | 4       | 0            |
| 2   | C     | 31    | 0        | 13       | 4       | 0            |
| 2   | D     | 31    | 0        | 13       | 4       | 0            |
| 2   | E     | 31    | 0        | 13       | 4       | 0            |
| 2   | F     | 31    | 0        | 13       | 3       | 0            |
| 2   | G     | 31    | 0        | 13       | 3       | 0            |
| 2   | H     | 31    | 0        | 13       | 2       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 30816 | 0        | 31768    | 611     | 4            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (611) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:206:THR:HG22 | 1:B:370:ARG:H   | 1.17                     | 1.09              |
| 1:H:206:THR:HG22 | 1:H:370:ARG:H   | 1.18                     | 1.08              |
| 1:E:206:THR:HG22 | 1:E:370:ARG:H   | 1.17                     | 1.08              |
| 1:A:206:THR:HG22 | 1:A:370:ARG:H   | 1.20                     | 1.07              |
| 1:C:206:THR:HG22 | 1:C:370:ARG:H   | 1.16                     | 1.05              |
| 1:D:206:THR:HG22 | 1:D:370:ARG:H   | 1.17                     | 1.05              |
| 1:F:206:THR:HG22 | 1:F:370:ARG:H   | 1.18                     | 1.04              |
| 1:G:206:THR:HG22 | 1:G:370:ARG:H   | 1.18                     | 1.02              |
| 1:E:201:ALA:HB2  | 1:F:497:GLN:OE1 | 1.64                     | 0.97              |
| 1:G:490:GLU:OE2  | 2:G:544:ANP:O2' | 1.84                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:490:GLU:OE2  | 2:E:544:ANP:O2'  | 1.86                     | 0.94              |
| 1:B:490:GLU:OE2  | 2:B:544:ANP:O2'  | 1.85                     | 0.94              |
| 1:A:201:ALA:HB2  | 1:B:497:GLN:OE1  | 1.66                     | 0.93              |
| 1:C:490:GLU:OE2  | 2:C:544:ANP:O2'  | 1.85                     | 0.93              |
| 1:A:490:GLU:OE2  | 2:A:544:ANP:O2'  | 1.86                     | 0.93              |
| 1:H:490:GLU:OE2  | 2:H:544:ANP:O2'  | 1.84                     | 0.93              |
| 1:D:490:GLU:OE2  | 2:D:544:ANP:O2'  | 1.86                     | 0.93              |
| 1:F:490:GLU:OE2  | 2:F:544:ANP:O2'  | 1.86                     | 0.91              |
| 1:C:201:ALA:HB2  | 1:D:497:GLN:OE1  | 1.78                     | 0.83              |
| 1:G:201:ALA:HB2  | 1:H:497:GLN:OE1  | 1.79                     | 0.82              |
| 1:A:497:GLN:OE1  | 1:H:201:ALA:HB2  | 1.81                     | 0.81              |
| 1:C:206:THR:HG22 | 1:C:370:ARG:N    | 1.95                     | 0.81              |
| 1:B:218:ARG:NH1  | 1:B:225:LYS:HB2  | 1.97                     | 0.79              |
| 1:G:206:THR:HG22 | 1:G:370:ARG:N    | 1.97                     | 0.79              |
| 1:H:206:THR:HG22 | 1:H:370:ARG:N    | 1.98                     | 0.78              |
| 1:E:206:THR:HG22 | 1:E:370:ARG:N    | 1.97                     | 0.78              |
| 1:F:206:THR:HG22 | 1:F:370:ARG:N    | 1.98                     | 0.77              |
| 1:G:258:LEU:HD12 | 1:H:264:GLN:HG2  | 1.66                     | 0.77              |
| 1:F:218:ARG:NH1  | 1:F:225:LYS:HB2  | 2.00                     | 0.77              |
| 1:H:218:ARG:NH1  | 1:H:225:LYS:HB2  | 2.00                     | 0.77              |
| 1:A:206:THR:HG22 | 1:A:370:ARG:N    | 1.99                     | 0.76              |
| 1:B:201:ALA:HB2  | 1:C:497:GLN:OE1  | 1.84                     | 0.76              |
| 1:C:218:ARG:NH1  | 1:C:225:LYS:HB2  | 2.00                     | 0.76              |
| 1:E:216:LYS:HD2  | 1:E:307:ARG:O    | 1.85                     | 0.76              |
| 1:C:216:LYS:HD2  | 1:C:307:ARG:O    | 1.85                     | 0.76              |
| 1:B:206:THR:HG22 | 1:B:370:ARG:N    | 1.97                     | 0.76              |
| 1:D:218:ARG:NH1  | 1:D:225:LYS:HB2  | 2.00                     | 0.76              |
| 1:D:201:ALA:HB2  | 1:E:497:GLN:OE1  | 1.85                     | 0.76              |
| 1:G:218:ARG:NH1  | 1:G:225:LYS:HB2  | 2.00                     | 0.76              |
| 1:D:153:ILE:HD11 | 1:D:400:ILE:HG21 | 1.67                     | 0.75              |
| 1:D:206:THR:HG22 | 1:D:370:ARG:N    | 1.97                     | 0.75              |
| 1:A:218:ARG:NH1  | 1:A:225:LYS:HB2  | 2.01                     | 0.75              |
| 1:F:216:LYS:HD2  | 1:F:307:ARG:O    | 1.87                     | 0.75              |
| 1:E:218:ARG:NH1  | 1:E:225:LYS:HB2  | 2.01                     | 0.74              |
| 1:G:216:LYS:HD2  | 1:G:307:ARG:O    | 1.88                     | 0.74              |
| 1:C:206:THR:CG2  | 1:C:370:ARG:H    | 1.96                     | 0.74              |
| 1:D:401:VAL:HB   | 1:D:407:THR:HG21 | 1.68                     | 0.74              |
| 1:A:216:LYS:HD2  | 1:A:307:ARG:O    | 1.87                     | 0.73              |
| 1:D:216:LYS:HD2  | 1:D:307:ARG:O    | 1.87                     | 0.72              |
| 1:H:153:ILE:HD11 | 1:H:400:ILE:HG21 | 1.71                     | 0.72              |
| 1:A:153:ILE:HD11 | 1:A:400:ILE:HG21 | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:216:LYS:HD2  | 1:B:307:ARG:O    | 1.88                     | 0.72              |
| 1:H:401:VAL:HB   | 1:H:407:THR:HG21 | 1.69                     | 0.72              |
| 1:B:206:THR:CG2  | 1:B:370:ARG:H    | 1.98                     | 0.72              |
| 1:H:216:LYS:HD2  | 1:H:307:ARG:O    | 1.89                     | 0.72              |
| 1:B:153:ILE:HD11 | 1:B:400:ILE:HG21 | 1.72                     | 0.71              |
| 1:B:468:ASN:O    | 1:B:469:LYS:HB3  | 1.90                     | 0.71              |
| 1:F:206:THR:CG2  | 1:F:370:ARG:H    | 2.01                     | 0.71              |
| 1:F:468:ASN:O    | 1:F:469:LYS:HB3  | 1.91                     | 0.71              |
| 1:G:153:ILE:HD11 | 1:G:400:ILE:HG21 | 1.72                     | 0.71              |
| 1:B:218:ARG:HH12 | 1:B:225:LYS:HB2  | 1.57                     | 0.70              |
| 1:E:468:ASN:O    | 1:E:469:LYS:HB3  | 1.91                     | 0.70              |
| 1:A:401:VAL:HB   | 1:A:407:THR:HG21 | 1.74                     | 0.70              |
| 1:C:258:LEU:HD12 | 1:D:264:GLN:HG2  | 1.72                     | 0.70              |
| 1:A:206:THR:CG2  | 1:A:370:ARG:H    | 2.02                     | 0.69              |
| 1:D:206:THR:CG2  | 1:D:370:ARG:H    | 2.01                     | 0.69              |
| 1:H:206:THR:CG2  | 1:H:370:ARG:H    | 2.01                     | 0.69              |
| 1:E:401:VAL:HB   | 1:E:407:THR:HG21 | 1.74                     | 0.69              |
| 1:C:468:ASN:O    | 1:C:469:LYS:HB3  | 1.91                     | 0.69              |
| 1:F:201:ALA:HB2  | 1:G:497:GLN:OE1  | 1.92                     | 0.69              |
| 1:E:206:THR:CG2  | 1:E:370:ARG:H    | 2.00                     | 0.69              |
| 1:G:401:VAL:HB   | 1:G:407:THR:HG21 | 1.74                     | 0.69              |
| 1:C:153:ILE:HD11 | 1:C:400:ILE:HG21 | 1.73                     | 0.69              |
| 1:A:201:ALA:HB2  | 1:B:497:GLN:CD   | 2.18                     | 0.68              |
| 1:H:468:ASN:O    | 1:H:469:LYS:HB3  | 1.92                     | 0.68              |
| 1:A:468:ASN:O    | 1:A:469:LYS:HB3  | 1.91                     | 0.68              |
| 1:G:206:THR:CG2  | 1:G:370:ARG:H    | 1.99                     | 0.68              |
| 1:G:468:ASN:O    | 1:G:469:LYS:HB3  | 1.92                     | 0.68              |
| 1:F:401:VAL:HB   | 1:F:407:THR:HG21 | 1.74                     | 0.68              |
| 1:F:153:ILE:HD11 | 1:F:400:ILE:HG21 | 1.75                     | 0.68              |
| 1:E:153:ILE:HD11 | 1:E:400:ILE:HG21 | 1.76                     | 0.68              |
| 1:C:401:VAL:HB   | 1:C:407:THR:HG21 | 1.76                     | 0.67              |
| 1:H:46:LYS:HG3   | 1:H:64:ILE:HD13  | 1.77                     | 0.67              |
| 1:B:401:VAL:HB   | 1:B:407:THR:HG21 | 1.75                     | 0.67              |
| 1:G:469:LYS:O    | 1:G:469:LYS:HG2  | 1.94                     | 0.67              |
| 1:B:469:LYS:O    | 1:B:469:LYS:HG2  | 1.95                     | 0.67              |
| 1:D:468:ASN:O    | 1:D:469:LYS:HB3  | 1.92                     | 0.67              |
| 1:F:173:ILE:HG23 | 1:F:208:LEU:HB2  | 1.78                     | 0.66              |
| 1:A:173:ILE:HG23 | 1:A:208:LEU:HB2  | 1.77                     | 0.66              |
| 1:D:34:THR:O     | 1:D:46:LYS:HE3   | 1.96                     | 0.66              |
| 1:B:34:THR:O     | 1:B:46:LYS:HE3   | 1.96                     | 0.66              |
| 1:E:201:ALA:HB2  | 1:F:497:GLN:CD   | 2.21                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:218:ARG:HH12 | 1:E:225:LYS:HB2  | 1.61                     | 0.66              |
| 1:F:469:LYS:HG2  | 1:F:469:LYS:O    | 1.95                     | 0.66              |
| 1:H:34:THR:O     | 1:H:46:LYS:HE3   | 1.96                     | 0.65              |
| 1:C:173:ILE:HG23 | 1:C:208:LEU:HB2  | 1.78                     | 0.65              |
| 1:E:46:LYS:HD3   | 1:F:514:ASP:HB3  | 1.77                     | 0.65              |
| 1:G:34:THR:O     | 1:G:46:LYS:HE3   | 1.97                     | 0.65              |
| 1:C:469:LYS:O    | 1:C:469:LYS:HG2  | 1.95                     | 0.65              |
| 1:A:46:LYS:HD3   | 1:B:514:ASP:HB3  | 1.78                     | 0.65              |
| 1:C:34:THR:O     | 1:C:46:LYS:HE3   | 1.97                     | 0.64              |
| 1:C:218:ARG:HH12 | 1:C:225:LYS:HB2  | 1.62                     | 0.64              |
| 1:C:258:LEU:HB3  | 1:D:268:MET:HE1  | 1.78                     | 0.64              |
| 1:E:173:ILE:HG23 | 1:E:208:LEU:HB2  | 1.77                     | 0.64              |
| 1:H:177:ALA:HB2  | 1:H:208:LEU:HD13 | 1.79                     | 0.64              |
| 1:A:34:THR:O     | 1:A:46:LYS:HE3   | 1.98                     | 0.64              |
| 1:G:258:LEU:HB3  | 1:H:268:MET:HE1  | 1.79                     | 0.64              |
| 1:A:218:ARG:HH12 | 1:A:225:LYS:HB2  | 1.62                     | 0.64              |
| 1:A:469:LYS:HG2  | 1:A:469:LYS:O    | 1.98                     | 0.64              |
| 1:C:257:LYS:HD3  | 1:C:260:GLU:OE1  | 1.98                     | 0.64              |
| 1:D:177:ALA:HB2  | 1:D:208:LEU:HD13 | 1.79                     | 0.64              |
| 1:H:218:ARG:HH12 | 1:H:225:LYS:HB2  | 1.62                     | 0.64              |
| 1:F:34:THR:O     | 1:F:46:LYS:HE3   | 1.98                     | 0.64              |
| 1:E:469:LYS:O    | 1:E:469:LYS:HG2  | 1.96                     | 0.64              |
| 1:F:218:ARG:HH12 | 1:F:225:LYS:HB2  | 1.60                     | 0.63              |
| 1:G:218:ARG:HH12 | 1:G:225:LYS:HB2  | 1.61                     | 0.63              |
| 1:H:173:ILE:HG23 | 1:H:208:LEU:HB2  | 1.81                     | 0.63              |
| 1:F:257:LYS:HD3  | 1:F:260:GLU:OE1  | 1.99                     | 0.63              |
| 1:A:257:LYS:HD3  | 1:A:260:GLU:OE1  | 1.99                     | 0.62              |
| 1:E:34:THR:O     | 1:E:46:LYS:HE3   | 1.97                     | 0.62              |
| 1:D:46:LYS:HG3   | 1:D:64:ILE:HD13  | 1.81                     | 0.62              |
| 1:E:225:LYS:HG2  | 1:E:225:LYS:O    | 1.99                     | 0.62              |
| 1:G:177:ALA:HB2  | 1:G:208:LEU:HD13 | 1.81                     | 0.62              |
| 1:B:257:LYS:HD3  | 1:B:260:GLU:OE1  | 2.00                     | 0.62              |
| 1:F:60:ASP:HB3   | 1:F:63:THR:OG1   | 2.00                     | 0.62              |
| 1:G:173:ILE:HG23 | 1:G:208:LEU:HB2  | 1.82                     | 0.61              |
| 1:B:173:ILE:HG23 | 1:B:208:LEU:HB2  | 1.80                     | 0.61              |
| 1:D:218:ARG:HH12 | 1:D:225:LYS:HB2  | 1.62                     | 0.61              |
| 1:C:46:LYS:HG3   | 1:C:64:ILE:HD13  | 1.82                     | 0.61              |
| 1:D:257:LYS:HD3  | 1:D:260:GLU:OE1  | 2.00                     | 0.61              |
| 1:E:257:LYS:HD3  | 1:E:260:GLU:OE1  | 2.00                     | 0.61              |
| 1:G:46:LYS:HG3   | 1:G:64:ILE:HD13  | 1.81                     | 0.61              |
| 1:E:60:ASP:HB3   | 1:E:63:THR:OG1   | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:257:LYS:HD3  | 1:H:260:GLU:OE1  | 2.00                     | 0.61              |
| 1:B:46:LYS:HD3   | 1:C:514:ASP:HB3  | 1.82                     | 0.61              |
| 1:G:257:LYS:HD3  | 1:G:260:GLU:OE1  | 2.01                     | 0.61              |
| 1:B:216:LYS:HE3  | 1:B:217:GLU:H    | 1.66                     | 0.61              |
| 1:D:173:ILE:HG23 | 1:D:208:LEU:HB2  | 1.82                     | 0.60              |
| 1:A:216:LYS:HE3  | 1:A:217:GLU:H    | 1.66                     | 0.60              |
| 1:A:60:ASP:HB3   | 1:A:63:THR:OG1   | 2.02                     | 0.60              |
| 1:B:60:ASP:HB3   | 1:B:63:THR:OG1   | 2.02                     | 0.60              |
| 1:D:259:MET:HG2  | 1:E:268:MET:HE2  | 1.83                     | 0.60              |
| 1:D:60:ASP:HB3   | 1:D:63:THR:OG1   | 2.02                     | 0.59              |
| 1:G:216:LYS:HE3  | 1:G:217:GLU:H    | 1.67                     | 0.59              |
| 1:F:216:LYS:HE3  | 1:F:217:GLU:H    | 1.67                     | 0.59              |
| 1:H:216:LYS:HE3  | 1:H:217:GLU:H    | 1.67                     | 0.59              |
| 1:C:177:ALA:HB2  | 1:C:208:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:225:LYS:O    | 1:A:225:LYS:HG2  | 2.02                     | 0.59              |
| 1:A:177:ALA:HB2  | 1:A:208:LEU:HD13 | 1.84                     | 0.59              |
| 1:H:469:LYS:O    | 1:H:469:LYS:HG2  | 2.02                     | 0.59              |
| 1:G:218:ARG:HH12 | 1:G:225:LYS:HE2  | 1.68                     | 0.59              |
| 1:F:46:LYS:HG3   | 1:F:64:ILE:HD13  | 1.85                     | 0.58              |
| 1:F:177:ALA:HB2  | 1:F:208:LEU:HD13 | 1.86                     | 0.58              |
| 1:F:503:ALA:O    | 1:F:507:GLU:HG3  | 2.03                     | 0.58              |
| 1:D:469:LYS:O    | 1:D:469:LYS:HG2  | 2.02                     | 0.58              |
| 1:B:503:ALA:O    | 1:B:507:GLU:HG3  | 2.04                     | 0.58              |
| 1:C:216:LYS:HE3  | 1:C:217:GLU:H    | 1.69                     | 0.58              |
| 1:A:268:MET:HE2  | 1:H:259:MET:HG2  | 1.86                     | 0.57              |
| 1:G:202:SER:C    | 1:G:204:ASP:H    | 2.12                     | 0.57              |
| 1:B:455:ILE:HG21 | 1:B:473:LEU:HD22 | 1.87                     | 0.57              |
| 1:C:202:SER:C    | 1:C:204:ASP:H    | 2.13                     | 0.57              |
| 1:E:46:LYS:HG3   | 1:E:64:ILE:HD13  | 1.86                     | 0.57              |
| 1:E:216:LYS:HE3  | 1:E:217:GLU:H    | 1.70                     | 0.57              |
| 1:H:60:ASP:HB3   | 1:H:63:THR:OG1   | 2.05                     | 0.57              |
| 1:A:46:LYS:HG3   | 1:A:64:ILE:HD13  | 1.86                     | 0.57              |
| 1:E:177:ALA:HB2  | 1:E:208:LEU:HD13 | 1.86                     | 0.57              |
| 1:F:438:GLU:C    | 1:F:441:PRO:HD2  | 2.30                     | 0.57              |
| 1:C:218:ARG:HH12 | 1:C:225:LYS:HE2  | 1.69                     | 0.57              |
| 1:C:503:ALA:O    | 1:C:507:GLU:HG3  | 2.05                     | 0.57              |
| 1:H:225:LYS:O    | 1:H:225:LYS:HG2  | 2.05                     | 0.57              |
| 1:C:60:ASP:HB3   | 1:C:63:THR:OG1   | 2.05                     | 0.56              |
| 1:D:225:LYS:O    | 1:D:225:LYS:HG2  | 2.04                     | 0.56              |
| 1:H:231:LYS:HD2  | 1:H:231:LYS:N    | 2.21                     | 0.56              |
| 1:D:216:LYS:HE3  | 1:D:217:GLU:H    | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:307:ARG:HG3  | 1:H:307:ARG:HH11 | 1.70                     | 0.56              |
| 1:F:46:LYS:HD3   | 1:G:514:ASP:HB3  | 1.86                     | 0.56              |
| 1:G:225:LYS:O    | 1:G:225:LYS:HG2  | 2.05                     | 0.56              |
| 1:C:46:LYS:HD3   | 1:D:514:ASP:HB3  | 1.87                     | 0.56              |
| 1:G:231:LYS:HD2  | 1:G:231:LYS:N    | 2.21                     | 0.55              |
| 1:A:503:ALA:O    | 1:A:507:GLU:HG3  | 2.07                     | 0.55              |
| 1:C:307:ARG:HG3  | 1:C:307:ARG:HH11 | 1.71                     | 0.55              |
| 1:G:503:ALA:O    | 1:G:507:GLU:HG3  | 2.05                     | 0.55              |
| 1:G:60:ASP:HB3   | 1:G:63:THR:OG1   | 2.07                     | 0.55              |
| 1:B:307:ARG:HG3  | 1:B:307:ARG:HH11 | 1.72                     | 0.55              |
| 1:E:195:ILE:HG23 | 1:E:369:ILE:HD12 | 1.89                     | 0.55              |
| 1:G:202:SER:OG   | 1:G:205:ASP:HB2  | 2.06                     | 0.55              |
| 1:A:202:SER:C    | 1:A:204:ASP:H    | 2.14                     | 0.55              |
| 1:C:206:THR:HG22 | 1:C:369:ILE:HA   | 1.89                     | 0.55              |
| 1:E:369:ILE:HD13 | 1:E:381:ALA:HA   | 1.89                     | 0.55              |
| 1:B:177:ALA:HB2  | 1:B:208:LEU:HD13 | 1.88                     | 0.55              |
| 1:A:307:ARG:HG3  | 1:A:307:ARG:HH11 | 1.72                     | 0.54              |
| 1:G:307:ARG:HG3  | 1:G:307:ARG:HH11 | 1.72                     | 0.54              |
| 1:C:231:LYS:HD2  | 1:C:231:LYS:N    | 2.23                     | 0.54              |
| 1:D:218:ARG:HH12 | 1:D:225:LYS:HE2  | 1.72                     | 0.54              |
| 1:F:225:LYS:O    | 1:F:225:LYS:HG2  | 2.08                     | 0.54              |
| 1:H:369:ILE:HD13 | 1:H:381:ALA:HA   | 1.89                     | 0.54              |
| 1:B:46:LYS:HG3   | 1:B:64:ILE:HD13  | 1.88                     | 0.54              |
| 1:B:202:SER:C    | 1:B:204:ASP:H    | 2.15                     | 0.54              |
| 1:D:307:ARG:HG3  | 1:D:307:ARG:HH11 | 1.71                     | 0.54              |
| 1:E:307:ARG:HH11 | 1:E:307:ARG:HG3  | 1.71                     | 0.54              |
| 1:F:202:SER:C    | 1:F:204:ASP:H    | 2.14                     | 0.54              |
| 1:F:202:SER:OG   | 1:F:205:ASP:HB2  | 2.08                     | 0.54              |
| 1:A:231:LYS:HD2  | 1:A:231:LYS:N    | 2.23                     | 0.54              |
| 1:C:202:SER:OG   | 1:C:205:ASP:HB2  | 2.07                     | 0.54              |
| 1:G:95:THR:HG23  | 2:G:544:ANP:O2B  | 2.08                     | 0.54              |
| 1:D:455:ILE:HG21 | 1:D:473:LEU:HD22 | 1.90                     | 0.54              |
| 1:H:65:LEU:HD23  | 1:H:68:MET:HE2   | 1.90                     | 0.54              |
| 1:H:202:SER:C    | 1:H:204:ASP:H    | 2.16                     | 0.54              |
| 1:B:195:ILE:HG23 | 1:B:369:ILE:HD12 | 1.90                     | 0.54              |
| 1:D:231:LYS:N    | 1:D:231:LYS:HD2  | 2.23                     | 0.54              |
| 1:G:65:LEU:HD23  | 1:G:68:MET:HE2   | 1.89                     | 0.54              |
| 1:H:202:SER:OG   | 1:H:205:ASP:HB2  | 2.07                     | 0.54              |
| 1:E:202:SER:C    | 1:E:204:ASP:H    | 2.16                     | 0.54              |
| 1:H:503:ALA:O    | 1:H:507:GLU:HG3  | 2.08                     | 0.54              |
| 1:D:202:SER:C    | 1:D:204:ASP:H    | 2.16                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:195:ILE:HG23 | 1:G:369:ILE:HD12 | 1.89                     | 0.54              |
| 1:H:232:ILE:HD12 | 1:H:321:THR:HG21 | 1.90                     | 0.54              |
| 1:G:206:THR:HG22 | 1:G:369:ILE:HA   | 1.90                     | 0.53              |
| 1:D:195:ILE:HG23 | 1:D:369:ILE:HD12 | 1.90                     | 0.53              |
| 1:B:438:GLU:C    | 1:B:441:PRO:HD2  | 2.32                     | 0.53              |
| 1:D:46:LYS:HD3   | 1:E:514:ASP:HB3  | 1.89                     | 0.53              |
| 1:F:369:ILE:HD13 | 1:F:381:ALA:HA   | 1.90                     | 0.53              |
| 1:B:65:LEU:HD23  | 1:B:68:MET:HE2   | 1.89                     | 0.53              |
| 1:B:225:LYS:O    | 1:B:225:LYS:HG2  | 2.08                     | 0.53              |
| 1:C:31:ILE:HD11  | 1:C:78:LEU:HB3   | 1.89                     | 0.53              |
| 1:D:202:SER:OG   | 1:D:205:ASP:HB2  | 2.08                     | 0.53              |
| 1:E:218:ARG:HH12 | 1:E:225:LYS:HE2  | 1.74                     | 0.53              |
| 1:C:49:VAL:HG21  | 1:D:73:PRO:HG3   | 1.89                     | 0.53              |
| 1:E:455:ILE:HG21 | 1:E:473:LEU:HD22 | 1.91                     | 0.53              |
| 1:C:455:ILE:HG21 | 1:C:473:LEU:HD22 | 1.91                     | 0.53              |
| 1:E:202:SER:OG   | 1:E:205:ASP:HB2  | 2.08                     | 0.53              |
| 1:F:307:ARG:HG3  | 1:F:307:ARG:HH11 | 1.72                     | 0.53              |
| 1:F:65:LEU:HD23  | 1:F:68:MET:HE2   | 1.90                     | 0.53              |
| 1:F:455:ILE:HG21 | 1:F:473:LEU:HD22 | 1.91                     | 0.53              |
| 1:G:31:ILE:HD11  | 1:G:78:LEU:HB3   | 1.90                     | 0.53              |
| 1:B:202:SER:OG   | 1:B:205:ASP:HB2  | 2.08                     | 0.52              |
| 1:C:195:ILE:HG23 | 1:C:369:ILE:HD12 | 1.91                     | 0.52              |
| 1:C:225:LYS:O    | 1:C:225:LYS:HG2  | 2.08                     | 0.52              |
| 1:F:218:ARG:HH12 | 1:F:225:LYS:HE2  | 1.74                     | 0.52              |
| 1:A:195:ILE:HG23 | 1:A:369:ILE:HD12 | 1.91                     | 0.52              |
| 1:B:198:LYS:HE3  | 1:B:353:MET:HE1  | 1.91                     | 0.52              |
| 1:B:231:LYS:HD2  | 1:B:231:LYS:N    | 2.25                     | 0.52              |
| 1:H:218:ARG:HH12 | 1:H:225:LYS:HE2  | 1.72                     | 0.52              |
| 1:B:31:ILE:HD11  | 1:B:78:LEU:HB3   | 1.91                     | 0.52              |
| 1:E:231:LYS:HD2  | 1:E:231:LYS:N    | 2.24                     | 0.52              |
| 1:D:232:ILE:HD12 | 1:D:321:THR:HG21 | 1.90                     | 0.52              |
| 1:A:218:ARG:HH12 | 1:A:225:LYS:HE2  | 1.75                     | 0.52              |
| 1:E:503:ALA:O    | 1:E:507:GLU:HG3  | 2.08                     | 0.52              |
| 1:H:31:ILE:HD11  | 1:H:78:LEU:HB3   | 1.92                     | 0.52              |
| 1:A:202:SER:OG   | 1:A:205:ASP:HB2  | 2.08                     | 0.52              |
| 1:A:206:THR:HG22 | 1:A:369:ILE:HA   | 1.92                     | 0.52              |
| 1:C:369:ILE:HD13 | 1:C:381:ALA:HA   | 1.92                     | 0.52              |
| 1:B:218:ARG:HH12 | 1:B:225:LYS:HE2  | 1.75                     | 0.52              |
| 1:H:455:ILE:HG21 | 1:H:473:LEU:HD22 | 1.91                     | 0.52              |
| 1:G:49:VAL:HG21  | 1:H:73:PRO:HG3   | 1.92                     | 0.52              |
| 1:G:369:ILE:HD13 | 1:G:381:ALA:HA   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:231:LYS:HD2  | 1:H:231:LYS:H    | 1.75                     | 0.52              |
| 1:B:369:ILE:HD13 | 1:B:381:ALA:HA   | 1.92                     | 0.51              |
| 1:C:65:LEU:HD23  | 1:C:68:MET:HE2   | 1.91                     | 0.51              |
| 1:D:369:ILE:HD13 | 1:D:381:ALA:HA   | 1.91                     | 0.51              |
| 1:G:455:ILE:HG21 | 1:G:473:LEU:HD22 | 1.92                     | 0.51              |
| 1:D:15:TYR:O     | 1:D:20:ALA:HB2   | 2.11                     | 0.51              |
| 1:D:49:VAL:HG21  | 1:E:73:PRO:HG3   | 1.91                     | 0.51              |
| 1:F:94:THR:H     | 2:F:544:ANP:HNB1 | 1.59                     | 0.51              |
| 1:D:503:ALA:O    | 1:D:507:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:56:VAL:HG13  | 1:B:56:VAL:O     | 2.10                     | 0.51              |
| 1:E:56:VAL:O     | 1:E:56:VAL:HG13  | 2.11                     | 0.51              |
| 1:B:201:ALA:HB2  | 1:C:497:GLN:CD   | 2.35                     | 0.51              |
| 1:D:150:LEU:HD22 | 1:D:391:VAL:HG13 | 1.93                     | 0.51              |
| 1:G:232:ILE:HD12 | 1:G:321:THR:HG21 | 1.92                     | 0.51              |
| 1:H:198:LYS:HE3  | 1:H:353:MET:HE1  | 1.93                     | 0.51              |
| 1:A:73:PRO:HG3   | 1:H:49:VAL:HG21  | 1.93                     | 0.51              |
| 1:A:178:VAL:HA   | 1:A:193:ILE:HD11 | 1.93                     | 0.51              |
| 1:A:369:ILE:HD13 | 1:A:381:ALA:HA   | 1.92                     | 0.50              |
| 1:A:455:ILE:HG21 | 1:A:473:LEU:HD22 | 1.93                     | 0.50              |
| 1:B:206:THR:HG22 | 1:B:369:ILE:HA   | 1.91                     | 0.50              |
| 1:G:94:THR:H     | 2:G:544:ANP:HNB1 | 1.59                     | 0.50              |
| 1:E:150:LEU:HD22 | 1:E:391:VAL:HG13 | 1.93                     | 0.50              |
| 1:G:243:GLU:HG2  | 1:H:246:THR:HG22 | 1.92                     | 0.50              |
| 1:E:15:TYR:O     | 1:E:20:ALA:HB2   | 2.10                     | 0.50              |
| 1:G:241:ILE:HD12 | 1:G:265:GLU:HG2  | 1.92                     | 0.50              |
| 1:D:65:LEU:HD23  | 1:D:68:MET:HE2   | 1.92                     | 0.50              |
| 1:E:206:THR:HG22 | 1:E:369:ILE:HA   | 1.92                     | 0.50              |
| 1:G:231:LYS:HD2  | 1:G:231:LYS:H    | 1.76                     | 0.50              |
| 1:B:94:THR:H     | 2:B:544:ANP:HNB1 | 1.59                     | 0.50              |
| 1:F:178:VAL:HA   | 1:F:193:ILE:HD11 | 1.94                     | 0.50              |
| 1:G:258:LEU:HD12 | 1:H:264:GLN:CG   | 2.40                     | 0.50              |
| 1:D:231:LYS:HD2  | 1:D:231:LYS:H    | 1.75                     | 0.50              |
| 1:H:195:ILE:HG23 | 1:H:369:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:150:LEU:HD22 | 1:A:391:VAL:HG13 | 1.94                     | 0.50              |
| 1:A:438:GLU:C    | 1:A:441:PRO:HD2  | 2.36                     | 0.50              |
| 1:D:94:THR:H     | 2:D:544:ANP:HNB1 | 1.60                     | 0.50              |
| 1:A:239:ILE:HD12 | 1:A:290:ILE:HG12 | 1.94                     | 0.49              |
| 1:D:31:ILE:HD11  | 1:D:78:LEU:HB3   | 1.93                     | 0.49              |
| 1:E:31:ILE:HD11  | 1:E:78:LEU:HB3   | 1.94                     | 0.49              |
| 1:H:56:VAL:HG13  | 1:H:56:VAL:O     | 2.12                     | 0.49              |
| 1:H:199:SER:HA   | 1:H:377:ILE:HD11 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:94:THR:H     | 2:H:544:ANP:HNB1 | 1.58                     | 0.49              |
| 1:A:347:LYS:HG2  | 1:A:352:SER:HB3  | 1.93                     | 0.49              |
| 1:C:94:THR:H     | 2:C:544:ANP:HNB1 | 1.60                     | 0.49              |
| 1:C:241:ILE:HD12 | 1:C:265:GLU:HG2  | 1.94                     | 0.49              |
| 1:E:94:THR:H     | 2:E:544:ANP:HNB1 | 1.60                     | 0.49              |
| 1:E:178:VAL:HA   | 1:E:193:ILE:HD11 | 1.93                     | 0.49              |
| 1:B:178:VAL:HA   | 1:B:193:ILE:HD11 | 1.94                     | 0.49              |
| 1:C:438:GLU:C    | 1:C:441:PRO:HD2  | 2.37                     | 0.49              |
| 1:F:206:THR:HG22 | 1:F:369:ILE:HA   | 1.94                     | 0.49              |
| 1:G:46:LYS:HD3   | 1:H:514:ASP:HB3  | 1.93                     | 0.49              |
| 1:H:438:GLU:C    | 1:H:441:PRO:HD2  | 2.37                     | 0.49              |
| 1:A:15:TYR:O     | 1:A:20:ALA:HB2   | 2.12                     | 0.49              |
| 1:F:231:LYS:HD2  | 1:F:231:LYS:N    | 2.27                     | 0.49              |
| 1:C:232:ILE:HD12 | 1:C:321:THR:HG21 | 1.94                     | 0.49              |
| 1:F:31:ILE:HD11  | 1:F:78:LEU:HB3   | 1.94                     | 0.49              |
| 1:F:195:ILE:HG23 | 1:F:369:ILE:HD12 | 1.92                     | 0.49              |
| 1:G:438:GLU:C    | 1:G:441:PRO:HD2  | 2.37                     | 0.49              |
| 1:F:150:LEU:HD22 | 1:F:391:VAL:HG13 | 1.94                     | 0.49              |
| 1:G:347:LYS:HG2  | 1:G:352:SER:HB3  | 1.94                     | 0.49              |
| 1:B:241:ILE:HD12 | 1:B:265:GLU:HG2  | 1.95                     | 0.49              |
| 1:D:198:LYS:HE3  | 1:D:353:MET:HE1  | 1.95                     | 0.49              |
| 1:F:201:ALA:HB2  | 1:G:497:GLN:CD   | 2.37                     | 0.49              |
| 1:D:206:THR:HG22 | 1:D:369:ILE:HA   | 1.96                     | 0.48              |
| 1:E:199:SER:HA   | 1:E:377:ILE:HD11 | 1.95                     | 0.48              |
| 1:D:155:MET:HE3  | 1:D:171:ALA:HB2  | 1.95                     | 0.48              |
| 1:E:438:GLU:C    | 1:E:441:PRO:HD2  | 2.38                     | 0.48              |
| 1:F:56:VAL:O     | 1:F:56:VAL:HG13  | 2.13                     | 0.48              |
| 1:H:150:LEU:HD22 | 1:H:391:VAL:HG13 | 1.94                     | 0.48              |
| 1:H:233:ALA:HB2  | 1:H:337:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:65:LEU:HD23  | 1:A:68:MET:HE2   | 1.94                     | 0.48              |
| 1:A:94:THR:H     | 2:A:544:ANP:HNB1 | 1.61                     | 0.48              |
| 1:G:56:VAL:O     | 1:G:56:VAL:HG13  | 2.13                     | 0.48              |
| 1:A:231:LYS:HD2  | 1:A:231:LYS:H    | 1.79                     | 0.48              |
| 1:B:199:SER:HA   | 1:B:377:ILE:HD11 | 1.94                     | 0.48              |
| 1:C:373:THR:HB   | 1:D:80:GLU:HB3   | 1.94                     | 0.48              |
| 1:D:438:GLU:C    | 1:D:441:PRO:HD2  | 2.38                     | 0.48              |
| 1:H:206:THR:HG22 | 1:H:369:ILE:HA   | 1.96                     | 0.48              |
| 1:D:199:SER:HA   | 1:D:377:ILE:HD11 | 1.94                     | 0.48              |
| 1:F:198:LYS:HE3  | 1:F:353:MET:HE1  | 1.95                     | 0.48              |
| 1:A:199:SER:HA   | 1:A:377:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:150:LEU:HD22 | 1:B:391:VAL:HG13 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:231:LYS:HD2  | 1:C:231:LYS:H    | 1.79                     | 0.48              |
| 1:E:269:LEU:HD23 | 1:E:293:LEU:HB2  | 1.95                     | 0.48              |
| 1:B:155:MET:HE3  | 1:B:171:ALA:HB2  | 1.96                     | 0.48              |
| 1:C:233:ALA:HB2  | 1:C:337:LEU:HD22 | 1.96                     | 0.48              |
| 1:G:199:SER:HA   | 1:G:377:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:269:LEU:HD23 | 1:A:293:LEU:HB2  | 1.96                     | 0.48              |
| 1:H:239:ILE:HD12 | 1:H:290:ILE:HG12 | 1.95                     | 0.48              |
| 1:H:241:ILE:HD12 | 1:H:265:GLU:HG2  | 1.96                     | 0.48              |
| 1:E:198:LYS:HE3  | 1:E:353:MET:HE1  | 1.96                     | 0.47              |
| 1:A:373:THR:HB   | 1:B:80:GLU:HB3   | 1.96                     | 0.47              |
| 1:E:347:LYS:HG2  | 1:E:352:SER:HB3  | 1.95                     | 0.47              |
| 1:F:232:ILE:HD12 | 1:F:321:THR:HG21 | 1.96                     | 0.47              |
| 1:A:514:ASP:HB3  | 1:H:46:LYS:HD3   | 1.95                     | 0.47              |
| 1:C:257:LYS:HD3  | 1:C:260:GLU:CD   | 2.40                     | 0.47              |
| 1:C:269:LEU:HD23 | 1:C:293:LEU:HB2  | 1.96                     | 0.47              |
| 1:C:347:LYS:HG2  | 1:C:352:SER:HB3  | 1.96                     | 0.47              |
| 1:F:199:SER:HA   | 1:F:377:ILE:HD11 | 1.95                     | 0.47              |
| 1:F:184:ASP:HA   | 1:F:185:GLU:HA   | 1.60                     | 0.47              |
| 1:F:348:ILE:HG23 | 1:F:348:ILE:O    | 2.14                     | 0.47              |
| 1:A:198:LYS:HE3  | 1:A:353:MET:HE1  | 1.96                     | 0.47              |
| 1:B:44:MET:HE2   | 1:B:44:MET:HA    | 1.96                     | 0.47              |
| 1:B:236:ASN:HB2  | 1:B:325:VAL:HG12 | 1.97                     | 0.47              |
| 1:C:56:VAL:O     | 1:C:56:VAL:HG13  | 2.14                     | 0.47              |
| 1:E:20:ALA:HB1   | 1:E:515:VAL:HG23 | 1.97                     | 0.47              |
| 1:E:65:LEU:HD23  | 1:E:68:MET:HE2   | 1.95                     | 0.47              |
| 1:A:56:VAL:HG13  | 1:A:56:VAL:O     | 2.15                     | 0.47              |
| 1:C:199:SER:HA   | 1:C:377:ILE:HD11 | 1.95                     | 0.47              |
| 1:G:348:ILE:HG23 | 1:G:348:ILE:O    | 2.14                     | 0.47              |
| 1:C:95:THR:HG23  | 2:C:544:ANP:O2B  | 2.15                     | 0.47              |
| 1:C:348:ILE:O    | 1:C:348:ILE:HG23 | 2.15                     | 0.47              |
| 1:F:44:MET:HA    | 1:F:44:MET:HE2   | 1.97                     | 0.47              |
| 1:G:198:LYS:HE3  | 1:G:353:MET:HE1  | 1.97                     | 0.47              |
| 1:D:233:ALA:HB2  | 1:D:337:LEU:HD22 | 1.97                     | 0.46              |
| 1:G:15:TYR:O     | 1:G:20:ALA:HB2   | 2.15                     | 0.46              |
| 1:G:211:GLY:HA3  | 1:G:356:VAL:O    | 2.15                     | 0.46              |
| 1:H:178:VAL:HA   | 1:H:193:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:241:ILE:HD12 | 1:A:265:GLU:HG2  | 1.97                     | 0.46              |
| 1:D:257:LYS:HD3  | 1:D:260:GLU:CD   | 2.41                     | 0.46              |
| 1:F:347:LYS:HG2  | 1:F:352:SER:HB3  | 1.97                     | 0.46              |
| 1:A:31:ILE:HD11  | 1:A:78:LEU:HB3   | 1.97                     | 0.46              |
| 1:C:198:LYS:HE3  | 1:C:353:MET:HE1  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:155:MET:HE3  | 1:H:171:ALA:HB2  | 1.98                     | 0.46              |
| 1:C:155:MET:HE1  | 1:C:167:LYS:O    | 2.16                     | 0.46              |
| 1:C:409:VAL:HG11 | 1:C:459:VAL:HG12 | 1.97                     | 0.46              |
| 1:D:239:ILE:HD12 | 1:D:290:ILE:HG12 | 1.97                     | 0.46              |
| 1:G:373:THR:HB   | 1:H:80:GLU:HB3   | 1.96                     | 0.46              |
| 1:A:20:ALA:HB1   | 1:A:515:VAL:HG23 | 1.98                     | 0.46              |
| 1:E:239:ILE:HD12 | 1:E:290:ILE:HG12 | 1.96                     | 0.46              |
| 1:A:497:GLN:CD   | 1:H:201:ALA:HB2  | 2.41                     | 0.46              |
| 1:E:45:ASP:OD1   | 1:E:59:ASN:HB2   | 2.15                     | 0.46              |
| 1:F:269:LEU:HD23 | 1:F:293:LEU:HB2  | 1.98                     | 0.46              |
| 1:G:201:ALA:HB2  | 1:H:497:GLN:CD   | 2.41                     | 0.46              |
| 1:H:347:LYS:HG2  | 1:H:352:SER:HB3  | 1.97                     | 0.46              |
| 1:D:348:ILE:O    | 1:D:348:ILE:HG23 | 2.16                     | 0.46              |
| 1:A:348:ILE:O    | 1:A:348:ILE:HG23 | 2.15                     | 0.46              |
| 1:A:409:VAL:HG11 | 1:A:459:VAL:HG12 | 1.98                     | 0.46              |
| 1:G:257:LYS:HD3  | 1:G:260:GLU:CD   | 2.41                     | 0.46              |
| 1:B:11:ASN:HA    | 1:B:12:MET:HA    | 1.54                     | 0.45              |
| 1:B:239:ILE:HD12 | 1:B:290:ILE:HG12 | 1.98                     | 0.45              |
| 1:B:347:LYS:HG2  | 1:B:352:SER:HB3  | 1.98                     | 0.45              |
| 1:D:11:ASN:HA    | 1:D:12:MET:HA    | 1.54                     | 0.45              |
| 1:E:11:ASN:HA    | 1:E:12:MET:HA    | 1.53                     | 0.45              |
| 1:F:239:ILE:HD12 | 1:F:290:ILE:HG12 | 1.98                     | 0.45              |
| 1:F:255:PRO:HG3  | 1:G:260:GLU:OE1  | 2.15                     | 0.45              |
| 1:C:216:LYS:HD3  | 1:C:306:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:241:ILE:HD12 | 1:D:265:GLU:HG2  | 1.97                     | 0.45              |
| 1:D:269:LEU:HD23 | 1:D:293:LEU:HB2  | 1.96                     | 0.45              |
| 1:F:236:ASN:HB2  | 1:F:325:VAL:HG12 | 1.98                     | 0.45              |
| 1:H:15:TYR:O     | 1:H:20:ALA:HB2   | 2.16                     | 0.45              |
| 1:H:155:MET:HE1  | 1:H:167:LYS:O    | 2.16                     | 0.45              |
| 1:H:283:VAL:HG22 | 1:H:304:VAL:HB   | 1.99                     | 0.45              |
| 1:H:348:ILE:O    | 1:H:348:ILE:HG23 | 2.15                     | 0.45              |
| 1:H:409:VAL:HG11 | 1:H:459:VAL:HG12 | 1.99                     | 0.45              |
| 1:A:257:LYS:HD3  | 1:A:260:GLU:CD   | 2.41                     | 0.45              |
| 1:C:211:GLY:HA3  | 1:C:356:VAL:O    | 2.15                     | 0.45              |
| 1:E:241:ILE:HD12 | 1:E:265:GLU:HG2  | 1.98                     | 0.45              |
| 1:G:218:ARG:NH1  | 1:G:225:LYS:HE2  | 2.31                     | 0.45              |
| 1:H:11:ASN:HA    | 1:H:12:MET:HA    | 1.54                     | 0.45              |
| 1:D:44:MET:HA    | 1:D:44:MET:HE2   | 1.98                     | 0.45              |
| 1:B:232:ILE:HD12 | 1:B:321:THR:HG21 | 1.98                     | 0.45              |
| 1:G:409:VAL:HG11 | 1:G:459:VAL:HG12 | 1.99                     | 0.45              |
| 1:H:257:LYS:HD3  | 1:H:260:GLU:CD   | 2.42                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:257:LYS:HD3  | 1:E:260:GLU:CD   | 2.42                     | 0.45              |
| 1:A:44:MET:HA    | 1:A:44:MET:HE2   | 1.98                     | 0.45              |
| 1:D:56:VAL:O     | 1:D:56:VAL:HG13  | 2.16                     | 0.45              |
| 1:E:231:LYS:HD2  | 1:E:231:LYS:H    | 1.81                     | 0.45              |
| 1:F:20:ALA:HB1   | 1:F:515:VAL:HG23 | 1.99                     | 0.45              |
| 1:F:95:THR:HG23  | 2:F:544:ANP:O2B  | 2.16                     | 0.45              |
| 1:G:178:VAL:HA   | 1:G:193:ILE:HD11 | 1.99                     | 0.45              |
| 1:H:184:ASP:HA   | 1:H:185:GLU:HA   | 1.62                     | 0.45              |
| 1:B:95:THR:HG23  | 2:B:544:ANP:O2B  | 2.16                     | 0.45              |
| 1:B:283:VAL:HG22 | 1:B:304:VAL:HB   | 1.98                     | 0.45              |
| 1:D:178:VAL:HA   | 1:D:193:ILE:HD11 | 1.98                     | 0.45              |
| 1:F:194:LYS:NZ   | 1:F:313:ASP:OD1  | 2.46                     | 0.45              |
| 1:F:233:ALA:HB2  | 1:F:337:LEU:HD22 | 1.99                     | 0.45              |
| 1:F:257:LYS:HD3  | 1:F:260:GLU:CD   | 2.42                     | 0.45              |
| 1:A:236:ASN:HB2  | 1:A:325:VAL:HG12 | 1.99                     | 0.45              |
| 1:C:15:TYR:O     | 1:C:20:ALA:HB2   | 2.17                     | 0.44              |
| 1:E:236:ASN:HB2  | 1:E:325:VAL:HG12 | 1.99                     | 0.44              |
| 1:F:155:MET:HE3  | 1:F:171:ALA:HB2  | 1.98                     | 0.44              |
| 1:G:20:ALA:HB1   | 1:G:515:VAL:HG23 | 1.99                     | 0.44              |
| 1:A:49:VAL:HG21  | 1:B:73:PRO:HG3   | 2.00                     | 0.44              |
| 1:B:233:ALA:HB2  | 1:B:337:LEU:HD22 | 1.99                     | 0.44              |
| 1:B:409:VAL:HG11 | 1:B:459:VAL:HG12 | 1.98                     | 0.44              |
| 1:C:184:ASP:HA   | 1:C:185:GLU:HA   | 1.61                     | 0.44              |
| 1:C:201:ALA:HB2  | 1:D:497:GLN:CD   | 2.39                     | 0.44              |
| 1:C:236:ASN:HB2  | 1:C:325:VAL:HG12 | 2.00                     | 0.44              |
| 1:D:283:VAL:HG22 | 1:D:304:VAL:HB   | 1.99                     | 0.44              |
| 1:H:44:MET:HE2   | 1:H:44:MET:HA    | 1.98                     | 0.44              |
| 1:H:211:GLY:HA3  | 1:H:356:VAL:O    | 2.17                     | 0.44              |
| 1:B:15:TYR:O     | 1:B:20:ALA:HB2   | 2.18                     | 0.44              |
| 1:B:255:PRO:HG3  | 1:C:260:GLU:OE1  | 2.18                     | 0.44              |
| 1:C:20:ALA:HB1   | 1:C:515:VAL:HG23 | 1.99                     | 0.44              |
| 1:C:150:LEU:HD22 | 1:C:391:VAL:HG13 | 2.00                     | 0.44              |
| 1:C:258:LEU:HD12 | 1:D:264:GLN:CG   | 2.43                     | 0.44              |
| 1:D:20:ALA:HB1   | 1:D:515:VAL:HG23 | 2.00                     | 0.44              |
| 1:D:227:VAL:CG1  | 1:D:230:ALA:HB2  | 2.48                     | 0.44              |
| 1:E:409:VAL:HG11 | 1:E:459:VAL:HG12 | 1.99                     | 0.44              |
| 1:F:231:LYS:HD2  | 1:F:231:LYS:H    | 1.83                     | 0.44              |
| 1:D:182:VAL:HG22 | 1:D:188:VAL:HG22 | 2.00                     | 0.44              |
| 1:F:211:GLY:HA3  | 1:F:356:VAL:O    | 2.18                     | 0.44              |
| 1:F:239:ILE:HD11 | 1:F:284:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:347:LYS:HG2  | 1:D:352:SER:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:44:MET:HE2   | 1:E:44:MET:HA    | 1.99                     | 0.44              |
| 1:F:241:ILE:HD12 | 1:F:265:GLU:HG2  | 2.00                     | 0.44              |
| 1:G:239:ILE:HD11 | 1:G:284:LEU:HD21 | 1.99                     | 0.44              |
| 1:E:211:GLY:HA3  | 1:E:356:VAL:O    | 2.18                     | 0.44              |
| 1:E:348:ILE:O    | 1:E:348:ILE:HG23 | 2.18                     | 0.44              |
| 1:C:194:LYS:NZ   | 1:C:313:ASP:OD1  | 2.46                     | 0.44              |
| 1:F:409:VAL:HG11 | 1:F:459:VAL:HG12 | 1.99                     | 0.44              |
| 1:A:327:THR:HB   | 1:H:296:HIS:HB2  | 2.00                     | 0.44              |
| 1:B:56:VAL:O     | 1:B:56:VAL:CG1   | 2.66                     | 0.44              |
| 1:D:201:ALA:HB2  | 1:E:497:GLN:CD   | 2.42                     | 0.44              |
| 1:D:409:VAL:HG11 | 1:D:459:VAL:HG12 | 1.99                     | 0.44              |
| 1:B:269:LEU:HD23 | 1:B:293:LEU:HB2  | 1.99                     | 0.43              |
| 1:C:243:GLU:HG2  | 1:D:246:THR:HG22 | 1.99                     | 0.43              |
| 1:G:269:LEU:HD23 | 1:G:293:LEU:HB2  | 2.00                     | 0.43              |
| 1:H:439:VAL:O    | 1:H:439:VAL:HG22 | 2.18                     | 0.43              |
| 1:B:239:ILE:HD11 | 1:B:284:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:255:PRO:HG3  | 1:E:260:GLU:OE1  | 2.19                     | 0.43              |
| 1:F:15:TYR:O     | 1:F:20:ALA:HB2   | 2.18                     | 0.43              |
| 1:F:155:MET:HE1  | 1:F:167:LYS:O    | 2.19                     | 0.43              |
| 1:H:182:VAL:HG22 | 1:H:188:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:216:LYS:HD3  | 1:A:306:ALA:HB1  | 1.99                     | 0.43              |
| 1:C:456:LEU:HG   | 1:C:460:ARG:HH21 | 1.83                     | 0.43              |
| 1:A:45:ASP:OD1   | 1:A:59:ASN:HB2   | 2.19                     | 0.43              |
| 1:A:259:MET:HG2  | 1:B:268:MET:HE2  | 2.01                     | 0.43              |
| 1:D:444:LEU:HD23 | 1:D:444:LEU:HA   | 1.87                     | 0.43              |
| 1:F:440:ILE:N    | 1:F:441:PRO:CD   | 2.81                     | 0.43              |
| 1:G:456:LEU:HG   | 1:G:460:ARG:HH21 | 1.83                     | 0.43              |
| 1:H:269:LEU:HD23 | 1:H:293:LEU:HB2  | 2.00                     | 0.43              |
| 1:B:257:LYS:HD3  | 1:B:260:GLU:CD   | 2.43                     | 0.43              |
| 1:D:194:LYS:NZ   | 1:D:313:ASP:OD1  | 2.48                     | 0.43              |
| 1:G:236:ASN:HB2  | 1:G:325:VAL:HG12 | 1.99                     | 0.43              |
| 1:H:239:ILE:HD11 | 1:H:284:LEU:HD21 | 2.00                     | 0.43              |
| 1:C:283:VAL:HG22 | 1:C:304:VAL:HB   | 1.99                     | 0.43              |
| 1:H:236:ASN:HB2  | 1:H:325:VAL:HG12 | 2.01                     | 0.43              |
| 1:B:155:MET:HE1  | 1:B:167:LYS:O    | 2.19                     | 0.43              |
| 1:C:218:ARG:NH1  | 1:C:225:LYS:HE2  | 2.32                     | 0.43              |
| 1:E:49:VAL:HG21  | 1:F:73:PRO:HG3   | 2.01                     | 0.43              |
| 1:B:20:ALA:HB1   | 1:B:515:VAL:HG23 | 2.00                     | 0.43              |
| 1:C:307:ARG:HH11 | 1:C:307:ARG:CG   | 2.31                     | 0.43              |
| 1:C:239:ILE:HD12 | 1:C:290:ILE:HG12 | 2.00                     | 0.43              |
| 1:B:348:ILE:O    | 1:B:348:ILE:HG23 | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:182:VAL:HG22 | 1:E:188:VAL:HG22 | 2.01                     | 0.43              |
| 1:E:373:THR:HB   | 1:F:80:GLU:HB3   | 2.01                     | 0.43              |
| 1:G:233:ALA:HB2  | 1:G:337:LEU:HD22 | 2.01                     | 0.43              |
| 1:A:402:SER:HB3  | 1:A:470:CYS:SG   | 2.59                     | 0.42              |
| 1:C:44:MET:HE2   | 1:C:44:MET:HA    | 2.00                     | 0.42              |
| 1:C:239:ILE:HD11 | 1:C:284:LEU:HD21 | 2.00                     | 0.42              |
| 1:H:227:VAL:CG1  | 1:H:230:ALA:HB2  | 2.49                     | 0.42              |
| 1:C:468:ASN:HD22 | 1:C:471:ALA:HB2  | 1.84                     | 0.42              |
| 1:E:402:SER:HB3  | 1:E:470:CYS:SG   | 2.59                     | 0.42              |
| 1:E:453:ILE:H    | 1:E:453:ILE:HG13 | 1.67                     | 0.42              |
| 1:A:11:ASN:HA    | 1:A:12:MET:HA    | 1.53                     | 0.42              |
| 1:B:211:GLY:HA3  | 1:B:356:VAL:O    | 2.19                     | 0.42              |
| 1:D:239:ILE:HD11 | 1:D:284:LEU:HD21 | 2.01                     | 0.42              |
| 1:F:283:VAL:HG22 | 1:F:304:VAL:HB   | 2.02                     | 0.42              |
| 1:A:284:LEU:O    | 1:A:305:ALA:HA   | 2.20                     | 0.42              |
| 1:B:194:LYS:NZ   | 1:B:313:ASP:OD1  | 2.46                     | 0.42              |
| 1:D:236:ASN:HB2  | 1:D:325:VAL:HG12 | 2.01                     | 0.42              |
| 1:A:194:LYS:NZ   | 1:A:313:ASP:OD1  | 2.47                     | 0.42              |
| 1:B:231:LYS:HD2  | 1:B:231:LYS:H    | 1.82                     | 0.42              |
| 1:G:227:VAL:CG1  | 1:G:230:ALA:HB2  | 2.50                     | 0.42              |
| 1:G:307:ARG:HH11 | 1:G:307:ARG:CG   | 2.31                     | 0.42              |
| 1:G:450:LEU:HB3  | 1:G:455:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:453:ILE:H    | 1:A:453:ILE:HG13 | 1.69                     | 0.42              |
| 1:E:259:MET:HG2  | 1:F:268:MET:HE2  | 2.02                     | 0.42              |
| 1:F:105:ARG:HH21 | 1:F:106:LYS:HE2  | 1.85                     | 0.42              |
| 1:H:281:ALA:HB2  | 1:H:337:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:184:ASP:HA   | 1:A:185:GLU:HA   | 1.62                     | 0.42              |
| 1:A:239:ILE:HD11 | 1:A:284:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:184:ASP:HA   | 1:B:185:GLU:HA   | 1.61                     | 0.42              |
| 1:G:155:MET:HE1  | 1:G:167:LYS:O    | 2.20                     | 0.42              |
| 1:G:239:ILE:HD12 | 1:G:290:ILE:HG12 | 2.01                     | 0.42              |
| 1:G:255:PRO:HD3  | 1:H:260:GLU:OE1  | 2.20                     | 0.42              |
| 1:A:260:GLU:OE1  | 1:H:255:PRO:HG3  | 2.20                     | 0.42              |
| 1:D:211:GLY:HA3  | 1:D:356:VAL:O    | 2.19                     | 0.42              |
| 1:F:11:ASN:HA    | 1:F:12:MET:HA    | 1.52                     | 0.42              |
| 1:F:45:ASP:OD1   | 1:F:59:ASN:HB2   | 2.20                     | 0.42              |
| 1:F:348:ILE:O    | 1:F:348:ILE:CG2  | 2.68                     | 0.42              |
| 1:D:440:ILE:HB   | 1:D:441:PRO:HD3  | 2.01                     | 0.42              |
| 1:E:456:LEU:HG   | 1:E:460:ARG:HH21 | 1.85                     | 0.42              |
| 1:F:105:ARG:NH2  | 1:F:106:LYS:HE2  | 2.35                     | 0.42              |
| 1:H:216:LYS:HD3  | 1:H:306:ALA:HB1  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:GLY:HA3  | 1:A:356:VAL:O    | 2.20                     | 0.41              |
| 1:A:232:ILE:HD12 | 1:A:321:THR:HG21 | 2.00                     | 0.41              |
| 1:F:284:LEU:O    | 1:F:305:ALA:HA   | 2.20                     | 0.41              |
| 1:H:468:ASN:HD22 | 1:H:471:ALA:HB2  | 1.86                     | 0.41              |
| 1:E:184:ASP:HA   | 1:E:185:GLU:HA   | 1.61                     | 0.41              |
| 1:E:239:ILE:HD11 | 1:E:284:LEU:HD21 | 2.02                     | 0.41              |
| 1:D:439:VAL:O    | 1:D:439:VAL:HG22 | 2.19                     | 0.41              |
| 1:B:307:ARG:HH11 | 1:B:307:ARG:CG   | 2.32                     | 0.41              |
| 1:D:296:HIS:HB2  | 1:E:327:THR:HB   | 2.03                     | 0.41              |
| 1:C:178:VAL:HA   | 1:C:193:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:476:PHE:HE2  | 2:C:544:ANP:N6   | 2.19                     | 0.41              |
| 1:D:216:LYS:HD3  | 1:D:306:ALA:HB1  | 2.03                     | 0.41              |
| 1:E:105:ARG:NH2  | 1:E:106:LYS:HE2  | 2.36                     | 0.41              |
| 1:A:201:ALA:HB2  | 1:B:497:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:296:HIS:HB2  | 1:B:327:THR:HB   | 2.03                     | 0.41              |
| 1:B:218:ARG:NH1  | 1:B:225:LYS:HE2  | 2.36                     | 0.41              |
| 1:D:468:ASN:HD22 | 1:D:471:ALA:HB2  | 1.85                     | 0.41              |
| 1:E:95:THR:HG23  | 2:E:544:ANP:O2B  | 2.20                     | 0.41              |
| 1:E:232:ILE:HD12 | 1:E:321:THR:HG21 | 2.02                     | 0.41              |
| 1:E:241:ILE:HD13 | 1:E:269:LEU:HD13 | 2.03                     | 0.41              |
| 1:G:11:ASN:HA    | 1:G:12:MET:HA    | 1.53                     | 0.41              |
| 1:G:202:SER:C    | 1:G:204:ASP:N    | 2.78                     | 0.41              |
| 1:G:468:ASN:HD22 | 1:G:471:ALA:HB2  | 1.85                     | 0.41              |
| 1:H:56:VAL:O     | 1:H:56:VAL:CG1   | 2.68                     | 0.41              |
| 1:B:439:VAL:O    | 1:B:439:VAL:HG22 | 2.20                     | 0.41              |
| 1:C:105:ARG:HH21 | 1:C:106:LYS:HE2  | 1.85                     | 0.41              |
| 1:D:47:MET:HB2   | 1:E:512:ILE:HD13 | 2.03                     | 0.41              |
| 1:D:456:LEU:HG   | 1:D:460:ARG:HH21 | 1.85                     | 0.41              |
| 1:G:197:LYS:HB3  | 1:G:377:ILE:HG21 | 2.03                     | 0.41              |
| 1:G:241:ILE:HD13 | 1:G:269:LEU:HD13 | 2.02                     | 0.41              |
| 1:H:326:ILE:HG22 | 1:H:328:ASN:H    | 1.85                     | 0.41              |
| 1:A:241:ILE:HD13 | 1:A:269:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:257:LYS:O    | 1:B:260:GLU:HB2  | 2.21                     | 0.41              |
| 1:B:284:LEU:O    | 1:B:305:ALA:HA   | 2.20                     | 0.41              |
| 1:B:476:PHE:HE2  | 2:B:544:ANP:N6   | 2.19                     | 0.41              |
| 1:C:227:VAL:CG1  | 1:C:230:ALA:HB2  | 2.51                     | 0.41              |
| 1:D:95:THR:HG23  | 2:D:544:ANP:O2B  | 2.21                     | 0.41              |
| 1:A:439:VAL:O    | 1:A:439:VAL:HG22 | 2.21                     | 0.40              |
| 1:D:155:MET:HE1  | 1:D:167:LYS:O    | 2.21                     | 0.40              |
| 1:E:397:ASP:OD1  | 1:E:493:ARG:HB2  | 2.21                     | 0.40              |
| 1:F:307:ARG:HH11 | 1:F:307:ARG:CG   | 2.32                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:283:VAL:HG22 | 1:G:304:VAL:HB   | 2.02                     | 0.40              |
| 1:G:348:ILE:O    | 1:G:348:ILE:CG2  | 2.69                     | 0.40              |
| 1:H:218:ARG:NH1  | 1:H:225:LYS:HE2  | 2.35                     | 0.40              |
| 1:H:348:ILE:O    | 1:H:348:ILE:CG2  | 2.69                     | 0.40              |
| 1:C:105:ARG:NH2  | 1:C:106:LYS:HE2  | 2.37                     | 0.40              |
| 1:D:450:LEU:HB3  | 1:D:455:ILE:HD11 | 2.03                     | 0.40              |
| 1:E:476:PHE:HE2  | 2:E:544:ANP:N6   | 2.19                     | 0.40              |
| 1:A:468:ASN:HD22 | 1:A:471:ALA:HB2  | 1.86                     | 0.40              |
| 1:C:155:MET:HE3  | 1:C:171:ALA:HB2  | 2.03                     | 0.40              |
| 1:D:105:ARG:HH21 | 1:D:106:LYS:HE2  | 1.86                     | 0.40              |
| 1:D:184:ASP:HA   | 1:D:185:GLU:HA   | 1.62                     | 0.40              |
| 1:D:476:PHE:HE2  | 2:D:544:ANP:N6   | 2.19                     | 0.40              |
| 1:G:56:VAL:O     | 1:G:56:VAL:CG1   | 2.70                     | 0.40              |
| 1:H:241:ILE:HD13 | 1:H:269:LEU:HD13 | 2.03                     | 0.40              |
| 1:A:182:VAL:HG22 | 1:A:188:VAL:HG22 | 2.04                     | 0.40              |
| 1:A:307:ARG:HH11 | 1:A:307:ARG:CG   | 2.35                     | 0.40              |
| 1:B:45:ASP:OD1   | 1:B:59:ASN:HB2   | 2.21                     | 0.40              |
| 1:E:216:LYS:HD3  | 1:E:306:ALA:HB1  | 2.03                     | 0.40              |
| 1:F:218:ARG:NH1  | 1:F:225:LYS:HE2  | 2.36                     | 0.40              |
| 1:F:468:ASN:HD22 | 1:F:471:ALA:HB2  | 1.85                     | 0.40              |
| 1:G:439:VAL:O    | 1:G:439:VAL:HG22 | 2.22                     | 0.40              |
| 1:H:307:ARG:HH11 | 1:H:307:ARG:CG   | 2.32                     | 0.40              |
| 1:B:440:ILE:N    | 1:B:441:PRO:CD   | 2.84                     | 0.40              |
| 1:C:11:ASN:HA    | 1:C:12:MET:HA    | 1.54                     | 0.40              |
| 1:E:31:ILE:HG21  | 1:E:75:ALA:HB1   | 2.02                     | 0.40              |
| 1:E:439:VAL:O    | 1:E:439:VAL:HG22 | 2.21                     | 0.40              |
| 1:G:243:GLU:HG2  | 1:H:246:THR:CG2  | 2.52                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:A:145:GLN:N | 1:C:185:GLU:CG[4_546]  | 2.02                     | 0.18              |
| 1:E:145:GLN:N | 1:G:185:GLU:CG[4_555]  | 2.04                     | 0.16              |
| 1:A:144:ALA:O | 1:C:185:GLU:OE2[4_546] | 2.07                     | 0.13              |
| 1:E:144:ALA:O | 1:G:185:GLU:OE2[4_555] | 2.08                     | 0.12              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 507/543 (93%)   | 488 (96%)  | 16 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | B     | 507/543 (93%)   | 487 (96%)  | 17 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | C     | 507/543 (93%)   | 490 (97%)  | 14 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | D     | 507/543 (93%)   | 487 (96%)  | 17 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | E     | 507/543 (93%)   | 489 (96%)  | 15 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | F     | 507/543 (93%)   | 487 (96%)  | 16 (3%)  | 4 (1%)   | 16          | 50 |
| 1   | G     | 507/543 (93%)   | 488 (96%)  | 16 (3%)  | 3 (1%)   | 21          | 56 |
| 1   | H     | 507/543 (93%)   | 488 (96%)  | 16 (3%)  | 3 (1%)   | 21          | 56 |
| All | All   | 4056/4344 (93%) | 3904 (96%) | 127 (3%) | 25 (1%)  | 21          | 56 |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 199 | SER  |
| 1   | A     | 203 | ILE  |
| 1   | A     | 465 | SER  |
| 1   | B     | 199 | SER  |
| 1   | B     | 203 | ILE  |
| 1   | B     | 465 | SER  |
| 1   | C     | 199 | SER  |
| 1   | C     | 203 | ILE  |
| 1   | C     | 465 | SER  |
| 1   | D     | 199 | SER  |
| 1   | D     | 203 | ILE  |
| 1   | D     | 465 | SER  |
| 1   | E     | 199 | SER  |
| 1   | E     | 203 | ILE  |
| 1   | E     | 465 | SER  |
| 1   | F     | 199 | SER  |
| 1   | F     | 203 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 465 | SER  |
| 1   | G     | 199 | SER  |
| 1   | G     | 203 | ILE  |
| 1   | G     | 465 | SER  |
| 1   | H     | 199 | SER  |
| 1   | H     | 203 | ILE  |
| 1   | H     | 465 | SER  |
| 1   | F     | 239 | ILE  |

### 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     | 410/434 (94%)   | 395 (96%)  | 15 (4%)  | 30          | 63 |
| 1   | B     | 410/434 (94%)   | 396 (97%)  | 14 (3%)  | 32          | 64 |
| 1   | C     | 410/434 (94%)   | 396 (97%)  | 14 (3%)  | 32          | 64 |
| 1   | D     | 410/434 (94%)   | 395 (96%)  | 15 (4%)  | 30          | 63 |
| 1   | E     | 410/434 (94%)   | 394 (96%)  | 16 (4%)  | 28          | 62 |
| 1   | F     | 410/434 (94%)   | 396 (97%)  | 14 (3%)  | 32          | 64 |
| 1   | G     | 410/434 (94%)   | 395 (96%)  | 15 (4%)  | 30          | 63 |
| 1   | H     | 410/434 (94%)   | 395 (96%)  | 15 (4%)  | 30          | 63 |
| All | All   | 3280/3472 (94%) | 3162 (96%) | 118 (4%) | 31          | 63 |

All (118) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 129 | GLN  |
| 1   | A     | 145 | GLN  |
| 1   | A     | 148 | GLU  |
| 1   | A     | 155 | MET  |
| 1   | A     | 168 | GLU  |
| 1   | A     | 203 | ILE  |
| 1   | A     | 216 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | ARG  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 292 | ASP  |
| 1   | A     | 327 | THR  |
| 1   | A     | 342 | LEU  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 469 | LYS  |
| 1   | A     | 481 | GLU  |
| 1   | B     | 39  | LEU  |
| 1   | B     | 129 | GLN  |
| 1   | B     | 145 | GLN  |
| 1   | B     | 148 | GLU  |
| 1   | B     | 155 | MET  |
| 1   | B     | 168 | GLU  |
| 1   | B     | 216 | LYS  |
| 1   | B     | 218 | ARG  |
| 1   | B     | 269 | LEU  |
| 1   | B     | 292 | ASP  |
| 1   | B     | 327 | THR  |
| 1   | B     | 342 | LEU  |
| 1   | B     | 365 | VAL  |
| 1   | B     | 481 | GLU  |
| 1   | C     | 129 | GLN  |
| 1   | C     | 145 | GLN  |
| 1   | C     | 148 | GLU  |
| 1   | C     | 155 | MET  |
| 1   | C     | 168 | GLU  |
| 1   | C     | 203 | ILE  |
| 1   | C     | 216 | LYS  |
| 1   | C     | 218 | ARG  |
| 1   | C     | 269 | LEU  |
| 1   | C     | 292 | ASP  |
| 1   | C     | 327 | THR  |
| 1   | C     | 342 | LEU  |
| 1   | C     | 365 | VAL  |
| 1   | C     | 481 | GLU  |
| 1   | D     | 39  | LEU  |
| 1   | D     | 129 | GLN  |
| 1   | D     | 145 | GLN  |
| 1   | D     | 148 | GLU  |
| 1   | D     | 155 | MET  |
| 1   | D     | 168 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 216 | LYS  |
| 1   | D     | 218 | ARG  |
| 1   | D     | 269 | LEU  |
| 1   | D     | 292 | ASP  |
| 1   | D     | 327 | THR  |
| 1   | D     | 342 | LEU  |
| 1   | D     | 365 | VAL  |
| 1   | D     | 469 | LYS  |
| 1   | D     | 481 | GLU  |
| 1   | E     | 39  | LEU  |
| 1   | E     | 44  | MET  |
| 1   | E     | 129 | GLN  |
| 1   | E     | 145 | GLN  |
| 1   | E     | 148 | GLU  |
| 1   | E     | 155 | MET  |
| 1   | E     | 168 | GLU  |
| 1   | E     | 216 | LYS  |
| 1   | E     | 218 | ARG  |
| 1   | E     | 269 | LEU  |
| 1   | E     | 292 | ASP  |
| 1   | E     | 327 | THR  |
| 1   | E     | 342 | LEU  |
| 1   | E     | 365 | VAL  |
| 1   | E     | 469 | LYS  |
| 1   | E     | 481 | GLU  |
| 1   | F     | 129 | GLN  |
| 1   | F     | 145 | GLN  |
| 1   | F     | 148 | GLU  |
| 1   | F     | 155 | MET  |
| 1   | F     | 168 | GLU  |
| 1   | F     | 203 | ILE  |
| 1   | F     | 216 | LYS  |
| 1   | F     | 218 | ARG  |
| 1   | F     | 269 | LEU  |
| 1   | F     | 292 | ASP  |
| 1   | F     | 327 | THR  |
| 1   | F     | 342 | LEU  |
| 1   | F     | 365 | VAL  |
| 1   | F     | 481 | GLU  |
| 1   | G     | 129 | GLN  |
| 1   | G     | 145 | GLN  |
| 1   | G     | 148 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 155 | MET  |
| 1   | G     | 168 | GLU  |
| 1   | G     | 203 | ILE  |
| 1   | G     | 216 | LYS  |
| 1   | G     | 218 | ARG  |
| 1   | G     | 269 | LEU  |
| 1   | G     | 292 | ASP  |
| 1   | G     | 327 | THR  |
| 1   | G     | 342 | LEU  |
| 1   | G     | 365 | VAL  |
| 1   | G     | 469 | LYS  |
| 1   | G     | 481 | GLU  |
| 1   | H     | 129 | GLN  |
| 1   | H     | 145 | GLN  |
| 1   | H     | 148 | GLU  |
| 1   | H     | 155 | MET  |
| 1   | H     | 168 | GLU  |
| 1   | H     | 203 | ILE  |
| 1   | H     | 216 | LYS  |
| 1   | H     | 218 | ARG  |
| 1   | H     | 269 | LEU  |
| 1   | H     | 292 | ASP  |
| 1   | H     | 327 | THR  |
| 1   | H     | 342 | LEU  |
| 1   | H     | 365 | VAL  |
| 1   | H     | 469 | LYS  |
| 1   | H     | 481 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 264 | GLN  |
| 1   | A     | 287 | GLN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 427 | GLN  |
| 1   | A     | 468 | ASN  |
| 1   | A     | 500 | GLN  |
| 1   | B     | 264 | GLN  |
| 1   | B     | 287 | GLN  |
| 1   | B     | 361 | HIS  |
| 1   | B     | 468 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 500 | GLN  |
| 1   | C     | 287 | GLN  |
| 1   | C     | 296 | HIS  |
| 1   | C     | 361 | HIS  |
| 1   | C     | 427 | GLN  |
| 1   | C     | 468 | ASN  |
| 1   | C     | 500 | GLN  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 296 | HIS  |
| 1   | D     | 361 | HIS  |
| 1   | D     | 427 | GLN  |
| 1   | D     | 468 | ASN  |
| 1   | D     | 500 | GLN  |
| 1   | E     | 264 | GLN  |
| 1   | E     | 296 | HIS  |
| 1   | E     | 361 | HIS  |
| 1   | E     | 427 | GLN  |
| 1   | E     | 468 | ASN  |
| 1   | E     | 500 | GLN  |
| 1   | F     | 264 | GLN  |
| 1   | F     | 361 | HIS  |
| 1   | F     | 427 | GLN  |
| 1   | F     | 468 | ASN  |
| 1   | F     | 500 | GLN  |
| 1   | G     | 264 | GLN  |
| 1   | G     | 296 | HIS  |
| 1   | G     | 361 | HIS  |
| 1   | G     | 427 | GLN  |
| 1   | G     | 468 | ASN  |
| 1   | G     | 500 | GLN  |
| 1   | H     | 264 | GLN  |
| 1   | H     | 296 | HIS  |
| 1   | H     | 361 | HIS  |
| 1   | H     | 427 | GLN  |
| 1   | H     | 468 | ASN  |
| 1   | H     | 500 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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 | $\# Z  > 2$ |
| 2   | ANP  | C     | 544 | 3    | 33,33,33     | 1.56 | 7 (21%)     | 45,52,52    | 1.19 | 2 (4%)      |
| 2   | ANP  | H     | 544 | 3    | 33,33,33     | 1.56 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |
| 2   | ANP  | E     | 544 | 3    | 33,33,33     | 1.57 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |
| 2   | ANP  | A     | 544 | 3    | 33,33,33     | 1.56 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |
| 2   | ANP  | G     | 544 | 3    | 33,33,33     | 1.57 | 7 (21%)     | 45,52,52    | 1.19 | 2 (4%)      |
| 2   | ANP  | D     | 544 | 3    | 33,33,33     | 1.57 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |
| 2   | ANP  | B     | 544 | 3    | 33,33,33     | 1.57 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |
| 2   | ANP  | F     | 544 | 3    | 33,33,33     | 1.57 | 7 (21%)     | 45,52,52    | 1.18 | 2 (4%)      |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ANP  | C     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | H     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | E     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | A     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ANP  | G     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | D     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | B     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |
| 2   | ANP  | F     | 544 | 3    | -       | 4/18/38/38 | 0/3/3/3 |

All (56) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 544 | ANP  | PB-O3A | 3.77  | 1.63        | 1.59     |
| 2   | G     | 544 | ANP  | PB-O3A | 3.75  | 1.63        | 1.59     |
| 2   | B     | 544 | ANP  | PB-O3A | 3.75  | 1.63        | 1.59     |
| 2   | A     | 544 | ANP  | PB-O3A | 3.74  | 1.63        | 1.59     |
| 2   | F     | 544 | ANP  | PB-O3A | 3.74  | 1.63        | 1.59     |
| 2   | D     | 544 | ANP  | PB-O3A | 3.73  | 1.63        | 1.59     |
| 2   | C     | 544 | ANP  | PB-O3A | 3.72  | 1.63        | 1.59     |
| 2   | H     | 544 | ANP  | PB-O3A | 3.72  | 1.63        | 1.59     |
| 2   | F     | 544 | ANP  | PA-O3A | 3.49  | 1.63        | 1.59     |
| 2   | G     | 544 | ANP  | PA-O3A | 3.49  | 1.63        | 1.59     |
| 2   | B     | 544 | ANP  | PA-O3A | 3.45  | 1.63        | 1.59     |
| 2   | B     | 544 | ANP  | PB-O2B | -3.44 | 1.47        | 1.56     |
| 2   | A     | 544 | ANP  | PA-O3A | 3.44  | 1.63        | 1.59     |
| 2   | D     | 544 | ANP  | PA-O3A | 3.44  | 1.63        | 1.59     |
| 2   | H     | 544 | ANP  | PA-O3A | 3.44  | 1.63        | 1.59     |
| 2   | G     | 544 | ANP  | PB-O2B | -3.43 | 1.47        | 1.56     |
| 2   | E     | 544 | ANP  | PA-O3A | 3.43  | 1.63        | 1.59     |
| 2   | H     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | A     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | D     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | E     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | C     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | F     | 544 | ANP  | PB-O2B | -3.42 | 1.47        | 1.56     |
| 2   | C     | 544 | ANP  | PA-O3A | 3.41  | 1.63        | 1.59     |
| 2   | F     | 544 | ANP  | PG-O2G | -2.89 | 1.49        | 1.56     |
| 2   | D     | 544 | ANP  | PG-O2G | -2.88 | 1.49        | 1.56     |
| 2   | B     | 544 | ANP  | PG-O2G | -2.87 | 1.49        | 1.56     |
| 2   | C     | 544 | ANP  | PG-O2G | -2.86 | 1.49        | 1.56     |
| 2   | A     | 544 | ANP  | PG-O2G | -2.86 | 1.49        | 1.56     |
| 2   | G     | 544 | ANP  | PG-O2G | -2.85 | 1.49        | 1.56     |
| 2   | E     | 544 | ANP  | PG-O2G | -2.84 | 1.49        | 1.56     |
| 2   | H     | 544 | ANP  | PG-O2G | -2.83 | 1.49        | 1.56     |
| 2   | D     | 544 | ANP  | PG-O3G | -2.81 | 1.49        | 1.56     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | C     | 544 | ANP  | PG-O3G | -2.81 | 1.49        | 1.56     |
| 2   | G     | 544 | ANP  | PG-O3G | -2.80 | 1.49        | 1.56     |
| 2   | E     | 544 | ANP  | PG-O3G | -2.79 | 1.49        | 1.56     |
| 2   | B     | 544 | ANP  | PG-O3G | -2.78 | 1.49        | 1.56     |
| 2   | A     | 544 | ANP  | PG-O3G | -2.78 | 1.49        | 1.56     |
| 2   | F     | 544 | ANP  | PG-O3G | -2.77 | 1.49        | 1.56     |
| 2   | H     | 544 | ANP  | PG-O3G | -2.76 | 1.49        | 1.56     |
| 2   | C     | 544 | ANP  | PG-O1G | 2.32  | 1.49        | 1.46     |
| 2   | F     | 544 | ANP  | PG-O1G | 2.32  | 1.49        | 1.46     |
| 2   | D     | 544 | ANP  | PG-O1G | 2.30  | 1.49        | 1.46     |
| 2   | E     | 544 | ANP  | PG-O1G | 2.29  | 1.49        | 1.46     |
| 2   | C     | 544 | ANP  | C4-N3  | 2.28  | 1.38        | 1.34     |
| 2   | A     | 544 | ANP  | PG-O1G | 2.28  | 1.49        | 1.46     |
| 2   | B     | 544 | ANP  | PG-O1G | 2.28  | 1.49        | 1.46     |
| 2   | G     | 544 | ANP  | PG-O1G | 2.28  | 1.49        | 1.46     |
| 2   | H     | 544 | ANP  | C4-N3  | 2.27  | 1.38        | 1.34     |
| 2   | B     | 544 | ANP  | C4-N3  | 2.27  | 1.38        | 1.34     |
| 2   | A     | 544 | ANP  | C4-N3  | 2.27  | 1.38        | 1.34     |
| 2   | E     | 544 | ANP  | C4-N3  | 2.27  | 1.38        | 1.34     |
| 2   | G     | 544 | ANP  | C4-N3  | 2.26  | 1.38        | 1.34     |
| 2   | H     | 544 | ANP  | PG-O1G | 2.25  | 1.49        | 1.46     |
| 2   | F     | 544 | ANP  | C4-N3  | 2.25  | 1.38        | 1.34     |
| 2   | D     | 544 | ANP  | C4-N3  | 2.23  | 1.38        | 1.34     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | C     | 544 | ANP  | O2B-PB-O1B | 4.60  | 119.74      | 109.87   |
| 2   | G     | 544 | ANP  | O2B-PB-O1B | 4.59  | 119.71      | 109.87   |
| 2   | F     | 544 | ANP  | O2B-PB-O1B | 4.59  | 119.71      | 109.87   |
| 2   | H     | 544 | ANP  | O2B-PB-O1B | 4.59  | 119.70      | 109.87   |
| 2   | E     | 544 | ANP  | O2B-PB-O1B | 4.58  | 119.69      | 109.87   |
| 2   | A     | 544 | ANP  | O2B-PB-O1B | 4.58  | 119.69      | 109.87   |
| 2   | B     | 544 | ANP  | O2B-PB-O1B | 4.58  | 119.68      | 109.87   |
| 2   | D     | 544 | ANP  | O2B-PB-O1B | 4.57  | 119.67      | 109.87   |
| 2   | H     | 544 | ANP  | O1B-PB-N3B | -2.23 | 108.49      | 111.77   |
| 2   | C     | 544 | ANP  | O1B-PB-N3B | -2.22 | 108.49      | 111.77   |
| 2   | B     | 544 | ANP  | O1B-PB-N3B | -2.21 | 108.52      | 111.77   |
| 2   | A     | 544 | ANP  | O1B-PB-N3B | -2.20 | 108.53      | 111.77   |
| 2   | E     | 544 | ANP  | O1B-PB-N3B | -2.20 | 108.53      | 111.77   |
| 2   | F     | 544 | ANP  | O1B-PB-N3B | -2.19 | 108.54      | 111.77   |
| 2   | G     | 544 | ANP  | O1B-PB-N3B | -2.19 | 108.54      | 111.77   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 544 | ANP  | O1B-PB-N3B | -2.19 | 108.55      | 111.77   |

There are no chirality outliers.

All (32) torsion outliers are listed below:

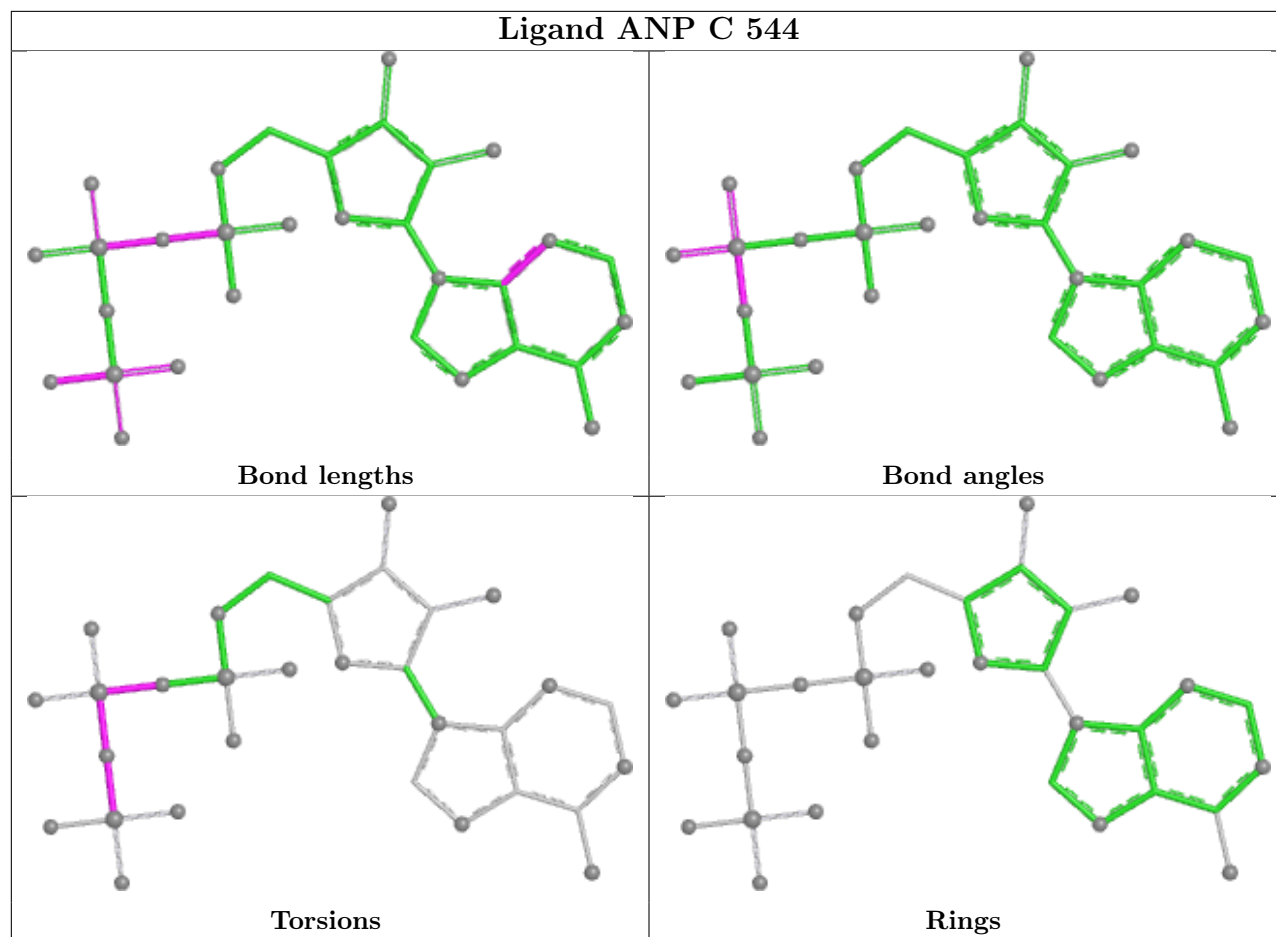
| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | A     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | A     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | A     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | B     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | B     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | B     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | C     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | C     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | C     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | D     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | D     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | D     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | E     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | E     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | E     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | F     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | F     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | F     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | G     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | G     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | G     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | H     | 544 | ANP  | PB-N3B-PG-O1G |
| 2   | H     | 544 | ANP  | PG-N3B-PB-O1B |
| 2   | H     | 544 | ANP  | PA-O3A-PB-O2B |
| 2   | A     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | B     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | C     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | D     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | E     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | F     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | G     | 544 | ANP  | PA-O3A-PB-O1B |
| 2   | H     | 544 | ANP  | PA-O3A-PB-O1B |

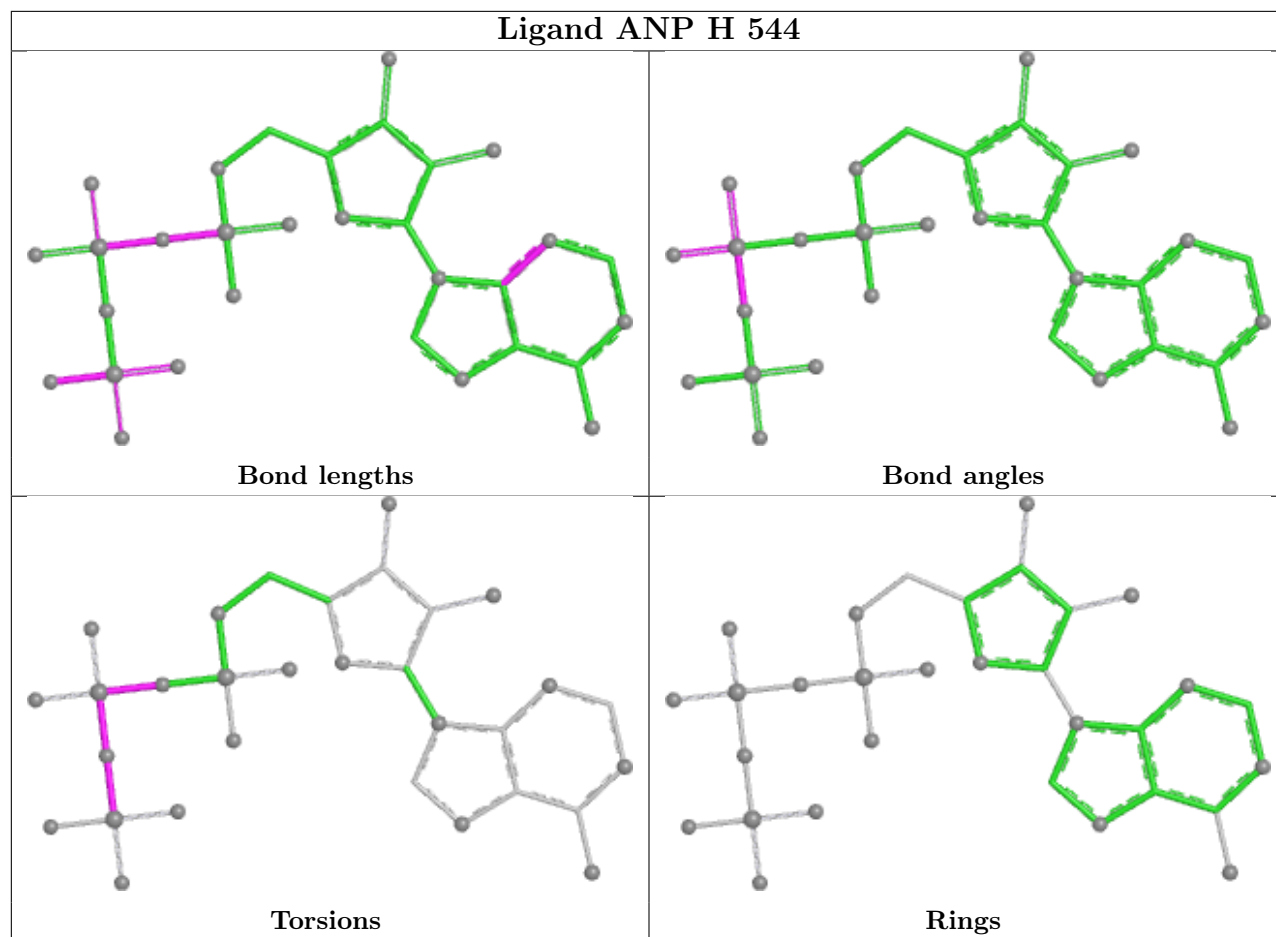
There are no ring outliers.

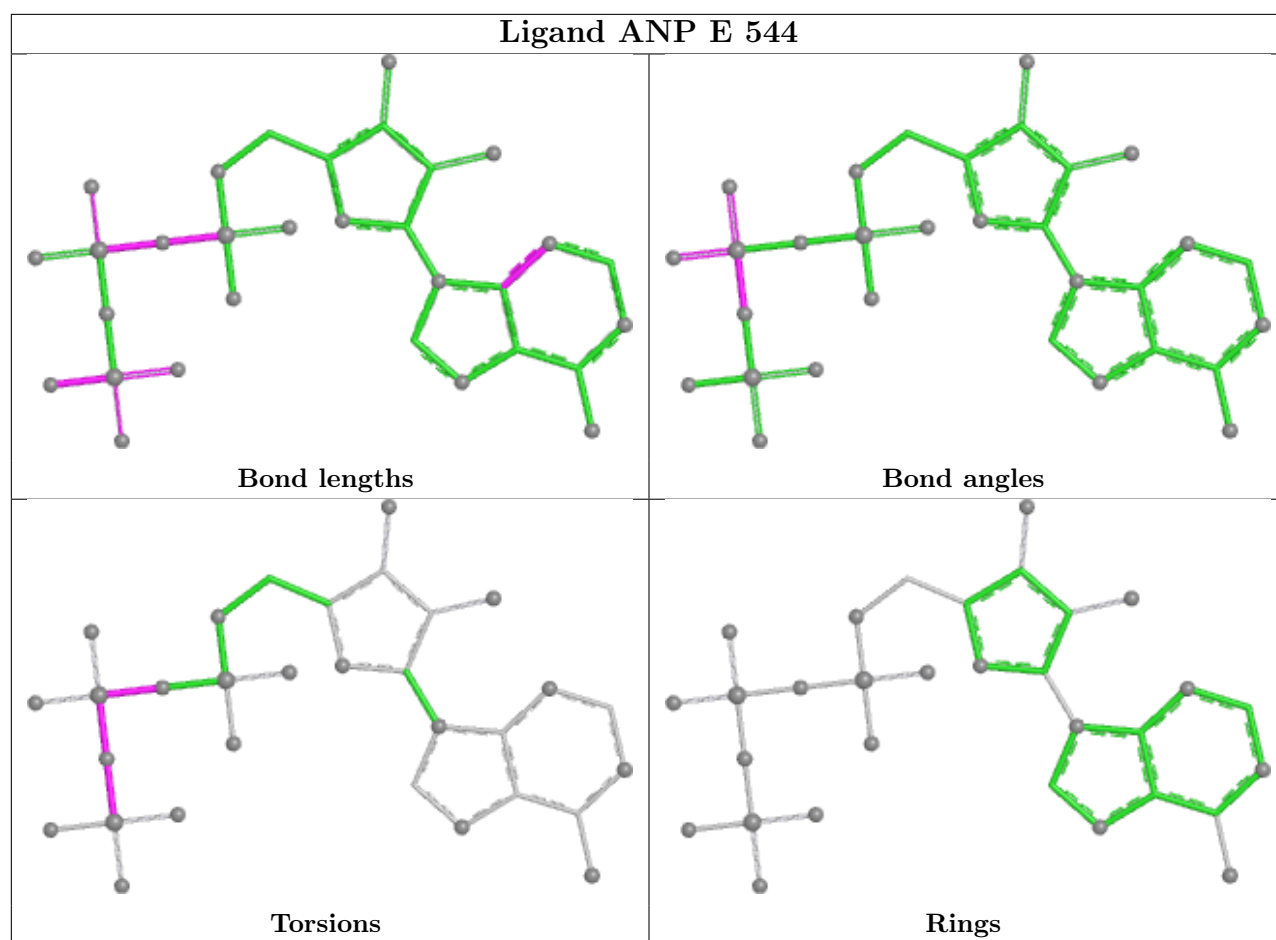
8 monomers are involved in 26 short contacts:

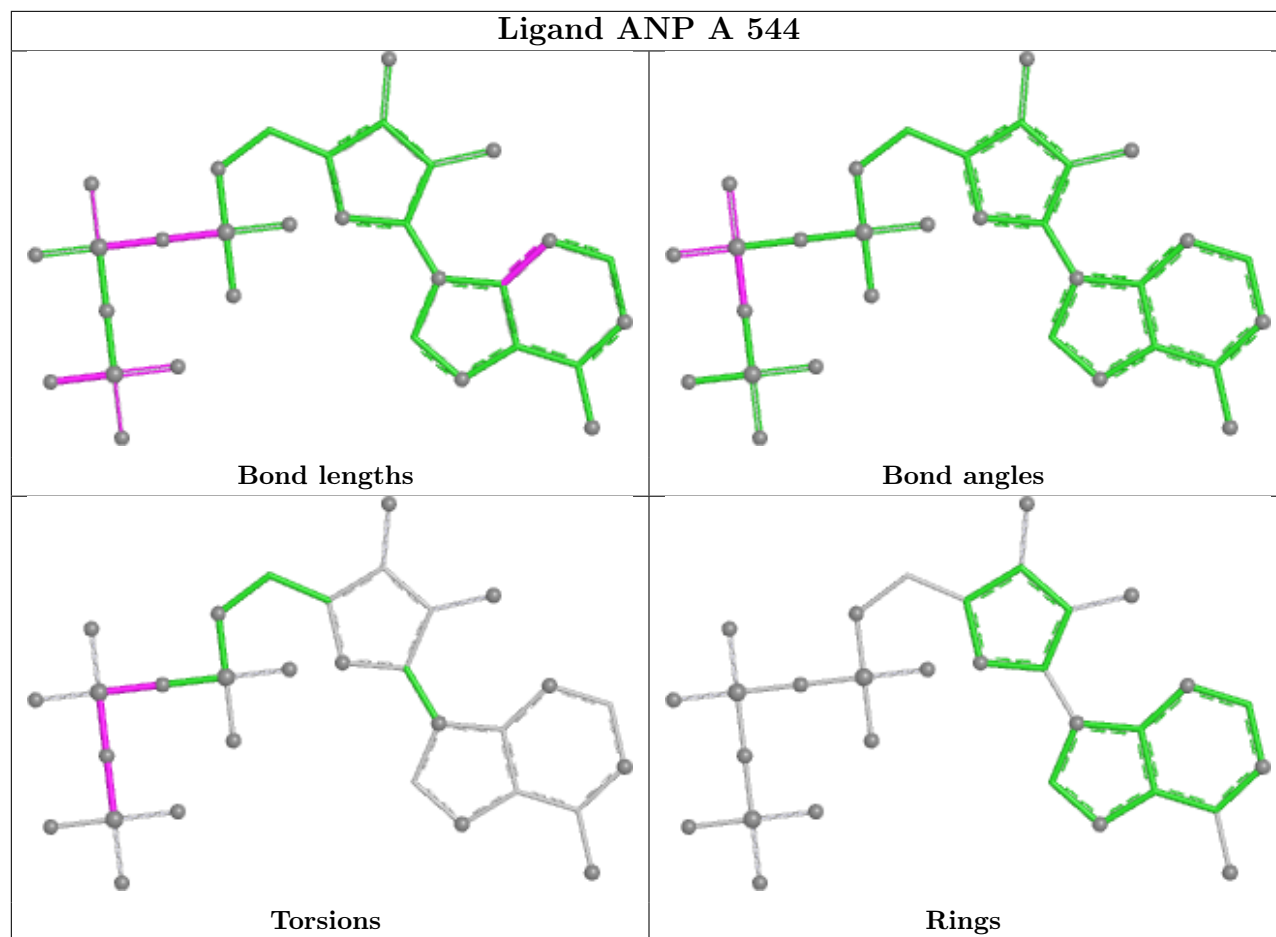
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 544 | ANP  | 4       | 0            |
| 2   | H     | 544 | ANP  | 2       | 0            |
| 2   | E     | 544 | ANP  | 4       | 0            |
| 2   | A     | 544 | ANP  | 2       | 0            |
| 2   | G     | 544 | ANP  | 3       | 0            |
| 2   | D     | 544 | ANP  | 4       | 0            |
| 2   | B     | 544 | ANP  | 4       | 0            |
| 2   | F     | 544 | ANP  | 3       | 0            |

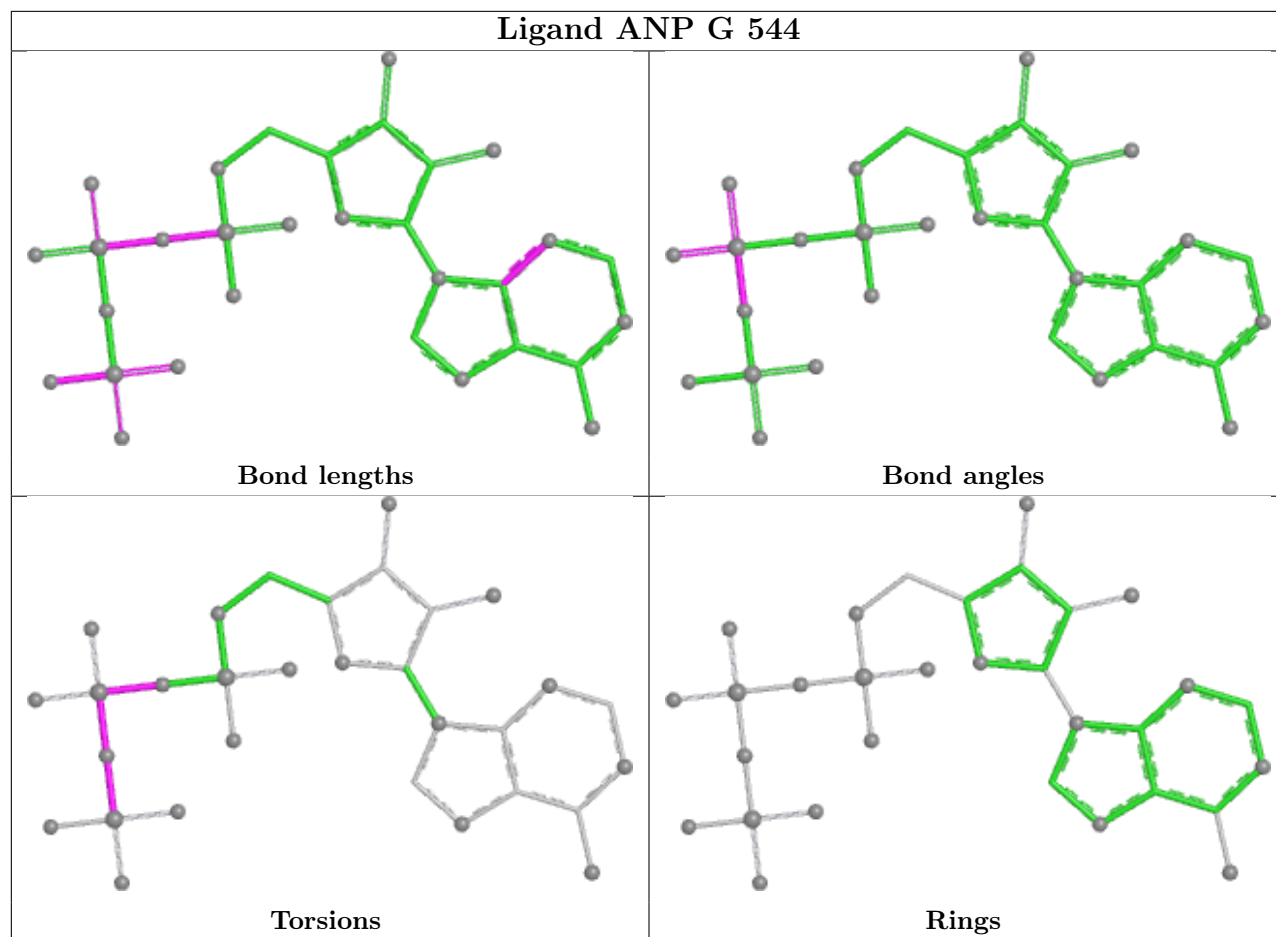
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

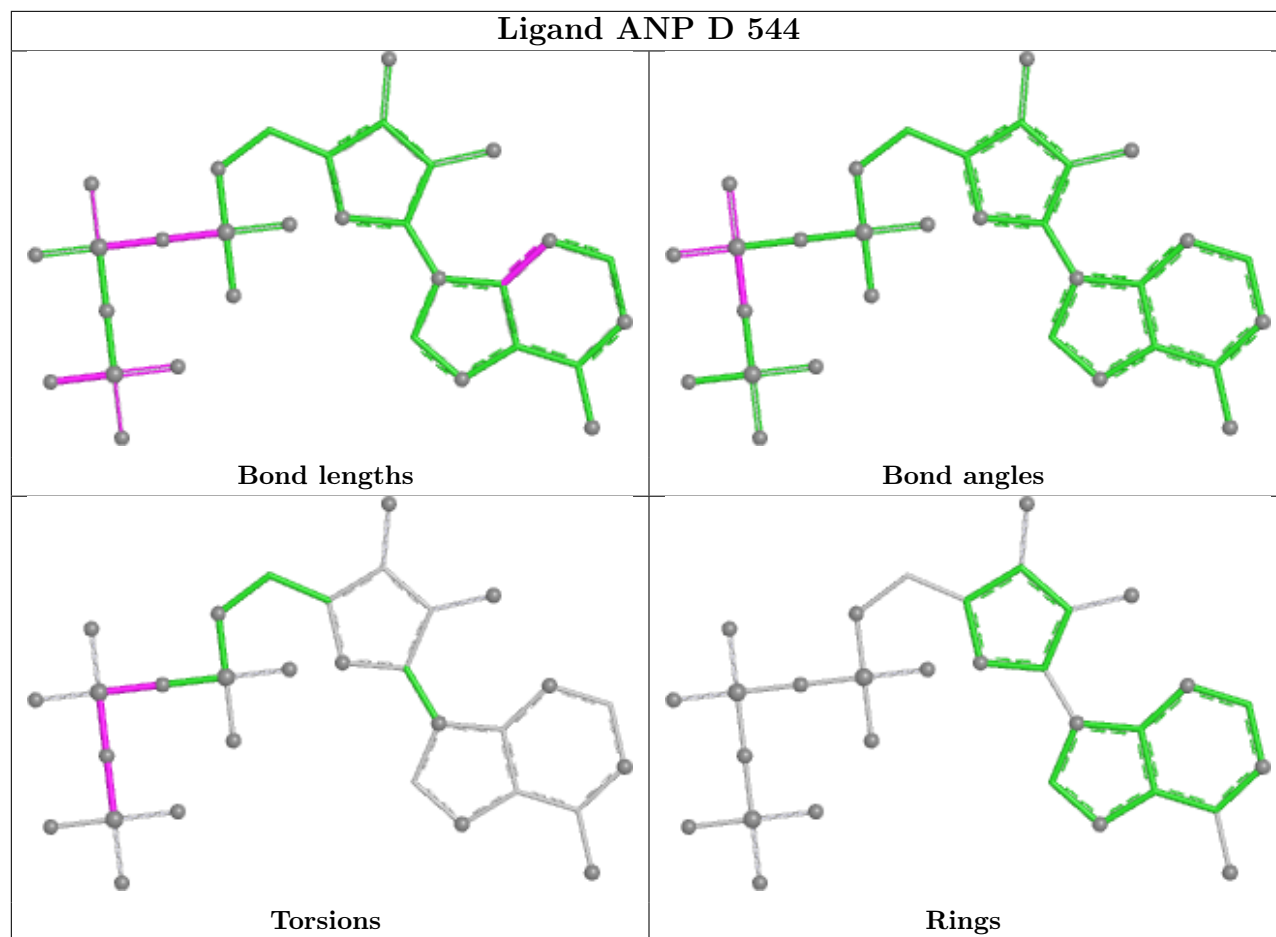


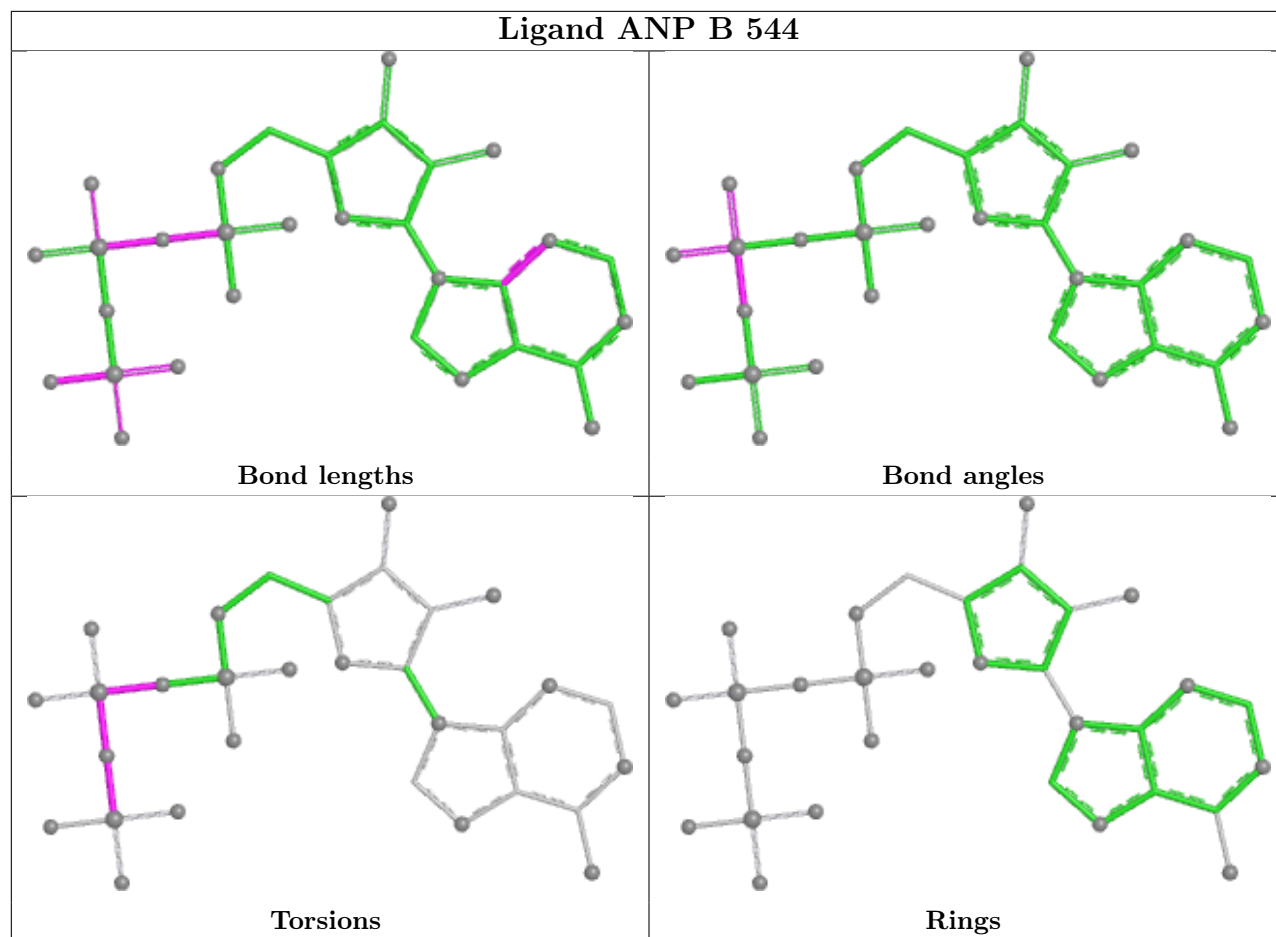


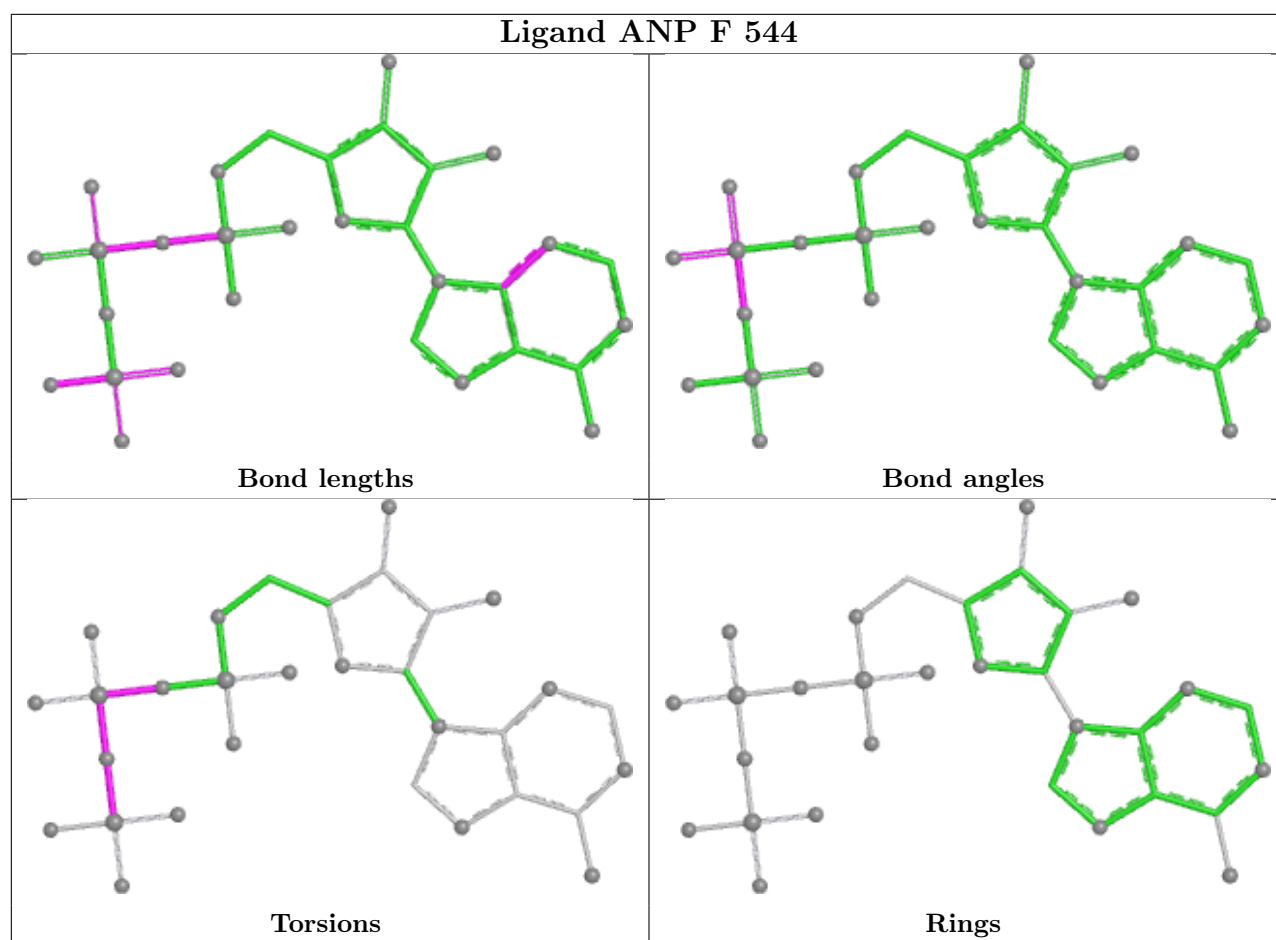












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 509/543 (93%)   | -0.17  | 1 (0%) 91 85 | 48, 89, 130, 187      | 0     |
| 1   | B     | 509/543 (93%)   | -0.19  | 1 (0%) 91 85 | 49, 89, 130, 186      | 0     |
| 1   | C     | 509/543 (93%)   | -0.12  | 0 100 100    | 48, 89, 130, 186      | 0     |
| 1   | D     | 509/543 (93%)   | -0.18  | 0 100 100    | 52, 91, 130, 187      | 0     |
| 1   | E     | 509/543 (93%)   | -0.15  | 2 (0%) 88 79 | 48, 88, 130, 187      | 0     |
| 1   | F     | 509/543 (93%)   | -0.18  | 1 (0%) 91 85 | 47, 89, 131, 186      | 0     |
| 1   | G     | 509/543 (93%)   | -0.12  | 0 100 100    | 48, 89, 130, 186      | 0     |
| 1   | H     | 509/543 (93%)   | -0.17  | 1 (0%) 91 85 | 52, 90, 131, 186      | 0     |
| All | All   | 4072/4344 (93%) | -0.16  | 6 (0%) 92 89 | 47, 90, 131, 187      | 0     |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 190 | LYS  | 2.5  |
| 1   | F     | 199 | SER  | 2.4  |
| 1   | H     | 16  | MET  | 2.2  |
| 1   | B     | 348 | ILE  | 2.2  |
| 1   | A     | 190 | LYS  | 2.1  |
| 1   | E     | 505 | SER  | 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 ⓘ

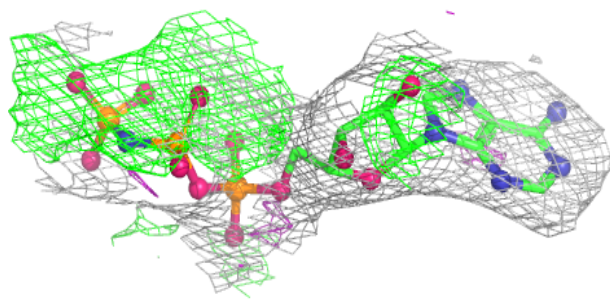
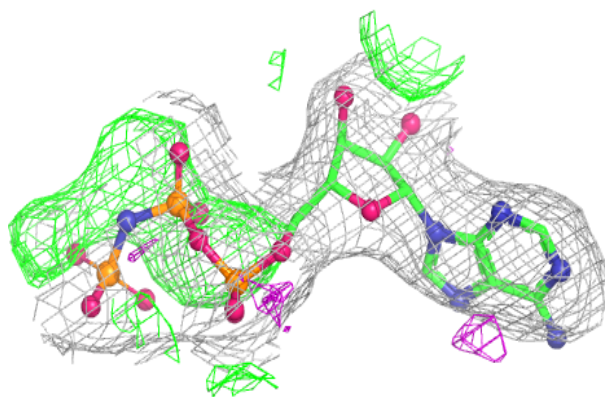
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | MG   | F     | 545 | 1/1   | 0.89 | 0.14 | 63,63,63,63                | 0     |
| 3   | MG   | B     | 545 | 1/1   | 0.90 | 0.15 | 74,74,74,74                | 0     |
| 2   | ANP  | F     | 544 | 31/31 | 0.91 | 0.12 | 38,81,97,98                | 0     |
| 3   | MG   | D     | 545 | 1/1   | 0.91 | 0.18 | 75,75,75,75                | 0     |
| 3   | MG   | A     | 545 | 1/1   | 0.91 | 0.13 | 61,61,61,61                | 0     |
| 2   | ANP  | B     | 544 | 31/31 | 0.92 | 0.11 | 39,80,102,107              | 0     |
| 2   | ANP  | D     | 544 | 31/31 | 0.92 | 0.12 | 45,89,117,118              | 0     |
| 2   | ANP  | A     | 544 | 31/31 | 0.92 | 0.11 | 45,70,89,97                | 0     |
| 2   | ANP  | H     | 544 | 31/31 | 0.92 | 0.12 | 47,84,112,115              | 0     |
| 3   | MG   | E     | 545 | 1/1   | 0.93 | 0.12 | 65,65,65,65                | 0     |
| 2   | ANP  | E     | 544 | 31/31 | 0.93 | 0.12 | 43,67,92,93                | 0     |
| 3   | MG   | H     | 545 | 1/1   | 0.93 | 0.15 | 57,57,57,57                | 0     |
| 2   | ANP  | G     | 544 | 31/31 | 0.94 | 0.11 | 41,75,93,101               | 0     |
| 2   | ANP  | C     | 544 | 31/31 | 0.94 | 0.10 | 41,77,100,103              | 0     |
| 3   | MG   | G     | 545 | 1/1   | 0.95 | 0.08 | 38,38,38,38                | 0     |
| 3   | MG   | C     | 545 | 1/1   | 0.95 | 0.10 | 52,52,52,52                | 0     |

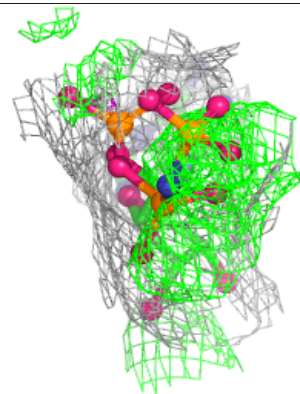
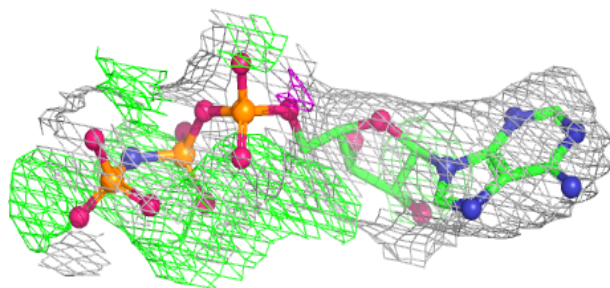
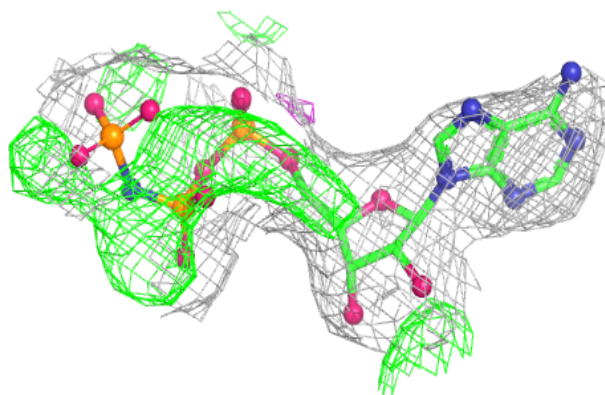
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP F 544:**

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

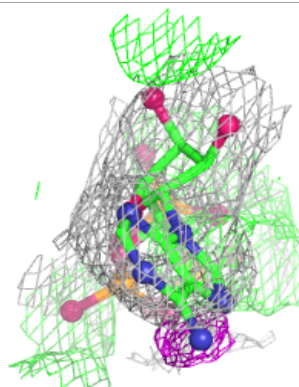
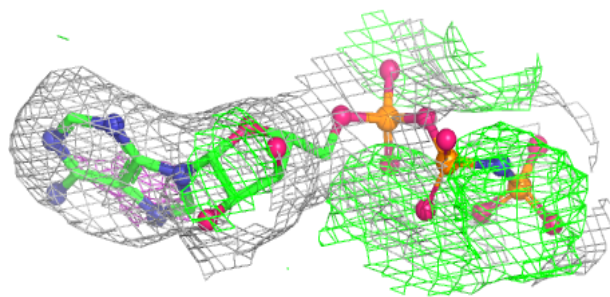
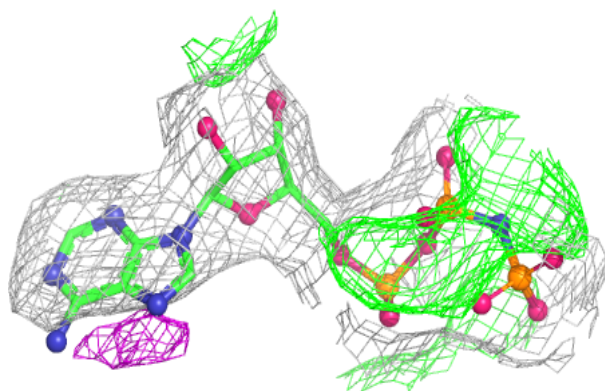
**Electron density around ANP B 544:**

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

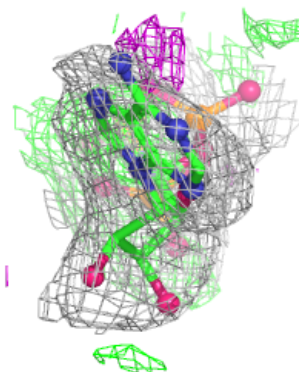
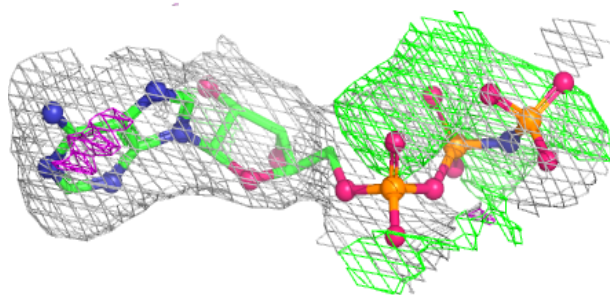
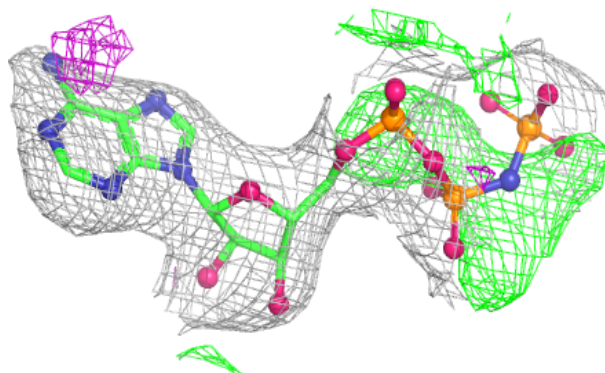


**Electron density around ANP D 544:**

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

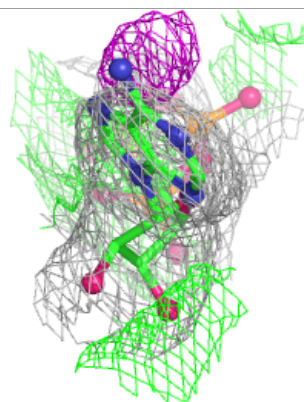
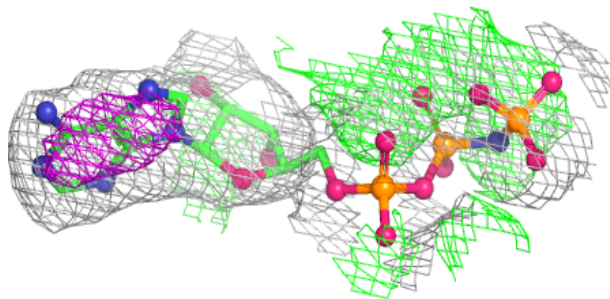
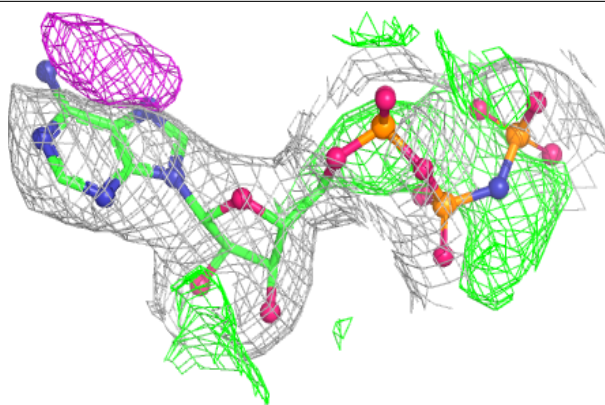
**Electron density around ANP A 544:**

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

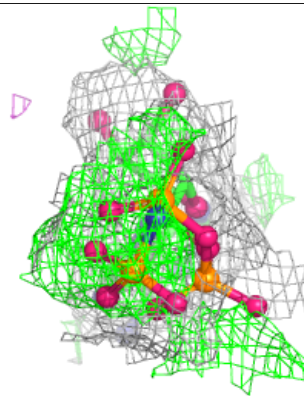
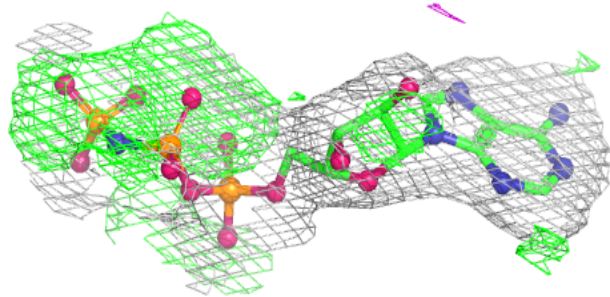
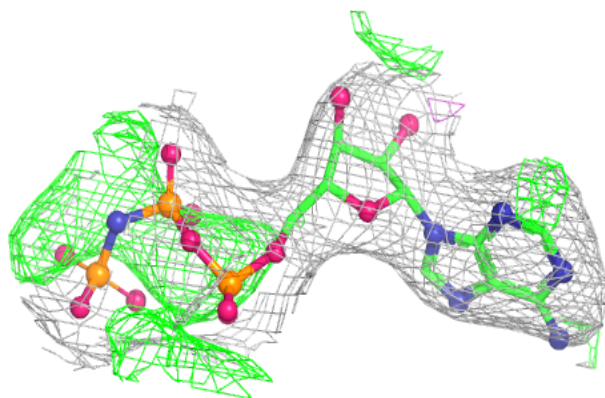


**Electron density around ANP H 544:**

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

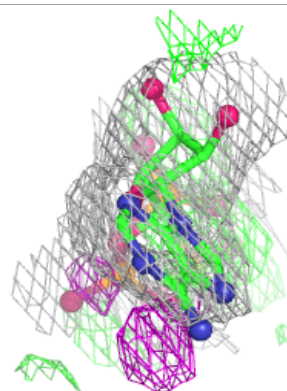
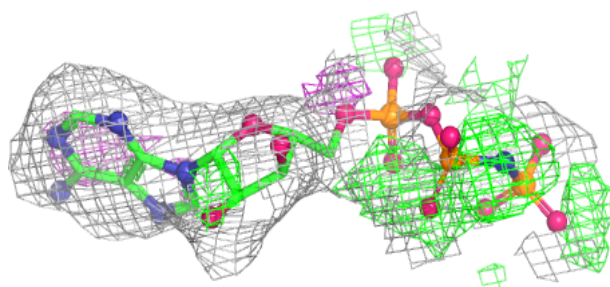
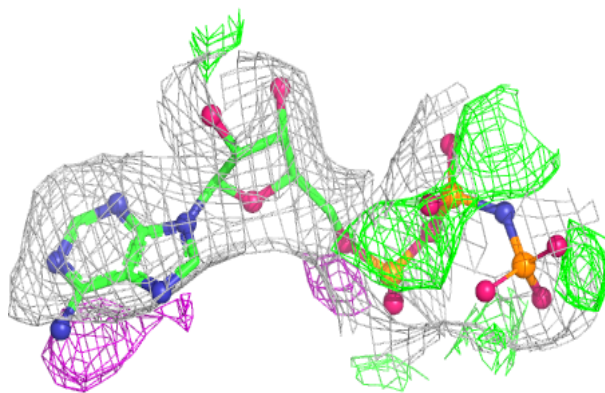
**Electron density around ANP E 544:**

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

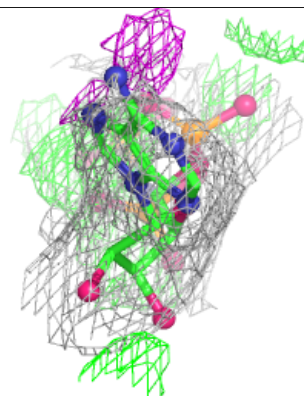
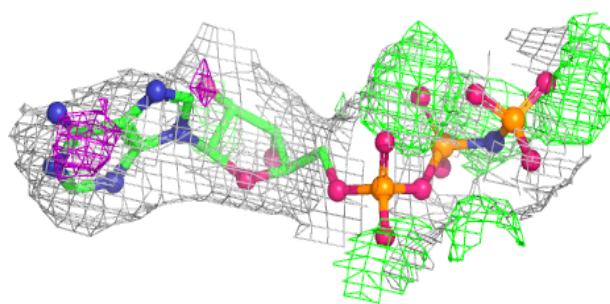
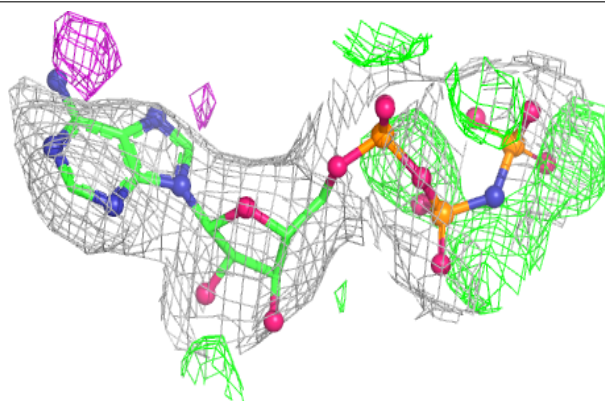


**Electron density around ANP G 544:**

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

**Electron density around ANP C 544:**

$2mF_o-DF_c$  (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.