



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 4R76 / pdb\_00004r76  
Title : Structure of the m17 leucyl aminopeptidase from malaria complexed with a hydroxamic acid-based inhibitor  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : 2014-08-27  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

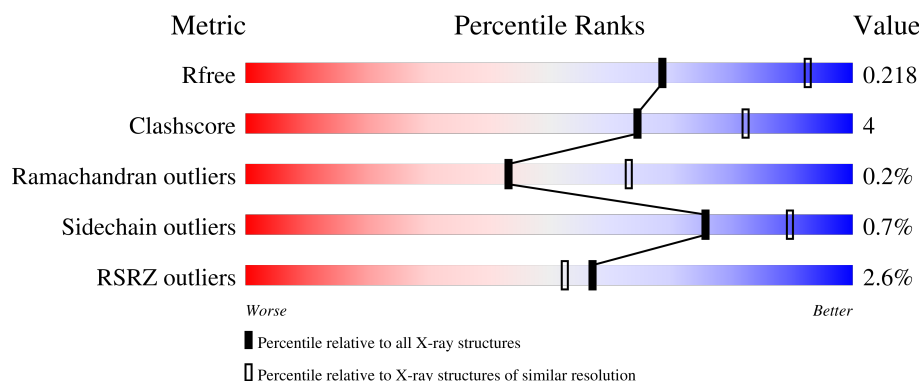
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 528    | <div> <div>0%</div> <div>86% 11% .</div> </div> |
| 1   | B     | 528    | <div> <div>4%</div> <div>86% 10% .</div> </div> |
| 1   | C     | 528    | <div> <div>2%</div> <div>88% 10% .</div> </div> |
| 1   | D     | 528    | <div> <div>2%</div> <div>87% 10% .</div> </div> |
| 1   | E     | 528    | <div> <div>2%</div> <div>85% 12% .</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 528    |                  |
| 1   | G     | 528    |                  |
| 1   | H     | 528    |                  |
| 1   | I     | 528    |                  |
| 1   | J     | 528    |                  |
| 1   | K     | 528    |                  |
| 1   | L     | 528    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5   | SO4  | A     | 1005 | -         | -        | X       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49162 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 M17 family aminopeptidase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 515      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3953  | 2542 | 634 | 758 | 19 |         |         |       |
| 1   | B     | 511      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3859  | 2484 | 625 | 731 | 19 |         |         |       |
| 1   | C     | 518      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3961  | 2547 | 639 | 756 | 19 |         |         |       |
| 1   | D     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3934  | 2533 | 633 | 748 | 20 |         |         |       |
| 1   | E     | 510      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3902  | 2514 | 625 | 744 | 19 |         |         |       |
| 1   | F     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3787  | 2440 | 611 | 717 | 19 |         |         |       |
| 1   | G     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3973  | 2552 | 638 | 764 | 19 |         |         |       |
| 1   | H     | 515      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3895  | 2504 | 630 | 742 | 19 |         |         |       |
| 1   | I     | 516      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3918  | 2521 | 630 | 748 | 19 |         |         |       |
| 1   | J     | 511      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3902  | 2513 | 629 | 741 | 19 |         |         |       |
| 1   | K     | 509      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3894  | 2508 | 624 | 743 | 19 |         |         |       |
| 1   | L     | 510      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3820  | 2455 | 614 | 732 | 19 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

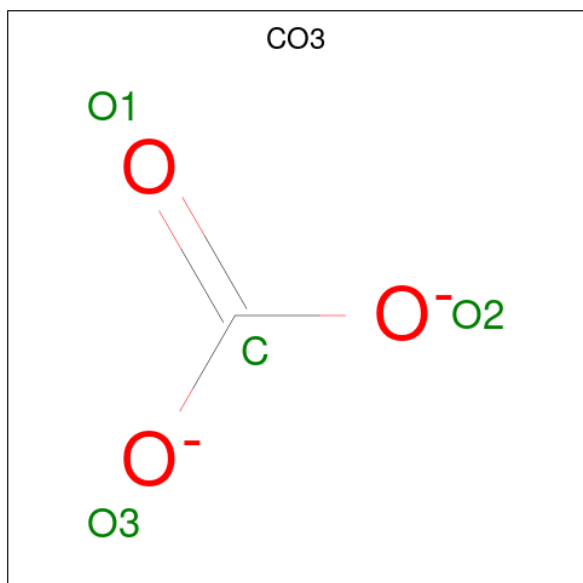
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | F     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | G     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | H     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | I     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | J     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | K     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | L     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).



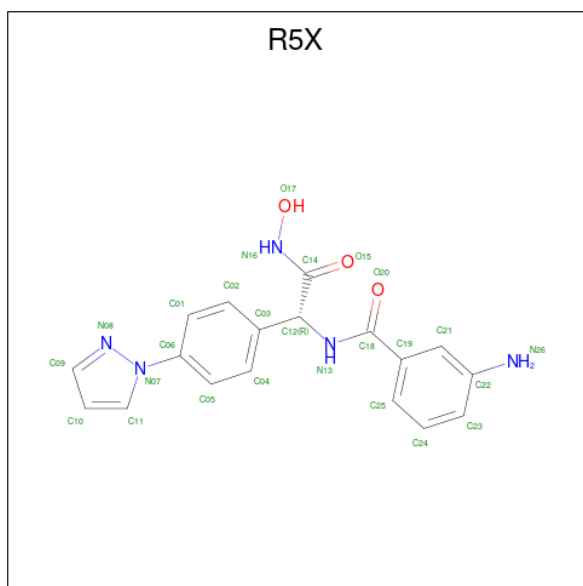
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

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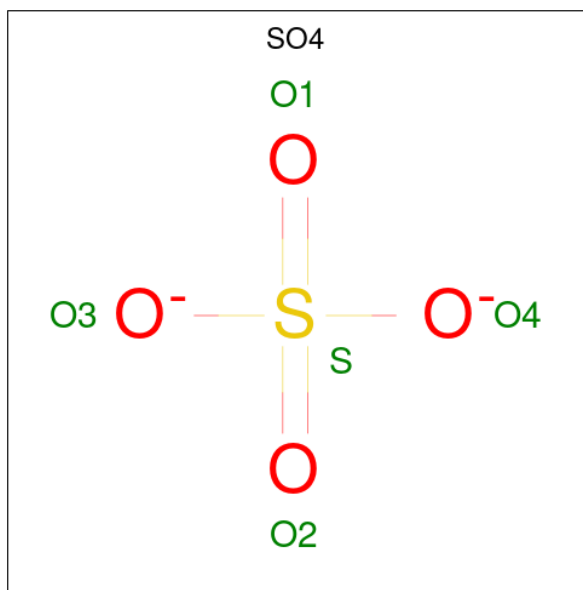
| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | B     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | C     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | D     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | E     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | F     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | G     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | H     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | I     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | J     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | K     | 1        | Total C O<br>4 1 3 | 0       | 0       |
| 3   | L     | 1        | Total C O<br>4 1 3 | 0       | 0       |

- Molecule 4 is 3-amino-N-{(1R)-2-(hydroxyamino)-2-oxo-1-[4-(1H-pyrazol-1-yl)phenyl]ethyl} benzamide (CCD ID: R5X) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>).



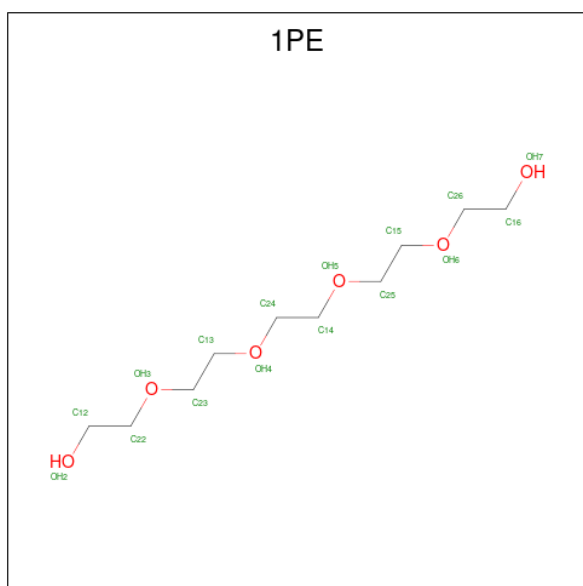
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |
| 4   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 26    | 18 | 5 | 3 |         |         |

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | A     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | H     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 5   | K     | 1        | Total O S<br>5 4 1 | 0       | 0       |

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 6   | B     | 1        | Total C O<br>10 6 4 | 0       | 0       |
| 6   | B     | 1        | Total C O<br>9 6 3  | 0       | 0       |
| 6   | E     | 1        | Total C O<br>10 6 4 | 0       | 0       |
| 6   | E     | 1        | Total C O<br>10 7 3 | 0       | 0       |
| 6   | F     | 1        | Total C O<br>8 6 2  | 0       | 0       |

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| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 6   | F     | 1        | Total C O<br>9 6 3  | 0       | 0       |
| 6   | F     | 1        | Total C O<br>9 6 3  | 0       | 0       |
| 6   | G     | 1        | Total C O<br>13 8 5 | 0       | 0       |
| 6   | G     | 1        | Total C O<br>10 6 4 | 0       | 0       |
| 6   | H     | 1        | Total C O<br>10 7 3 | 0       | 0       |
| 6   | I     | 1        | Total C O<br>10 6 4 | 0       | 0       |
| 6   | I     | 1        | Total C O<br>11 8 3 | 0       | 0       |
| 6   | J     | 1        | Total C O<br>10 6 4 | 0       | 0       |
| 6   | K     | 1        | Total C O<br>13 8 5 | 0       | 0       |
| 6   | L     | 1        | Total C O<br>7 4 3  | 0       | 0       |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 7   | A     | 170      | Total O<br>170 170 | 0       | 0       |
| 7   | B     | 125      | Total O<br>125 125 | 0       | 0       |
| 7   | C     | 155      | Total O<br>155 155 | 0       | 0       |
| 7   | D     | 174      | Total O<br>174 174 | 0       | 0       |
| 7   | E     | 151      | Total O<br>151 151 | 0       | 0       |
| 7   | F     | 119      | Total O<br>119 119 | 0       | 0       |
| 7   | G     | 150      | Total O<br>150 150 | 0       | 0       |
| 7   | H     | 133      | Total O<br>133 133 | 0       | 0       |
| 7   | I     | 143      | Total O<br>143 143 | 0       | 0       |

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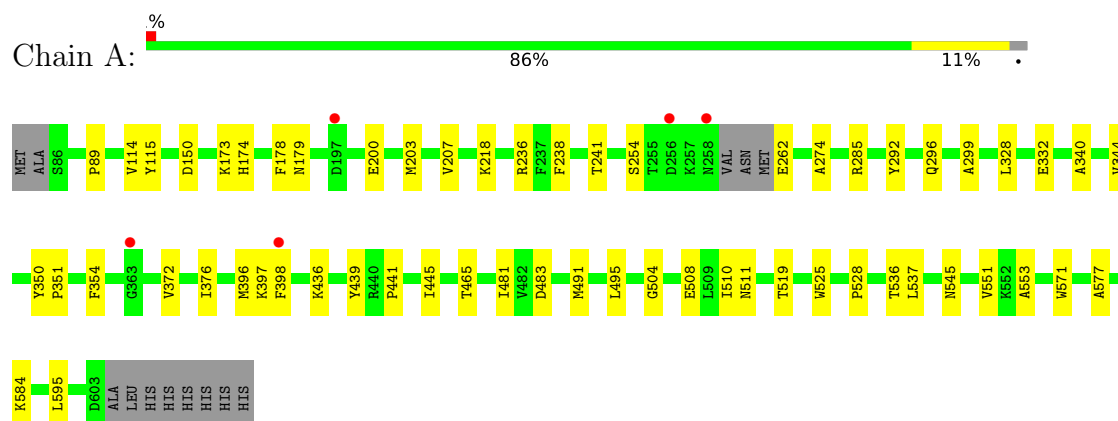
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | J     | 171      | Total<br>171 | O<br>171 | 0       | 0       |
| 7   | K     | 163      | Total<br>163 | O<br>163 | 0       | 0       |
| 7   | L     | 142      | Total<br>142 | O<br>142 | 0       | 0       |

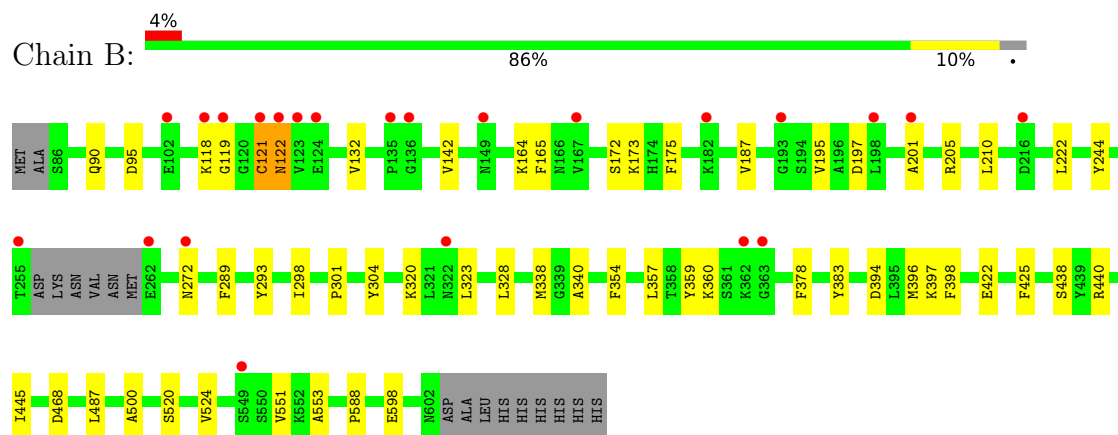
### 3 Residue-property plots

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.

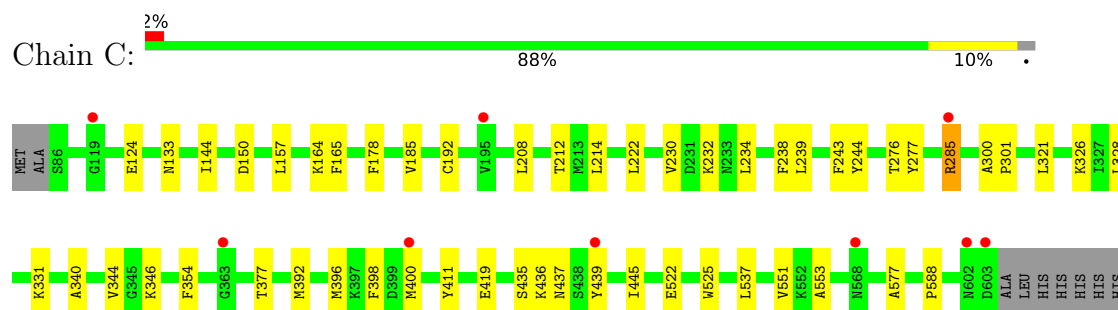
#### • Molecule 1: M17 family aminopeptidase



#### • Molecule 1: M17 family aminopeptidase



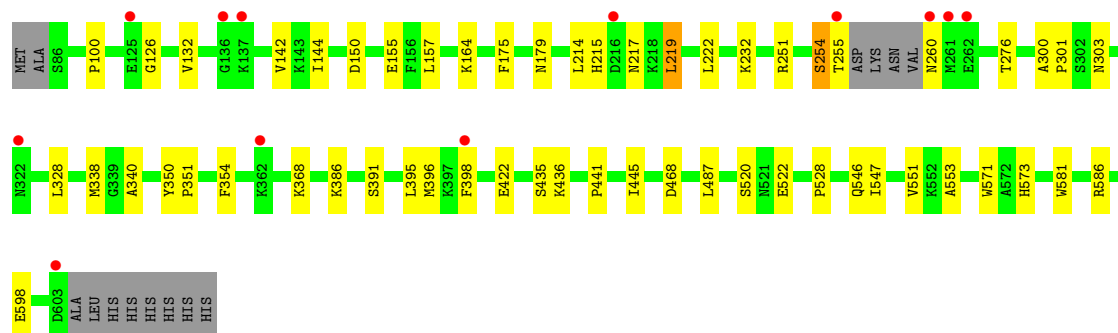
#### • Molecule 1: M17 family aminopeptidase



HIS

- Molecule 1: M17 family aminopeptidase

Chain D:  2% 87% 10%



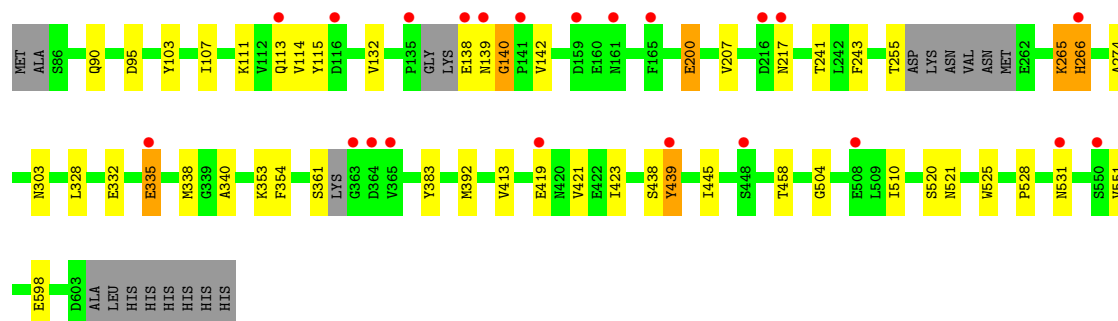
- Molecule 1: M17 family aminopeptidase

Chain E:  2% 85% 12%



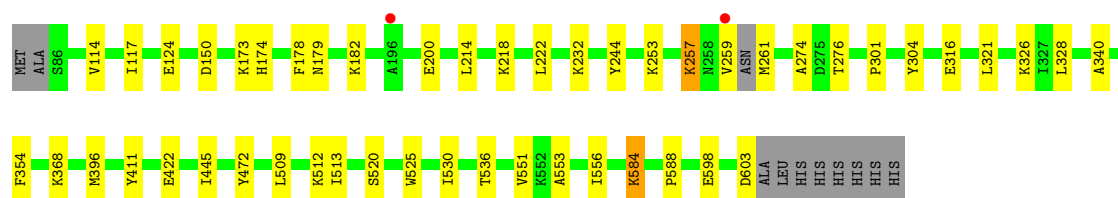
- Molecule 1: M17 family aminopeptidase

Chain F:  4% 87% 8%

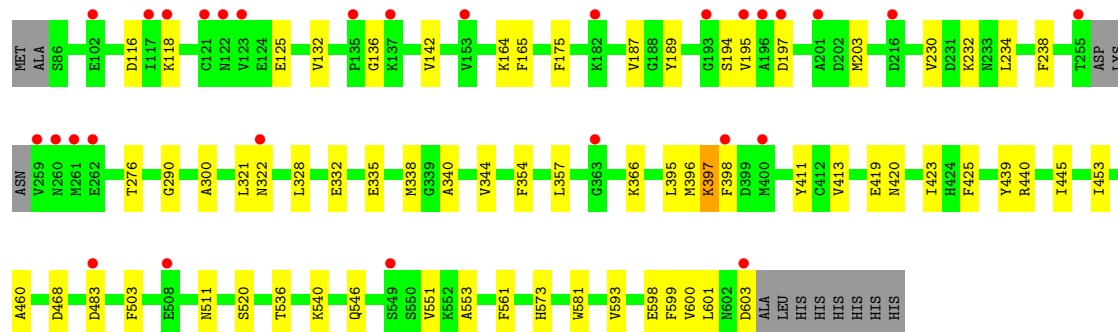
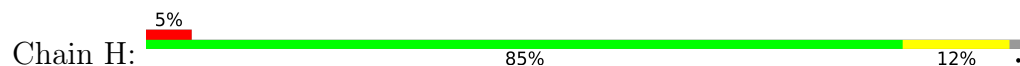


- Molecule 1: M17 family aminopeptidase

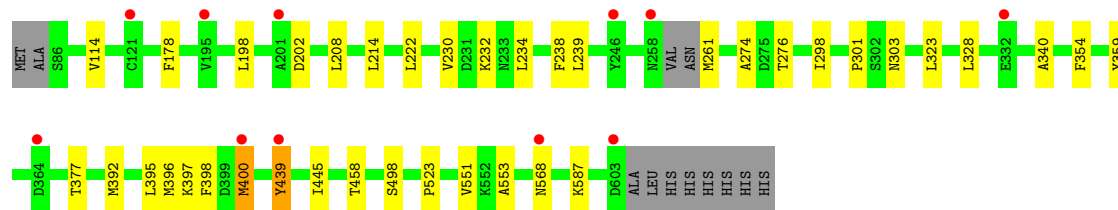
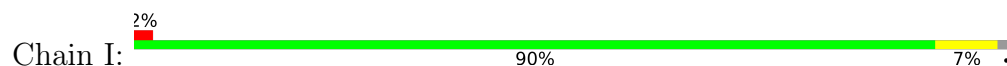
Chain G:  89% 9%



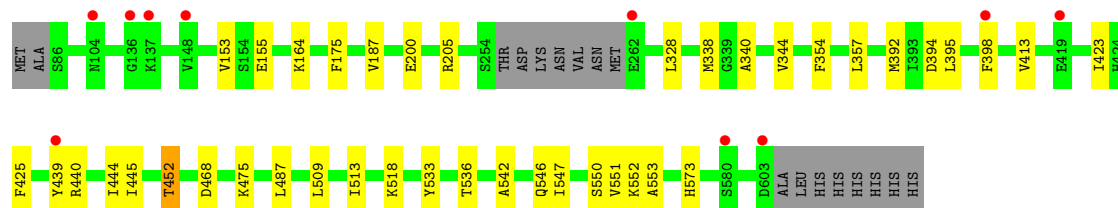
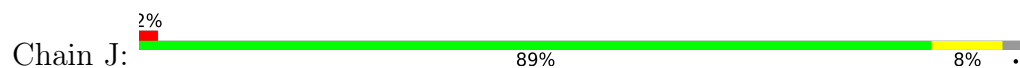
• Molecule 1: M17 family aminopeptidase



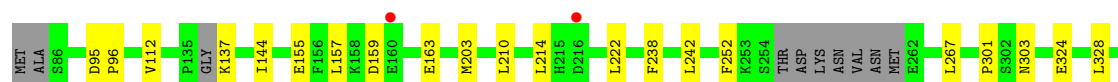
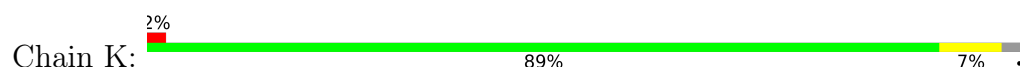
• Molecule 1: M17 family aminopeptidase

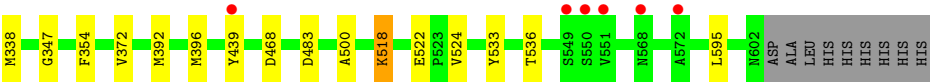


• Molecule 1: M17 family aminopeptidase

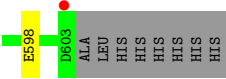
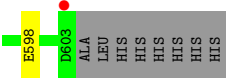
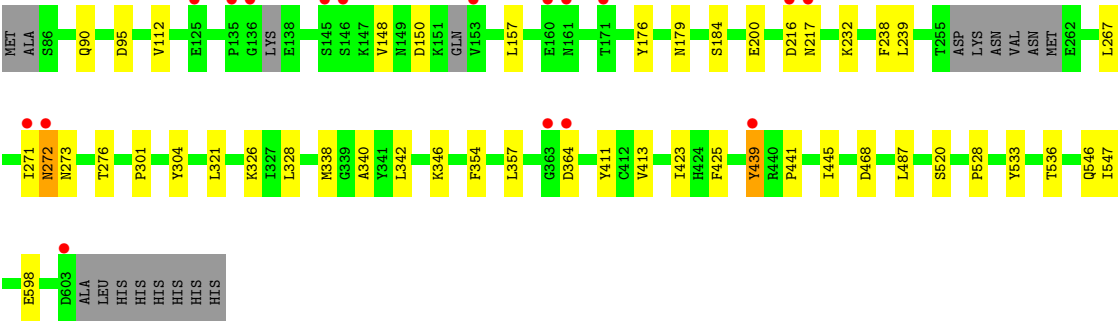
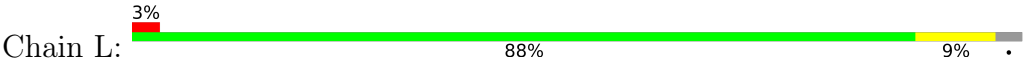


• Molecule 1: M17 family aminopeptidase





● Molecule 1: M17 family aminopeptidase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 174.04Å 177.41Å 231.77Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 36.21 – 2.50<br>36.21 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.4 (36.21-2.50)<br>72.5 (36.21-2.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.25 (at 2.51Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.4_1496                                           | Depositor        |
| R, $R_{free}$                                                           | 0.207 , 0.248<br>0.209 , 0.218                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1839 reflections (0.87%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 20.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.184                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 43.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for k,h,-l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 49162                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0131e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, R5X, 1PE, ZN, SO4

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     | 0.26         | 0/4033      | 0.70        | 0/5469          |
| 1   | B     | 0.27         | 0/3936      | 0.71        | 2/5349 (0.0%)   |
| 1   | C     | 0.26         | 0/4042      | 0.70        | 2/5485 (0.0%)   |
| 1   | D     | 0.27         | 0/4011      | 0.72        | 2/5439 (0.0%)   |
| 1   | E     | 0.27         | 0/3978      | 0.71        | 0/5396          |
| 1   | F     | 0.30         | 0/3862      | 0.74        | 4/5257 (0.1%)   |
| 1   | G     | 0.26         | 0/4050      | 0.70        | 0/5491          |
| 1   | H     | 0.27         | 0/3970      | 0.71        | 1/5394 (0.0%)   |
| 1   | I     | 0.27         | 0/3995      | 0.70        | 0/5422          |
| 1   | J     | 0.26         | 0/3979      | 0.71        | 0/5398          |
| 1   | K     | 0.26         | 0/3970      | 0.70        | 0/5386          |
| 1   | L     | 0.27         | 0/3895      | 0.71        | 0/5299          |
| All | All   | 0.27         | 0/47721     | 0.71        | 11/64785 (0.0%) |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 140 | GLY  | CA-C-N | 5.65  | 125.62      | 120.03   |
| 1   | F     | 140 | GLY  | C-N-CA | 5.65  | 125.62      | 120.03   |
| 1   | B     | 121 | CYS  | CA-C-N | -5.29 | 113.93      | 122.81   |
| 1   | B     | 121 | CYS  | C-N-CA | -5.29 | 113.93      | 122.81   |
| 1   | D     | 522 | GLU  | CA-C-N | 5.28  | 125.53      | 119.83   |
| 1   | D     | 522 | GLU  | C-N-CA | 5.28  | 125.53      | 119.83   |
| 1   | F     | 265 | LYS  | CA-C-N | -5.20 | 113.79      | 122.21   |
| 1   | F     | 265 | LYS  | C-N-CA | -5.20 | 113.79      | 122.21   |
| 1   | C     | 522 | GLU  | CA-C-N | 5.18  | 125.10      | 119.76   |
| 1   | C     | 522 | GLU  | C-N-CA | 5.18  | 125.10      | 119.76   |
| 1   | H     | 397 | LYS  | N-CA-C | -5.14 | 106.27      | 112.54   |

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     | 3953  | 0        | 3884     | 36      | 1            |
| 1   | B     | 3859  | 0        | 3745     | 32      | 0            |
| 1   | C     | 3961  | 0        | 3887     | 35      | 0            |
| 1   | D     | 3934  | 0        | 3865     | 35      | 0            |
| 1   | E     | 3902  | 0        | 3832     | 35      | 0            |
| 1   | F     | 3787  | 0        | 3598     | 32      | 0            |
| 1   | G     | 3973  | 0        | 3902     | 30      | 1            |
| 1   | H     | 3895  | 0        | 3777     | 44      | 0            |
| 1   | I     | 3918  | 0        | 3815     | 25      | 0            |
| 1   | J     | 3902  | 0        | 3826     | 28      | 0            |
| 1   | K     | 3894  | 0        | 3818     | 23      | 0            |
| 1   | L     | 3820  | 0        | 3646     | 30      | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 4     | 0        | 0        | 0       | 0            |
| 3   | B     | 4     | 0        | 0        | 0       | 0            |
| 3   | C     | 4     | 0        | 0        | 0       | 0            |
| 3   | D     | 4     | 0        | 0        | 0       | 0            |
| 3   | E     | 4     | 0        | 0        | 0       | 0            |
| 3   | F     | 4     | 0        | 0        | 0       | 0            |
| 3   | G     | 4     | 0        | 0        | 0       | 0            |
| 3   | H     | 4     | 0        | 0        | 0       | 0            |
| 3   | I     | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | J     | 4     | 0        | 0        | 0       | 0            |
| 3   | K     | 4     | 0        | 0        | 0       | 0            |
| 3   | L     | 4     | 0        | 0        | 0       | 0            |
| 4   | A     | 26    | 0        | 16       | 1       | 0            |
| 4   | B     | 26    | 0        | 16       | 1       | 0            |
| 4   | C     | 26    | 0        | 16       | 3       | 0            |
| 4   | D     | 26    | 0        | 16       | 1       | 0            |
| 4   | E     | 26    | 0        | 16       | 1       | 0            |
| 4   | F     | 26    | 0        | 16       | 1       | 0            |
| 4   | G     | 26    | 0        | 16       | 0       | 0            |
| 4   | H     | 26    | 0        | 16       | 0       | 0            |
| 4   | I     | 26    | 0        | 16       | 2       | 0            |
| 4   | J     | 26    | 0        | 16       | 3       | 0            |
| 4   | K     | 26    | 0        | 16       | 2       | 0            |
| 4   | L     | 26    | 0        | 16       | 2       | 0            |
| 5   | A     | 10    | 0        | 0        | 2       | 0            |
| 5   | E     | 10    | 0        | 0        | 0       | 0            |
| 5   | F     | 5     | 0        | 0        | 0       | 0            |
| 5   | H     | 5     | 0        | 0        | 0       | 0            |
| 5   | K     | 5     | 0        | 0        | 0       | 0            |
| 6   | B     | 19    | 0        | 23       | 1       | 0            |
| 6   | E     | 20    | 0        | 23       | 0       | 0            |
| 6   | F     | 26    | 0        | 28       | 1       | 0            |
| 6   | G     | 23    | 0        | 29       | 2       | 0            |
| 6   | H     | 10    | 0        | 10       | 0       | 0            |
| 6   | I     | 21    | 0        | 24       | 0       | 0            |
| 6   | J     | 10    | 0        | 13       | 0       | 0            |
| 6   | K     | 13    | 0        | 17       | 0       | 0            |
| 6   | L     | 7     | 0        | 9        | 0       | 0            |
| 7   | A     | 170   | 0        | 0        | 6       | 0            |
| 7   | B     | 125   | 0        | 0        | 1       | 0            |
| 7   | C     | 155   | 0        | 0        | 2       | 0            |
| 7   | D     | 174   | 0        | 0        | 2       | 0            |
| 7   | E     | 151   | 0        | 0        | 1       | 0            |
| 7   | F     | 119   | 0        | 0        | 1       | 0            |
| 7   | G     | 150   | 0        | 0        | 2       | 0            |
| 7   | H     | 133   | 0        | 0        | 7       | 0            |
| 7   | I     | 143   | 0        | 0        | 1       | 0            |
| 7   | J     | 171   | 0        | 0        | 4       | 0            |
| 7   | K     | 163   | 0        | 0        | 2       | 0            |
| 7   | L     | 142   | 0        | 0        | 1       | 0            |
| All | All   | 49162 | 0        | 45963    | 360     | 1            |

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 4.

All (360) 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:E:395:LEU:O    | 1:E:397:LYS:N    | 2.15                     | 0.79              |
| 1:J:328:LEU:HB2  | 1:J:354:PHE:HB3  | 1.65                     | 0.77              |
| 1:C:392:MET:HE3  | 4:C:1004:R5X:H8  | 1.67                     | 0.76              |
| 1:G:326:LYS:NZ   | 1:G:472:TYR:OH   | 2.20                     | 0.73              |
| 1:L:176:TYR:OH   | 1:L:217:ASN:OD1  | 2.07                     | 0.72              |
| 1:H:335:GLU:OE2  | 1:H:335:GLU:CG   | 2.38                     | 0.72              |
| 1:C:164:LYS:NZ   | 1:E:184:SER:OG   | 2.23                     | 0.71              |
| 1:C:328:LEU:HB2  | 1:C:354:PHE:HB3  | 1.71                     | 0.71              |
| 1:H:335:GLU:CG   | 1:H:335:GLU:OE1  | 2.38                     | 0.71              |
| 1:I:392:MET:HE3  | 4:I:1004:R5X:H1  | 1.71                     | 0.71              |
| 1:G:368:LYS:NZ   | 1:G:422:GLU:OE1  | 2.25                     | 0.70              |
| 1:K:328:LEU:HB2  | 1:K:354:PHE:HB3  | 1.75                     | 0.69              |
| 1:I:328:LEU:HB2  | 1:I:354:PHE:HB3  | 1.75                     | 0.69              |
| 1:H:328:LEU:HB2  | 1:H:354:PHE:HB3  | 1.74                     | 0.69              |
| 1:D:126:GLY:HA2  | 1:D:219:LEU:HG   | 1.76                     | 0.68              |
| 1:D:132:VAL:HG21 | 1:D:142:VAL:HG13 | 1.76                     | 0.68              |
| 1:L:232:LYS:NZ   | 7:L:1209:HOH:O   | 2.27                     | 0.67              |
| 1:E:328:LEU:HB2  | 1:E:354:PHE:HB3  | 1.77                     | 0.67              |
| 1:I:340:ALA:HA   | 1:I:445:ILE:HD12 | 1.77                     | 0.67              |
| 1:J:392:MET:HE3  | 4:J:1004:R5X:H1  | 1.77                     | 0.67              |
| 1:I:214:LEU:HD21 | 1:I:222:LEU:HD22 | 1.77                     | 0.66              |
| 1:L:90:GLN:NE2   | 1:L:95:ASP:O     | 2.24                     | 0.66              |
| 1:A:173:LYS:NZ   | 7:A:1104:HOH:O   | 2.29                     | 0.66              |
| 1:H:366:LYS:HG3  | 1:H:420:ASN:HB3  | 1.76                     | 0.65              |
| 1:F:328:LEU:HB2  | 1:F:354:PHE:HB3  | 1.76                     | 0.65              |
| 1:G:173:LYS:NZ   | 7:G:1111:HOH:O   | 2.30                     | 0.65              |
| 1:C:300:ALA:O    | 7:C:1101:HOH:O   | 2.14                     | 0.65              |
| 1:L:328:LEU:HB2  | 1:L:354:PHE:HB3  | 1.78                     | 0.64              |
| 1:I:551:VAL:HG12 | 1:I:553:ALA:H    | 1.63                     | 0.64              |
| 1:I:178:PHE:HZ   | 1:K:155:GLU:HG2  | 1.63                     | 0.64              |
| 1:H:136:GLY:N    | 7:H:1139:HOH:O   | 2.31                     | 0.64              |
| 1:H:332:GLU:OE1  | 7:H:1137:HOH:O   | 2.15                     | 0.63              |
| 1:H:322:ASN:OD1  | 7:H:1228:HOH:O   | 2.14                     | 0.63              |
| 1:E:161:ASN:HA   | 1:E:164:LYS:HE2  | 1.81                     | 0.62              |
| 1:I:439:TYR:OH   | 1:I:458:THR:O    | 2.17                     | 0.62              |
| 1:B:122:ASN:N    | 1:B:122:ASN:HD22 | 1.97                     | 0.62              |
| 1:E:340:ALA:HA   | 1:E:445:ILE:HD12 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:144:ILE:HG13 | 1:K:157:LEU:HD22 | 1.82                     | 0.62              |
| 1:G:253:LYS:HB2  | 1:G:257:LYS:HE3  | 1.83                     | 0.61              |
| 1:A:577:ALA:HB1  | 4:A:1004:R5X:H9  | 1.83                     | 0.61              |
| 1:H:232:LYS:NZ   | 1:H:276:THR:O    | 2.33                     | 0.61              |
| 1:H:551:VAL:HG12 | 1:H:553:ALA:H    | 1.66                     | 0.61              |
| 1:B:328:LEU:HB2  | 1:B:354:PHE:HB3  | 1.83                     | 0.60              |
| 1:B:440:ARG:NH1  | 7:B:1106:HOH:O   | 2.31                     | 0.60              |
| 1:C:340:ALA:HA   | 1:C:445:ILE:HD12 | 1.83                     | 0.60              |
| 1:F:340:ALA:HA   | 1:F:445:ILE:HD12 | 1.82                     | 0.60              |
| 1:D:100:PRO:O    | 1:D:251:ARG:NH1  | 2.29                     | 0.60              |
| 1:H:460:ALA:O    | 1:H:546:GLN:NE2  | 2.34                     | 0.60              |
| 1:B:551:VAL:HG12 | 1:B:553:ALA:H    | 1.66                     | 0.60              |
| 1:E:232:LYS:NZ   | 1:E:276:THR:O    | 2.35                     | 0.60              |
| 1:G:232:LYS:NZ   | 1:G:276:THR:O    | 2.33                     | 0.60              |
| 1:H:335:GLU:OE2  | 1:H:335:GLU:OE1  | 2.20                     | 0.59              |
| 1:I:232:LYS:NZ   | 1:I:276:THR:O    | 2.34                     | 0.59              |
| 1:E:112:VAL:HG22 | 1:E:267:LEU:HB3  | 1.84                     | 0.59              |
| 1:H:338:MET:HE3  | 1:H:468:ASP:HB3  | 1.83                     | 0.59              |
| 1:I:261:MET:N    | 7:I:1105:HOH:O   | 2.34                     | 0.59              |
| 1:H:321:LEU:HD11 | 1:H:411:TYR:HA   | 1.83                     | 0.59              |
| 1:H:511:ASN:ND2  | 7:H:1124:HOH:O   | 2.35                     | 0.58              |
| 1:A:178:PHE:HZ   | 1:D:155:GLU:HG2  | 1.68                     | 0.58              |
| 1:L:112:VAL:HG22 | 1:L:267:LEU:HB3  | 1.86                     | 0.58              |
| 1:D:520:SER:HB3  | 1:D:598:GLU:HG3  | 1.86                     | 0.58              |
| 1:A:203:MET:HE2  | 1:A:238:PHE:HD1  | 1.69                     | 0.58              |
| 1:G:214:LEU:HD21 | 1:G:222:LEU:HD22 | 1.86                     | 0.57              |
| 1:B:340:ALA:HA   | 1:B:445:ILE:HD12 | 1.87                     | 0.57              |
| 1:B:132:VAL:HG21 | 1:B:142:VAL:HG13 | 1.87                     | 0.57              |
| 1:L:340:ALA:HA   | 1:L:445:ILE:HD12 | 1.84                     | 0.57              |
| 1:D:328:LEU:HB2  | 1:D:354:PHE:HB3  | 1.87                     | 0.56              |
| 1:F:138:GLU:N    | 1:F:140:GLY:H    | 2.03                     | 0.56              |
| 1:G:259:VAL:O    | 1:G:261:MET:N    | 2.39                     | 0.56              |
| 1:J:395:LEU:O    | 1:J:398:PHE:HB3  | 2.05                     | 0.56              |
| 1:H:300:ALA:O    | 7:H:1102:HOH:O   | 2.17                     | 0.56              |
| 1:A:328:LEU:HB2  | 1:A:354:PHE:HB3  | 1.87                     | 0.56              |
| 1:B:357:LEU:HB2  | 1:B:425:PHE:HB2  | 1.87                     | 0.56              |
| 1:L:520:SER:HB3  | 1:L:598:GLU:HG3  | 1.87                     | 0.56              |
| 1:B:320:LYS:NZ   | 6:B:1005:1PE:OH4 | 2.35                     | 0.56              |
| 1:A:504:GLY:HA3  | 1:A:510:ILE:HD11 | 1.87                     | 0.55              |
| 1:D:214:LEU:HD21 | 1:D:222:LEU:HD22 | 1.88                     | 0.55              |
| 1:F:439:TYR:OH   | 1:F:458:THR:O    | 2.24                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:230:VAL:HG12 | 1:I:234:LEU:HD23 | 1.88                     | 0.55              |
| 1:J:475:LYS:NZ   | 7:J:1232:HOH:O   | 2.39                     | 0.55              |
| 1:A:551:VAL:HG12 | 1:A:553:ALA:H    | 1.70                     | 0.55              |
| 1:H:600:VAL:O    | 1:H:603:ASP:HB3  | 2.06                     | 0.55              |
| 1:C:232:LYS:NZ   | 1:C:276:THR:O    | 2.39                     | 0.55              |
| 1:F:132:VAL:HG21 | 1:F:142:VAL:HG13 | 1.89                     | 0.55              |
| 1:A:262:GLU:N    | 7:A:1219:HOH:O   | 2.40                     | 0.55              |
| 1:C:326:LYS:HE2  | 1:C:328:LEU:HD21 | 1.89                     | 0.55              |
| 1:D:232:LYS:NZ   | 1:D:276:THR:O    | 2.38                     | 0.55              |
| 1:A:218:LYS:O    | 1:D:164:LYS:NZ   | 2.39                     | 0.55              |
| 1:A:340:ALA:HA   | 1:A:445:ILE:HD12 | 1.88                     | 0.55              |
| 1:H:164:LYS:NZ   | 1:L:184:SER:OG   | 2.40                     | 0.55              |
| 1:K:392:MET:HE3  | 4:K:1004:R5X:H1  | 1.87                     | 0.55              |
| 1:F:113:GLN:OE1  | 1:F:115:TYR:OH   | 2.24                     | 0.55              |
| 1:D:217:ASN:HD21 | 1:D:219:LEU:HB2  | 1.72                     | 0.54              |
| 1:H:483:ASP:OD2  | 1:H:573:HIS:ND1  | 2.26                     | 0.54              |
| 1:I:238:PHE:HD2  | 1:I:239:LEU:HD12 | 1.73                     | 0.54              |
| 1:G:551:VAL:HG12 | 1:G:553:ALA:H    | 1.72                     | 0.54              |
| 1:G:178:PHE:HZ   | 1:J:155:GLU:HG2  | 1.73                     | 0.54              |
| 1:H:340:ALA:HA   | 1:H:445:ILE:HD12 | 1.89                     | 0.54              |
| 1:E:543:ASP:CG   | 1:F:255:THR:H    | 2.16                     | 0.54              |
| 1:L:413:VAL:HG11 | 1:L:423:ILE:HD12 | 1.89                     | 0.54              |
| 1:F:90:GLN:NE2   | 1:F:95:ASP:O     | 2.38                     | 0.53              |
| 1:C:230:VAL:O    | 1:C:277:TYR:OH   | 2.19                     | 0.53              |
| 1:B:122:ASN:N    | 1:B:122:ASN:ND2  | 2.57                     | 0.53              |
| 1:G:328:LEU:HB2  | 1:G:354:PHE:HB3  | 1.90                     | 0.53              |
| 1:F:114:VAL:HG12 | 1:F:274:ALA:HB1  | 1.90                     | 0.53              |
| 1:L:533:TYR:O    | 1:L:536:THR:HG22 | 2.09                     | 0.53              |
| 1:C:214:LEU:HD21 | 1:C:222:LEU:HD22 | 1.90                     | 0.53              |
| 1:D:551:VAL:HG12 | 1:D:553:ALA:H    | 1.74                     | 0.52              |
| 1:B:175:PHE:N    | 1:B:187:VAL:O    | 2.39                     | 0.52              |
| 1:J:164:LYS:NZ   | 7:J:1206:HOH:O   | 2.40                     | 0.52              |
| 1:F:265:LYS:C    | 1:F:266:HIS:CD2  | 2.87                     | 0.52              |
| 1:D:441:PRO:HB2  | 1:E:394:ASP:HA   | 1.92                     | 0.52              |
| 1:E:451:LYS:NZ   | 1:E:564:GLU:O    | 2.37                     | 0.52              |
| 1:B:500:ALA:HB3  | 1:B:524:VAL:HG22 | 1.92                     | 0.52              |
| 1:K:533:TYR:O    | 1:K:536:THR:HG22 | 2.09                     | 0.52              |
| 1:B:121:CYS:C    | 1:B:122:ASN:HD22 | 2.18                     | 0.51              |
| 1:J:357:LEU:HB2  | 1:J:425:PHE:HB2  | 1.91                     | 0.51              |
| 1:A:511:ASN:ND2  | 7:A:1238:HOH:O   | 2.40                     | 0.51              |
| 1:L:216:ASP:C    | 1:L:217:ASN:HD22 | 2.17                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:244:TYR:OH   | 1:B:588:PRO:O     | 2.29                     | 0.51              |
| 1:C:243:PHE:CE2  | 1:C:285:ARG:HG2   | 2.45                     | 0.51              |
| 1:C:392:MET:CE   | 4:C:1004:R5X:H8   | 2.40                     | 0.51              |
| 1:F:520:SER:HB3  | 1:F:598:GLU:HG3   | 1.91                     | 0.51              |
| 1:K:203:MET:HE2  | 1:K:238:PHE:HD1   | 1.75                     | 0.51              |
| 1:E:238:PHE:HD2  | 1:E:239:LEU:HD12  | 1.75                     | 0.51              |
| 1:F:504:GLY:HA3  | 1:F:510:ILE:HD11  | 1.93                     | 0.51              |
| 1:K:439:TYR:H    | 1:K:439:TYR:HD2   | 1.59                     | 0.50              |
| 1:A:299:ALA:O    | 1:A:397:LYS:NZ    | 2.37                     | 0.50              |
| 1:G:512:LYS:NZ   | 1:G:603:ASP:OD1   | 2.40                     | 0.50              |
| 1:E:144:ILE:HG13 | 1:E:157:LEU:HD22  | 1.93                     | 0.50              |
| 1:H:540:LYS:NZ   | 1:I:587:LYS:HD3   | 2.27                     | 0.50              |
| 1:F:265:LYS:C    | 1:F:266:HIS:HD2   | 2.19                     | 0.50              |
| 1:A:536:THR:HG21 | 1:A:551:VAL:HG23  | 1.93                     | 0.50              |
| 1:K:137:LYS:N    | 7:K:1186:HOH:O    | 2.45                     | 0.50              |
| 1:K:392:MET:CE   | 4:K:1004:R5X:H1   | 2.42                     | 0.50              |
| 1:I:114:VAL:HG12 | 1:I:274:ALA:HB1   | 1.94                     | 0.49              |
| 1:L:546:GLN:HG2  | 1:L:547:ILE:HG23  | 1.93                     | 0.49              |
| 1:C:243:PHE:HE2  | 1:C:285:ARG:HG2   | 1.77                     | 0.49              |
| 1:F:111:LYS:O    | 1:F:266:HIS:HB3   | 2.11                     | 0.49              |
| 1:B:520:SER:HB3  | 1:B:598:GLU:HG3   | 1.94                     | 0.49              |
| 1:J:440:ARG:NH1  | 7:J:1127:HOH:O    | 2.42                     | 0.49              |
| 1:L:321:LEU:HD11 | 1:L:411:TYR:HA    | 1.94                     | 0.49              |
| 1:C:244:TYR:OH   | 1:C:588:PRO:O     | 2.31                     | 0.49              |
| 1:H:175:PHE:N    | 1:H:187:VAL:O     | 2.39                     | 0.49              |
| 1:H:230:VAL:HG12 | 1:H:234:LEU:HD23  | 1.95                     | 0.48              |
| 1:A:396:MET:SD   | 1:A:398:PHE:HE2   | 2.36                     | 0.48              |
| 1:C:238:PHE:HD2  | 1:C:239:LEU:HD12  | 1.78                     | 0.48              |
| 1:L:238:PHE:HD2  | 1:L:239:LEU:HD12  | 1.77                     | 0.48              |
| 1:A:376:ILE:HD11 | 1:A:465:THR:HG21  | 1.95                     | 0.48              |
| 1:D:338:MET:HE3  | 1:D:468:ASP:HB3   | 1.93                     | 0.48              |
| 1:G:411:TYR:HE1  | 6:G:1005:1PE:H252 | 1.78                     | 0.48              |
| 1:H:203:MET:HE2  | 1:H:238:PHE:HD1   | 1.79                     | 0.48              |
| 1:J:340:ALA:HA   | 1:J:445:ILE:HD12  | 1.95                     | 0.48              |
| 1:H:503:PHE:O    | 1:H:573:HIS:N     | 2.39                     | 0.48              |
| 1:L:271:ILE:O    | 1:L:272:ASN:HB3   | 2.13                     | 0.48              |
| 1:E:204:LYS:HG2  | 1:E:241:THR:HG21  | 1.94                     | 0.48              |
| 1:J:550:SER:O    | 1:J:552:LYS:HD2   | 2.13                     | 0.48              |
| 1:D:571:TRP:CZ2  | 1:D:573:HIS:HB2   | 2.49                     | 0.48              |
| 1:B:210:LEU:HD21 | 1:B:222:LEU:HD21  | 1.95                     | 0.48              |
| 1:J:551:VAL:HG12 | 1:J:553:ALA:H     | 1.79                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:338:MET:HE3  | 1:K:468:ASP:HB3   | 1.96                     | 0.48              |
| 1:A:236:ARG:NH2  | 1:A:519:THR:O     | 2.42                     | 0.47              |
| 1:G:321:LEU:HD11 | 1:G:411:TYR:HA    | 1.96                     | 0.47              |
| 1:H:175:PHE:HD1  | 1:L:176:TYR:HB2   | 1.79                     | 0.47              |
| 1:E:198:LEU:HD22 | 1:E:202:ASP:HB3   | 1.94                     | 0.47              |
| 1:D:386:LYS:HB3  | 1:D:391:SER:HB2   | 1.97                     | 0.47              |
| 1:B:323:LEU:HD22 | 1:B:359:TYR:HB2   | 1.96                     | 0.47              |
| 1:L:338:MET:HE3  | 1:L:468:ASP:HB3   | 1.96                     | 0.47              |
| 1:J:444:ILE:HB   | 1:K:301:PRO:HG2   | 1.97                     | 0.47              |
| 1:A:254:SER:O    | 7:A:1267:HOH:O    | 2.20                     | 0.47              |
| 1:C:551:VAL:HG12 | 1:C:553:ALA:H     | 1.80                     | 0.47              |
| 1:G:525:TRP:CZ3  | 1:L:528:PRO:HB3   | 2.50                     | 0.47              |
| 1:H:165:PHE:HB3  | 1:H:189:TYR:OH    | 2.15                     | 0.47              |
| 1:J:413:VAL:HG11 | 1:J:423:ILE:HD12  | 1.96                     | 0.47              |
| 1:K:210:LEU:HD23 | 1:K:242:LEU:HD13  | 1.96                     | 0.47              |
| 1:G:536:THR:HG21 | 1:G:551:VAL:HG23  | 1.97                     | 0.47              |
| 1:H:194:SER:HB2  | 7:H:1139:HOH:O    | 2.15                     | 0.47              |
| 1:I:395:LEU:O    | 1:I:397:LYS:N     | 2.47                     | 0.47              |
| 1:J:344:VAL:HA   | 1:J:439:TYR:CE2   | 2.49                     | 0.47              |
| 1:A:114:VAL:HG12 | 1:A:274:ALA:HB1   | 1.97                     | 0.47              |
| 1:E:372:VAL:O    | 1:E:483:ASP:HA    | 2.15                     | 0.47              |
| 1:F:303:ASN:O    | 7:F:1121:HOH:O    | 2.20                     | 0.46              |
| 1:A:441:PRO:HB2  | 1:B:394:ASP:HA    | 1.97                     | 0.46              |
| 1:B:338:MET:HE3  | 1:B:468:ASP:HB3   | 1.97                     | 0.46              |
| 1:F:439:TYR:H    | 1:F:439:TYR:HD2   | 1.64                     | 0.46              |
| 1:C:577:ALA:HB1  | 4:C:1004:R5X:H9   | 1.98                     | 0.46              |
| 1:H:599:PHE:O    | 1:H:603:ASP:HB2   | 2.15                     | 0.46              |
| 1:J:392:MET:CE   | 4:J:1004:R5X:H1   | 2.44                     | 0.46              |
| 1:G:316:GLU:HG3  | 6:G:1006:1PE:H142 | 1.98                     | 0.46              |
| 1:D:260:ASN:N    | 7:D:1186:HOH:O    | 2.49                     | 0.46              |
| 1:H:413:VAL:HG11 | 1:H:423:ILE:HD12  | 1.98                     | 0.46              |
| 1:C:133:ASN:HB3  | 1:C:192:CYS:HB2   | 1.97                     | 0.46              |
| 1:D:254:SER:HA   | 1:D:255:THR:HA    | 1.56                     | 0.46              |
| 1:D:395:LEU:HD11 | 1:D:581:TRP:CG    | 2.51                     | 0.46              |
| 1:I:498:SER:O    | 1:I:523:PRO:HG2   | 2.16                     | 0.46              |
| 1:C:178:PHE:HZ   | 1:E:155:GLU:HG2   | 1.80                     | 0.45              |
| 1:F:413:VAL:HG11 | 1:F:423:ILE:HD12  | 1.97                     | 0.45              |
| 1:C:331:LYS:HD2  | 1:C:331:LYS:HA    | 1.74                     | 0.45              |
| 1:F:200:GLU:HG3  | 1:F:521:ASN:O     | 2.16                     | 0.45              |
| 1:A:491:MET:HE1  | 1:A:495:LEU:HD12  | 1.98                     | 0.45              |
| 1:G:340:ALA:HA   | 1:G:445:ILE:HD12  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:509:LEU:O    | 1:G:513:ILE:HG12 | 2.16                     | 0.45              |
| 1:C:144:ILE:HD12 | 1:C:157:LEU:HB3  | 1.99                     | 0.45              |
| 1:J:153:VAL:HG13 | 1:J:187:VAL:HG21 | 1.98                     | 0.45              |
| 1:K:112:VAL:HG22 | 1:K:267:LEU:HB3  | 1.99                     | 0.45              |
| 1:A:207:VAL:HG11 | 1:A:241:THR:HG22 | 1.98                     | 0.45              |
| 1:E:307:PRO:HD3  | 1:E:377:THR:OG1  | 2.17                     | 0.45              |
| 1:E:311:SER:HB2  | 1:E:327:ILE:HD12 | 1.99                     | 0.45              |
| 1:G:326:LYS:HE2  | 1:G:326:LYS:HB3  | 1.85                     | 0.45              |
| 1:B:360:LYS:HG2  | 1:B:422:GLU:HG3  | 1.98                     | 0.45              |
| 1:C:321:LEU:HD11 | 1:C:411:TYR:HA   | 1.97                     | 0.45              |
| 1:D:144:ILE:HG13 | 1:D:157:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:301:PRO:HB2  | 1:D:303:ASN:OD1  | 2.17                     | 0.45              |
| 1:G:301:PRO:HG2  | 1:G:304:TYR:CD2  | 2.52                     | 0.45              |
| 1:H:164:LYS:HE3  | 1:H:165:PHE:CE2  | 2.52                     | 0.45              |
| 1:K:522:GLU:OE1  | 1:K:595:LEU:N    | 2.50                     | 0.45              |
| 1:A:525:TRP:CZ3  | 1:F:528:PRO:HB3  | 2.52                     | 0.44              |
| 1:D:487:LEU:HD22 | 1:D:573:HIS:CE1  | 2.51                     | 0.44              |
| 1:E:114:VAL:HG12 | 1:E:274:ALA:HB1  | 1.98                     | 0.44              |
| 1:E:439:TYR:H    | 1:E:439:TYR:HD2  | 1.64                     | 0.44              |
| 1:G:174:HIS:HB3  | 1:J:175:PHE:CD2  | 2.53                     | 0.44              |
| 1:H:132:VAL:HG21 | 1:H:142:VAL:HG13 | 1.98                     | 0.44              |
| 1:I:392:MET:CE   | 4:I:1004:R5X:H1  | 2.43                     | 0.44              |
| 1:F:332:GLU:O    | 1:F:335:GLU:HG2  | 2.18                     | 0.44              |
| 1:H:520:SER:HB3  | 1:H:598:GLU:HG3  | 1.98                     | 0.44              |
| 1:K:95:ASP:HA    | 1:K:96:PRO:HD3   | 1.89                     | 0.44              |
| 1:A:150:ASP:OD1  | 1:A:179:ASN:HB2  | 2.17                     | 0.44              |
| 1:G:114:VAL:HG12 | 1:G:274:ALA:HB1  | 1.99                     | 0.44              |
| 1:H:601:LEU:C    | 1:H:603:ASP:H    | 2.25                     | 0.44              |
| 1:L:148:VAL:HG21 | 1:L:157:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:537:LEU:HA   | 1:A:545:ASN:HB2  | 2.00                     | 0.44              |
| 1:C:230:VAL:HG12 | 1:C:234:LEU:HD23 | 1.99                     | 0.44              |
| 1:C:377:THR:HA   | 1:C:400:MET:HE2  | 2.00                     | 0.44              |
| 1:D:546:GLN:HG2  | 1:D:547:ILE:HG23 | 2.00                     | 0.44              |
| 1:E:152:GLN:HG2  | 1:E:180:ASP:OD2  | 2.18                     | 0.44              |
| 1:J:394:ASP:HA   | 1:L:441:PRO:HB2  | 1.99                     | 0.44              |
| 1:J:487:LEU:O    | 4:J:1004:R5X:H10 | 2.18                     | 0.44              |
| 1:B:173:LYS:HE3  | 1:F:217:ASN:OD1  | 2.18                     | 0.44              |
| 1:D:396:MET:SD   | 1:D:398:PHE:HE2  | 2.41                     | 0.44              |
| 1:K:518:LYS:HD3  | 1:K:518:LYS:HA   | 1.75                     | 0.44              |
| 1:C:124:GLU:O    | 1:C:185:VAL:HG12 | 2.18                     | 0.43              |
| 1:L:90:GLN:HB3   | 1:L:95:ASP:HB2   | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:347:GLY:N    | 7:E:1195:HOH:O   | 2.43                     | 0.43              |
| 1:G:218:LYS:HD2  | 1:J:164:LYS:HA   | 2.00                     | 0.43              |
| 1:H:195:VAL:HG12 | 1:H:197:ASP:H    | 1.82                     | 0.43              |
| 1:J:487:LEU:HD22 | 1:J:573:HIS:CE1  | 2.52                     | 0.43              |
| 1:L:326:LYS:HE3  | 1:L:328:LEU:HD11 | 2.00                     | 0.43              |
| 1:C:164:LYS:HE3  | 1:C:165:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:344:VAL:HA   | 1:C:439:TYR:CE2  | 2.53                     | 0.43              |
| 1:C:396:MET:SD   | 1:C:398:PHE:HE2  | 2.41                     | 0.43              |
| 1:E:368:LYS:HG2  | 1:E:422:GLU:HB3  | 2.00                     | 0.43              |
| 1:E:344:VAL:HA   | 1:E:439:TYR:CE2  | 2.53                     | 0.43              |
| 1:K:347:GLY:N    | 7:K:1196:HOH:O   | 2.41                     | 0.43              |
| 1:H:357:LEU:HB2  | 1:H:425:PHE:HB2  | 2.01                     | 0.43              |
| 1:H:440:ARG:NH1  | 7:H:1135:HOH:O   | 2.39                     | 0.43              |
| 1:I:568:ASN:OD1  | 1:I:568:ASN:O    | 2.37                     | 0.43              |
| 1:L:357:LEU:HB2  | 1:L:425:PHE:HB2  | 2.00                     | 0.43              |
| 1:H:290:GLY:C    | 1:H:593:VAL:HG11 | 2.44                     | 0.43              |
| 1:J:546:GLN:HG2  | 1:J:547:ILE:HG23 | 2.01                     | 0.43              |
| 1:A:344:VAL:HA   | 1:A:439:TYR:CE2  | 2.54                     | 0.43              |
| 1:E:244:TYR:OH   | 1:E:588:PRO:O    | 2.36                     | 0.43              |
| 1:G:244:TYR:OH   | 1:G:588:PRO:O    | 2.36                     | 0.43              |
| 1:K:372:VAL:O    | 1:K:483:ASP:HA   | 2.18                     | 0.43              |
| 1:L:487:LEU:O    | 4:L:1004:R5X:H10 | 2.18                     | 0.43              |
| 1:G:182:LYS:NZ   | 7:G:1217:HOH:O   | 2.50                     | 0.43              |
| 1:E:522:GLU:HA   | 1:E:523:PRO:HD3  | 1.86                     | 0.43              |
| 1:H:116:ASP:OD2  | 1:H:118:LYS:HD2  | 2.19                     | 0.43              |
| 1:J:509:LEU:O    | 1:J:513:ILE:HG12 | 2.19                     | 0.43              |
| 1:L:232:LYS:HE2  | 1:L:276:THR:O    | 2.18                     | 0.43              |
| 1:B:90:GLN:NE2   | 1:B:95:ASP:O     | 2.51                     | 0.42              |
| 1:D:386:LYS:HE3  | 1:D:396:MET:SD   | 2.59                     | 0.42              |
| 1:F:207:VAL:HG11 | 1:F:241:THR:HG22 | 2.01                     | 0.42              |
| 1:H:453:ILE:HD13 | 1:H:561:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:372:VAL:O    | 1:A:483:ASP:HA   | 2.19                     | 0.42              |
| 1:C:525:TRP:CZ3  | 1:D:528:PRO:HB3  | 2.54                     | 0.42              |
| 1:F:383:TYR:HE2  | 1:F:438:SER:HB2  | 1.84                     | 0.42              |
| 1:C:208:LEU:O    | 1:C:212:THR:HG23 | 2.18                     | 0.42              |
| 1:E:129:ILE:HG21 | 1:E:190:VAL:HG23 | 2.01                     | 0.42              |
| 1:F:361:SER:OG   | 1:F:419:GLU:HA   | 2.19                     | 0.42              |
| 1:J:452:THR:HG22 | 1:J:542:ALA:HB1  | 2.01                     | 0.42              |
| 1:A:332:GLU:OE1  | 1:A:332:GLU:N    | 2.51                     | 0.42              |
| 1:B:383:TYR:HE2  | 1:B:438:SER:HB2  | 1.84                     | 0.42              |
| 1:H:395:LEU:O    | 1:H:397:LYS:N    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:208:LEU:HD23 | 1:I:208:LEU:HA    | 1.91                     | 0.42              |
| 1:E:150:ASP:OD1  | 1:E:179:ASN:HB2   | 2.20                     | 0.42              |
| 1:I:377:THR:HA   | 1:I:400:MET:HG2   | 2.02                     | 0.42              |
| 1:I:400:MET:HE3  | 1:I:400:MET:HB2   | 1.82                     | 0.42              |
| 1:L:150:ASP:OD1  | 1:L:179:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:441:PRO:HD2  | 1:B:378:PHE:CZ    | 2.55                     | 0.42              |
| 1:F:111:LYS:HA   | 1:F:111:LYS:HD2   | 1.74                     | 0.42              |
| 1:F:338:MET:HE1  | 1:F:354:PHE:CE2   | 2.55                     | 0.42              |
| 1:G:530:ILE:HD12 | 1:G:556:ILE:HD13  | 2.01                     | 0.42              |
| 1:D:340:ALA:HA   | 1:D:445:ILE:HD12  | 2.02                     | 0.42              |
| 1:D:586:ARG:NH1  | 7:D:1191:HOH:O    | 2.53                     | 0.42              |
| 1:E:520:SER:HB3  | 1:E:598:GLU:HG3   | 2.02                     | 0.42              |
| 1:I:198:LEU:HD22 | 1:I:202:ASP:HB3   | 2.01                     | 0.42              |
| 1:G:520:SER:HB3  | 1:G:598:GLU:HG3   | 2.02                     | 0.42              |
| 1:L:342:LEU:O    | 1:L:346:LYS:HG3   | 2.19                     | 0.42              |
| 1:B:301:PRO:HG2  | 1:B:304:TYR:CD2   | 2.55                     | 0.41              |
| 1:C:300:ALA:HA   | 1:C:301:PRO:HD3   | 1.86                     | 0.41              |
| 1:B:164:LYS:HE3  | 1:B:165:PHE:CZ    | 2.55                     | 0.41              |
| 1:E:396:MET:HA   | 1:E:398:PHE:CE2   | 2.55                     | 0.41              |
| 1:G:150:ASP:OD1  | 1:G:179:ASN:HB2   | 2.19                     | 0.41              |
| 1:I:323:LEU:HD22 | 1:I:359:TYR:HB2   | 2.02                     | 0.41              |
| 1:J:205:ARG:NH1  | 7:J:1215:HOH:O    | 2.54                     | 0.41              |
| 1:L:273:ASN:O    | 1:L:276:THR:HG22  | 2.20                     | 0.41              |
| 1:B:289:PHE:O    | 1:B:293:TYR:N     | 2.41                     | 0.41              |
| 1:C:150:ASP:N    | 7:C:1171:HOH:O    | 2.53                     | 0.41              |
| 1:F:138:GLU:HA   | 1:F:139:ASN:HA    | 1.70                     | 0.41              |
| 1:H:344:VAL:HA   | 1:H:439:TYR:CE2   | 2.55                     | 0.41              |
| 1:K:159:ASP:O    | 1:K:163:GLU:HB2   | 2.20                     | 0.41              |
| 1:A:174:HIS:HB3  | 1:D:175:PHE:CD2   | 2.55                     | 0.41              |
| 1:B:118:LYS:HE3  | 1:B:272:ASN:HD22  | 1.84                     | 0.41              |
| 1:I:301:PRO:HB2  | 1:I:303:ASN:OD1   | 2.20                     | 0.41              |
| 1:L:301:PRO:HG2  | 1:L:304:TYR:HD2   | 1.84                     | 0.41              |
| 5:A:1005:SO4:O1  | 1:C:436:LYS:HE3   | 2.21                     | 0.41              |
| 1:D:350:TYR:HA   | 1:D:351:PRO:HD3   | 1.90                     | 0.41              |
| 1:D:487:LEU:O    | 4:D:1004:R5X:H10  | 2.21                     | 0.41              |
| 1:F:103:TYR:CD2  | 6:F:1005:1PE:H141 | 2.54                     | 0.41              |
| 1:G:301:PRO:HG2  | 1:G:304:TYR:HD2   | 1.86                     | 0.41              |
| 1:A:89:PRO:HG2   | 1:A:350:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:436:LYS:NZ   | 5:A:1005:SO4:O1   | 2.54                     | 0.41              |
| 7:A:1113:HOH:O   | 1:B:397:LYS:NZ    | 2.50                     | 0.41              |
| 1:C:537:LEU:HD23 | 1:C:537:LEU:HA    | 1.93                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:435:SER:OG   | 1:D:436:LYS:N    | 2.53                     | 0.41              |
| 1:E:435:SER:OG   | 1:E:436:LYS:N    | 2.53                     | 0.41              |
| 1:H:398:PHE:CE1  | 1:H:581:TRP:HB2  | 2.55                     | 0.41              |
| 1:K:301:PRO:HB2  | 1:K:303:ASN:OD1  | 2.20                     | 0.41              |
| 1:C:435:SER:OG   | 1:C:436:LYS:N    | 2.53                     | 0.41              |
| 1:G:584:LYS:HE2  | 1:G:584:LYS:HB3  | 1.86                     | 0.41              |
| 1:J:533:TYR:O    | 1:J:536:THR:HG22 | 2.20                     | 0.41              |
| 1:A:292:TYR:O    | 1:A:296:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:195:VAL:HG12 | 1:B:197:ASP:H    | 1.86                     | 0.41              |
| 1:D:150:ASP:OD1  | 1:D:179:ASN:HB2  | 2.21                     | 0.41              |
| 1:E:300:ALA:HA   | 1:E:301:PRO:HD3  | 1.90                     | 0.41              |
| 1:J:338:MET:HE3  | 1:J:468:ASP:HB3  | 2.02                     | 0.41              |
| 4:L:1004:R5X:H11 | 4:L:1004:R5X:H15 | 1.56                     | 0.41              |
| 1:A:285:ARG:NH2  | 7:A:1125:HOH:O   | 2.54                     | 0.41              |
| 1:B:201:ALA:O    | 1:B:205:ARG:HG3  | 2.20                     | 0.41              |
| 1:D:300:ALA:HA   | 1:D:301:PRO:HD3  | 1.90                     | 0.41              |
| 1:F:107:ILE:HG21 | 1:F:243:PHE:HB3  | 2.03                     | 0.41              |
| 1:I:298:ILE:HG23 | 1:I:398:PHE:HA   | 2.02                     | 0.41              |
| 1:L:439:TYR:HD2  | 1:L:439:TYR:H    | 1.69                     | 0.41              |
| 1:D:441:PRO:HD2  | 1:E:378:PHE:CZ   | 2.57                     | 0.40              |
| 1:E:301:PRO:HB2  | 1:E:303:ASN:OD1  | 2.20                     | 0.40              |
| 1:F:353:LYS:HA   | 1:F:353:LYS:HD3  | 1.87                     | 0.40              |
| 1:K:500:ALA:HB3  | 1:K:524:VAL:HG22 | 2.03                     | 0.40              |
| 1:B:487:LEU:O    | 4:B:1004:R5X:H10 | 2.21                     | 0.40              |
| 1:C:346:LYS:HB3  | 1:C:437:ASN:O    | 2.20                     | 0.40              |
| 1:A:481:ILE:O    | 1:A:571:TRP:HA   | 2.22                     | 0.40              |
| 1:A:528:PRO:HB3  | 1:F:525:TRP:CE3  | 2.56                     | 0.40              |
| 1:B:298:ILE:HG23 | 1:B:398:PHE:HA   | 2.04                     | 0.40              |
| 1:H:540:LYS:HZ1  | 1:I:587:LYS:HD3  | 1.85                     | 0.40              |
| 1:K:214:LEU:HD21 | 1:K:222:LEU:HD22 | 2.02                     | 0.40              |
| 1:A:350:TYR:HA   | 1:A:351:PRO:HD2  | 1.94                     | 0.40              |
| 1:D:368:LYS:NZ   | 1:D:422:GLU:OE1  | 2.54                     | 0.40              |
| 1:E:487:LEU:O    | 4:E:1004:R5X:H10 | 2.22                     | 0.40              |
| 1:F:392:MET:CE   | 4:F:1004:R5X:H1  | 2.52                     | 0.40              |
| 1:H:536:THR:HG21 | 1:H:551:VAL:HG23 | 2.04                     | 0.40              |
| 1:J:452:THR:HG21 | 1:K:252:PHE:O    | 2.21                     | 0.40              |

All (1) 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:115:TYR:OH | 1:G:124:GLU:OE1[2_564] | 2.17                     | 0.03              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 512/528 (97%)   | 493 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | B     | 507/528 (96%)   | 489 (96%)  | 16 (3%)  | 2 (0%)   | 30          | 49  |
| 1   | C     | 517/528 (98%)   | 502 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 1   | D     | 510/528 (97%)   | 493 (97%)  | 16 (3%)  | 1 (0%)   | 43          | 63  |
| 1   | E     | 504/528 (96%)   | 491 (97%)  | 12 (2%)  | 1 (0%)   | 43          | 63  |
| 1   | F     | 501/528 (95%)   | 486 (97%)  | 14 (3%)  | 1 (0%)   | 43          | 63  |
| 1   | G     | 513/528 (97%)   | 498 (97%)  | 14 (3%)  | 1 (0%)   | 43          | 63  |
| 1   | H     | 511/528 (97%)   | 490 (96%)  | 19 (4%)  | 2 (0%)   | 30          | 49  |
| 1   | I     | 512/528 (97%)   | 495 (97%)  | 16 (3%)  | 1 (0%)   | 43          | 63  |
| 1   | J     | 507/528 (96%)   | 493 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 1   | K     | 503/528 (95%)   | 487 (97%)  | 15 (3%)  | 1 (0%)   | 43          | 63  |
| 1   | L     | 502/528 (95%)   | 484 (96%)  | 16 (3%)  | 2 (0%)   | 30          | 49  |
| All | All   | 6099/6336 (96%) | 5901 (97%) | 186 (3%) | 12 (0%)  | 43          | 63  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 396 | MET  |
| 1   | F     | 551 | VAL  |
| 1   | H     | 396 | MET  |
| 1   | I     | 396 | MET  |
| 1   | B     | 119 | GLY  |
| 1   | K     | 396 | MET  |
| 1   | L     | 364 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 254 | SER  |
| 1   | G     | 396 | MET  |
| 1   | H     | 125 | GLU  |
| 1   | L     | 272 | ASN  |
| 1   | B     | 396 | MET  |

### 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     | 422/455 (93%)   | 418 (99%)  | 4 (1%)   | 70          | 87 |
| 1   | B     | 402/455 (88%)   | 400 (100%) | 2 (0%)   | 81          | 92 |
| 1   | C     | 421/455 (92%)   | 419 (100%) | 2 (0%)   | 81          | 92 |
| 1   | D     | 417/455 (92%)   | 415 (100%) | 2 (0%)   | 81          | 92 |
| 1   | E     | 415/455 (91%)   | 411 (99%)  | 4 (1%)   | 68          | 86 |
| 1   | F     | 382/455 (84%)   | 376 (98%)  | 6 (2%)   | 55          | 79 |
| 1   | G     | 425/455 (93%)   | 421 (99%)  | 4 (1%)   | 70          | 87 |
| 1   | H     | 406/455 (89%)   | 405 (100%) | 1 (0%)   | 87          | 95 |
| 1   | I     | 411/455 (90%)   | 409 (100%) | 2 (0%)   | 81          | 92 |
| 1   | J     | 412/455 (90%)   | 409 (99%)  | 3 (1%)   | 76          | 89 |
| 1   | K     | 414/455 (91%)   | 412 (100%) | 2 (0%)   | 81          | 92 |
| 1   | L     | 393/455 (86%)   | 391 (100%) | 2 (0%)   | 81          | 92 |
| All | All   | 4920/5460 (90%) | 4886 (99%) | 34 (1%)  | 76          | 89 |

All (34) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 200 | GLU  |
| 1   | A     | 508 | GLU  |
| 1   | A     | 584 | LYS  |
| 1   | A     | 595 | LEU  |
| 1   | B     | 122 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 172 | SER  |
| 1   | C     | 285 | ARG  |
| 1   | C     | 419 | GLU  |
| 1   | D     | 215 | HIS  |
| 1   | D     | 219 | LEU  |
| 1   | E     | 102 | GLU  |
| 1   | E     | 169 | LEU  |
| 1   | E     | 204 | LYS  |
| 1   | E     | 547 | ILE  |
| 1   | F     | 200 | GLU  |
| 1   | F     | 266 | HIS  |
| 1   | F     | 335 | GLU  |
| 1   | F     | 421 | VAL  |
| 1   | F     | 439 | TYR  |
| 1   | F     | 531 | ASN  |
| 1   | G     | 117 | ILE  |
| 1   | G     | 200 | GLU  |
| 1   | G     | 257 | LYS  |
| 1   | G     | 584 | LYS  |
| 1   | H     | 419 | GLU  |
| 1   | I     | 400 | MET  |
| 1   | I     | 439 | TYR  |
| 1   | J     | 200 | GLU  |
| 1   | J     | 452 | THR  |
| 1   | J     | 518 | LYS  |
| 1   | K     | 324 | GLU  |
| 1   | K     | 518 | LYS  |
| 1   | L     | 200 | GLU  |
| 1   | L     | 439 | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 134 | ASN  |
| 1   | A     | 437 | ASN  |
| 1   | B     | 104 | ASN  |
| 1   | B     | 122 | ASN  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 420 | ASN  |
| 1   | C     | 104 | ASN  |
| 1   | C     | 260 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 134 | ASN  |
| 1   | D     | 152 | GLN  |
| 1   | D     | 161 | ASN  |
| 1   | D     | 420 | ASN  |
| 1   | E     | 134 | ASN  |
| 1   | E     | 174 | HIS  |
| 1   | F     | 152 | GLN  |
| 1   | F     | 174 | HIS  |
| 1   | F     | 266 | HIS  |
| 1   | F     | 420 | ASN  |
| 1   | G     | 134 | ASN  |
| 1   | G     | 437 | ASN  |
| 1   | G     | 521 | ASN  |
| 1   | H     | 322 | ASN  |
| 1   | I     | 215 | HIS  |
| 1   | J     | 437 | ASN  |
| 1   | K     | 134 | ASN  |
| 1   | K     | 166 | ASN  |
| 1   | K     | 420 | ASN  |
| 1   | K     | 437 | ASN  |
| 1   | K     | 521 | ASN  |
| 1   | L     | 104 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 24 are monoatomic - leaving 46 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 | $\# Z  > 2$ |
| 3   | CO3  | G     | 1002 | -    | 3,3,3        | 0.85 | 0           | 2,3,3       | 0.14 | 0           |
| 3   | CO3  | H     | 1002 | -    | 3,3,3        | 0.79 | 0           | 2,3,3       | 0.06 | 0           |
| 3   | CO3  | K     | 1002 | -    | 3,3,3        | 0.82 | 0           | 2,3,3       | 0.17 | 0           |
| 5   | SO4  | E     | 1005 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.13 | 0           |
| 6   | 1PE  | B     | 1006 | -    | 8,8,15       | 0.47 | 0           | 7,7,14      | 0.31 | 0           |
| 6   | 1PE  | I     | 1006 | -    | 10,10,15     | 0.47 | 0           | 9,9,14      | 0.34 | 0           |
| 4   | R5X  | D     | 1004 | 2    | 27,28,28     | 2.93 | 5 (18%)     | 36,38,38    | 1.60 | 4 (11%)     |
| 6   | 1PE  | G     | 1005 | -    | 12,12,15     | 0.43 | 0           | 11,11,14    | 0.42 | 0           |
| 5   | SO4  | K     | 1005 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.06 | 0           |
| 4   | R5X  | B     | 1004 | 2    | 27,28,28     | 3.04 | 5 (18%)     | 36,38,38    | 1.68 | 8 (22%)     |
| 6   | 1PE  | F     | 1005 | -    | 7,7,15       | 0.52 | 0           | 6,6,14      | 0.31 | 0           |
| 4   | R5X  | G     | 1004 | 2    | 27,28,28     | 3.00 | 6 (22%)     | 36,38,38    | 1.70 | 9 (25%)     |
| 3   | CO3  | I     | 1002 | -    | 3,3,3        | 0.83 | 0           | 2,3,3       | 0.15 | 0           |
| 4   | R5X  | H     | 1004 | 2    | 27,28,28     | 2.93 | 5 (18%)     | 36,38,38    | 1.73 | 7 (19%)     |
| 6   | 1PE  | J     | 1005 | -    | 9,9,15       | 0.44 | 0           | 8,8,14      | 0.31 | 0           |
| 4   | R5X  | K     | 1004 | 2    | 27,28,28     | 3.10 | 5 (18%)     | 36,38,38    | 1.56 | 6 (16%)     |
| 5   | SO4  | A     | 1006 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.07 | 0           |
| 5   | SO4  | E     | 1008 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.15 | 0           |
| 6   | 1PE  | I     | 1005 | -    | 9,9,15       | 0.44 | 0           | 8,8,14      | 0.27 | 0           |
| 4   | R5X  | J     | 1004 | 2    | 27,28,28     | 3.02 | 5 (18%)     | 36,38,38    | 1.59 | 4 (11%)     |
| 4   | R5X  | E     | 1004 | 2    | 27,28,28     | 3.01 | 5 (18%)     | 36,38,38    | 1.58 | 5 (13%)     |
| 4   | R5X  | L     | 1004 | 2    | 27,28,28     | 2.89 | 5 (18%)     | 36,38,38    | 1.86 | 10 (27%)    |
| 5   | SO4  | A     | 1005 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.08 | 0           |
| 5   | SO4  | H     | 1005 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.05 | 0           |
| 6   | 1PE  | L     | 1005 | -    | 6,6,15       | 0.41 | 0           | 5,5,14      | 0.36 | 0           |
| 6   | 1PE  | K     | 1006 | -    | 12,12,15     | 0.44 | 0           | 11,11,14    | 0.30 | 0           |
| 6   | 1PE  | E     | 1007 | -    | 9,9,15       | 0.47 | 0           | 8,8,14      | 0.31 | 0           |
| 3   | CO3  | F     | 1002 | -    | 3,3,3        | 0.84 | 0           | 2,3,3       | 0.13 | 0           |
| 4   | R5X  | I     | 1004 | 2    | 27,28,28     | 3.10 | 6 (22%)     | 36,38,38    | 1.43 | 4 (11%)     |
| 3   | CO3  | J     | 1002 | -    | 3,3,3        | 0.82 | 0           | 2,3,3       | 0.06 | 0           |
| 3   | CO3  | C     | 1002 | -    | 3,3,3        | 0.82 | 0           | 2,3,3       | 0.18 | 0           |
| 3   | CO3  | B     | 1002 | -    | 3,3,3        | 0.78 | 0           | 2,3,3       | 0.07 | 0           |
| 4   | R5X  | F     | 1004 | 2    | 27,28,28     | 2.93 | 5 (18%)     | 36,38,38    | 1.73 | 8 (22%)     |
| 6   | 1PE  | F     | 1006 | -    | 8,8,15       | 0.47 | 0           | 7,7,14      | 0.27 | 0           |
| 6   | 1PE  | G     | 1006 | -    | 9,9,15       | 0.43 | 0           | 8,8,14      | 0.29 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CO3  | A     | 1002 | -    | 3,3,3        | 0.85 | 0        | 2,3,3       | 0.17 | 0        |
| 3   | CO3  | E     | 1002 | -    | 3,3,3        | 0.81 | 0        | 2,3,3       | 0.12 | 0        |
| 4   | R5X  | C     | 1004 | 2    | 27,28,28     | 3.18 | 5 (18%)  | 36,38,38    | 1.71 | 9 (25%)  |
| 6   | 1PE  | B     | 1005 | -    | 9,9,15       | 0.46 | 0        | 8,8,14      | 0.23 | 0        |
| 3   | CO3  | L     | 1002 | -    | 3,3,3        | 0.84 | 0        | 2,3,3       | 0.11 | 0        |
| 3   | CO3  | D     | 1002 | -    | 3,3,3        | 0.81 | 0        | 2,3,3       | 0.08 | 0        |
| 6   | 1PE  | H     | 1006 | -    | 9,9,15       | 0.46 | 0        | 8,8,14      | 0.39 | 0        |
| 4   | R5X  | A     | 1004 | 2    | 27,28,28     | 3.07 | 5 (18%)  | 36,38,38    | 1.73 | 9 (25%)  |
| 6   | 1PE  | F     | 1007 | -    | 8,8,15       | 0.47 | 0        | 7,7,14      | 0.36 | 0        |
| 6   | 1PE  | E     | 1006 | -    | 9,9,15       | 0.44 | 0        | 8,8,14      | 0.28 | 0        |
| 5   | SO4  | F     | 1008 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.09 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 6   | 1PE  | B     | 1006 | -    | -       | 1/6/6/13   | -       |
| 6   | 1PE  | I     | 1006 | -    | -       | 3/8/8/13   | -       |
| 4   | R5X  | D     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | G     | 1005 | -    | -       | 4/10/10/13 | -       |
| 4   | R5X  | B     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | F     | 1005 | -    | -       | 0/5/5/13   | -       |
| 4   | R5X  | G     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 4   | R5X  | H     | 1004 | 2    | -       | 3/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | J     | 1005 | -    | -       | 0/7/7/13   | -       |
| 4   | R5X  | K     | 1004 | 2    | -       | 0/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | I     | 1005 | -    | -       | 0/7/7/13   | -       |
| 4   | R5X  | J     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 4   | R5X  | E     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 4   | R5X  | L     | 1004 | 2    | -       | 4/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | L     | 1005 | -    | -       | 2/4/4/13   | -       |
| 6   | 1PE  | K     | 1006 | -    | -       | 1/10/10/13 | -       |
| 6   | 1PE  | E     | 1007 | -    | -       | 1/7/7/13   | -       |
| 4   | R5X  | I     | 1004 | 2    | -       | 1/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | G     | 1006 | -    | -       | 1/7/7/13   | -       |
| 6   | 1PE  | F     | 1006 | -    | -       | 0/6/6/13   | -       |
| 4   | R5X  | F     | 1004 | 2    | -       | 3/22/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | R5X  | C     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | B     | 1005 | -    | -       | 1/7/7/13   | -       |
| 6   | 1PE  | H     | 1006 | -    | -       | 2/7/7/13   | -       |
| 4   | R5X  | A     | 1004 | 2    | -       | 2/22/22/22 | 0/3/3/3 |
| 6   | 1PE  | F     | 1007 | -    | -       | 0/6/6/13   | -       |
| 6   | 1PE  | E     | 1006 | -    | -       | 0/7/7/13   | -       |

All (62) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 4   | C     | 1004 | R5X  | N07-N08 | -11.97 | 1.19        | 1.36     |
| 4   | A     | 1004 | R5X  | N07-N08 | -11.36 | 1.20        | 1.36     |
| 4   | B     | 1004 | R5X  | N07-N08 | -11.05 | 1.20        | 1.36     |
| 4   | K     | 1004 | R5X  | N07-N08 | -10.90 | 1.21        | 1.36     |
| 4   | I     | 1004 | R5X  | N07-N08 | -10.73 | 1.21        | 1.36     |
| 4   | G     | 1004 | R5X  | N07-N08 | -10.68 | 1.21        | 1.36     |
| 4   | J     | 1004 | R5X  | N07-N08 | -10.56 | 1.21        | 1.36     |
| 4   | E     | 1004 | R5X  | N07-N08 | -10.45 | 1.21        | 1.36     |
| 4   | D     | 1004 | R5X  | N07-N08 | -10.12 | 1.22        | 1.36     |
| 4   | H     | 1004 | R5X  | N07-N08 | -10.09 | 1.22        | 1.36     |
| 4   | F     | 1004 | R5X  | N07-N08 | -10.05 | 1.22        | 1.36     |
| 4   | L     | 1004 | R5X  | N07-N08 | -9.88  | 1.22        | 1.36     |
| 4   | K     | 1004 | R5X  | C03-C12 | -8.55  | 1.39        | 1.52     |
| 4   | I     | 1004 | R5X  | C03-C12 | -8.34  | 1.39        | 1.52     |
| 4   | J     | 1004 | R5X  | C03-C12 | -8.29  | 1.39        | 1.52     |
| 4   | E     | 1004 | R5X  | C03-C12 | -8.29  | 1.39        | 1.52     |
| 4   | D     | 1004 | R5X  | C03-C12 | -8.03  | 1.40        | 1.52     |
| 4   | F     | 1004 | R5X  | C03-C12 | -8.02  | 1.40        | 1.52     |
| 4   | L     | 1004 | R5X  | C03-C12 | -8.02  | 1.40        | 1.52     |
| 4   | C     | 1004 | R5X  | C03-C12 | -7.96  | 1.40        | 1.52     |
| 4   | B     | 1004 | R5X  | C03-C12 | -7.94  | 1.40        | 1.52     |
| 4   | H     | 1004 | R5X  | C03-C12 | -7.91  | 1.40        | 1.52     |
| 4   | A     | 1004 | R5X  | C03-C12 | -7.86  | 1.40        | 1.52     |
| 4   | G     | 1004 | R5X  | C03-C12 | -7.75  | 1.40        | 1.52     |
| 4   | K     | 1004 | R5X  | C06-N07 | -5.21  | 1.33        | 1.43     |
| 4   | I     | 1004 | R5X  | C06-N07 | -5.13  | 1.33        | 1.43     |
| 4   | E     | 1004 | R5X  | C06-N07 | -5.09  | 1.33        | 1.43     |
| 4   | D     | 1004 | R5X  | C06-N07 | -5.09  | 1.33        | 1.43     |
| 4   | J     | 1004 | R5X  | C06-N07 | -5.07  | 1.33        | 1.43     |
| 4   | H     | 1004 | R5X  | C06-N07 | -5.06  | 1.33        | 1.43     |
| 4   | C     | 1004 | R5X  | C06-N07 | -5.04  | 1.33        | 1.43     |
| 4   | L     | 1004 | R5X  | C06-N07 | -5.02  | 1.33        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | A     | 1004 | R5X  | C06-N07 | -5.02 | 1.33        | 1.43     |
| 4   | F     | 1004 | R5X  | C06-N07 | -5.01 | 1.33        | 1.43     |
| 4   | I     | 1004 | R5X  | C19-C18 | -4.95 | 1.39        | 1.50     |
| 4   | E     | 1004 | R5X  | C19-C18 | -4.95 | 1.39        | 1.50     |
| 4   | G     | 1004 | R5X  | C19-C18 | -4.93 | 1.39        | 1.50     |
| 4   | B     | 1004 | R5X  | C06-N07 | -4.92 | 1.33        | 1.43     |
| 4   | G     | 1004 | R5X  | C06-N07 | -4.92 | 1.33        | 1.43     |
| 4   | D     | 1004 | R5X  | C19-C18 | -4.91 | 1.39        | 1.50     |
| 4   | H     | 1004 | R5X  | C19-C18 | -4.91 | 1.39        | 1.50     |
| 4   | A     | 1004 | R5X  | C19-C18 | -4.88 | 1.39        | 1.50     |
| 4   | K     | 1004 | R5X  | C19-C18 | -4.86 | 1.39        | 1.50     |
| 4   | J     | 1004 | R5X  | C19-C18 | -4.85 | 1.39        | 1.50     |
| 4   | L     | 1004 | R5X  | C19-C18 | -4.84 | 1.39        | 1.50     |
| 4   | F     | 1004 | R5X  | C19-C18 | -4.83 | 1.39        | 1.50     |
| 4   | C     | 1004 | R5X  | C19-C18 | -4.82 | 1.39        | 1.50     |
| 4   | B     | 1004 | R5X  | C19-C18 | -4.81 | 1.39        | 1.50     |
| 4   | I     | 1004 | R5X  | O17-N16 | 3.16  | 1.47        | 1.40     |
| 4   | K     | 1004 | R5X  | C10-C09 | -2.29 | 1.32        | 1.39     |
| 4   | C     | 1004 | R5X  | C10-C09 | -2.28 | 1.32        | 1.39     |
| 4   | F     | 1004 | R5X  | C10-C09 | -2.28 | 1.32        | 1.39     |
| 4   | J     | 1004 | R5X  | C10-C09 | -2.27 | 1.32        | 1.39     |
| 4   | A     | 1004 | R5X  | C10-C09 | -2.27 | 1.32        | 1.39     |
| 4   | E     | 1004 | R5X  | C10-C09 | -2.26 | 1.33        | 1.39     |
| 4   | B     | 1004 | R5X  | C10-C09 | -2.25 | 1.33        | 1.39     |
| 4   | H     | 1004 | R5X  | C10-C09 | -2.24 | 1.33        | 1.39     |
| 4   | D     | 1004 | R5X  | C10-C09 | -2.24 | 1.33        | 1.39     |
| 4   | G     | 1004 | R5X  | C10-C09 | -2.23 | 1.33        | 1.39     |
| 4   | I     | 1004 | R5X  | C10-C09 | -2.23 | 1.33        | 1.39     |
| 4   | L     | 1004 | R5X  | C10-C09 | -2.22 | 1.33        | 1.39     |
| 4   | G     | 1004 | R5X  | O17-N16 | 2.16  | 1.45        | 1.40     |

All (83) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 4   | J     | 1004 | R5X  | C09-N08-N07 | 6.47 | 110.25      | 103.94   |
| 4   | F     | 1004 | R5X  | C09-N08-N07 | 6.45 | 110.23      | 103.94   |
| 4   | L     | 1004 | R5X  | C09-N08-N07 | 6.40 | 110.18      | 103.94   |
| 4   | K     | 1004 | R5X  | C09-N08-N07 | 6.35 | 110.13      | 103.94   |
| 4   | D     | 1004 | R5X  | C09-N08-N07 | 6.34 | 110.12      | 103.94   |
| 4   | H     | 1004 | R5X  | C09-N08-N07 | 6.32 | 110.10      | 103.94   |
| 4   | B     | 1004 | R5X  | C09-N08-N07 | 6.30 | 110.08      | 103.94   |
| 4   | I     | 1004 | R5X  | C09-N08-N07 | 6.24 | 110.03      | 103.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | E     | 1004 | R5X  | C09-N08-N07 | 6.24  | 110.02      | 103.94   |
| 4   | G     | 1004 | R5X  | C09-N08-N07 | 6.23  | 110.02      | 103.94   |
| 4   | C     | 1004 | R5X  | C09-N08-N07 | 6.16  | 109.94      | 103.94   |
| 4   | A     | 1004 | R5X  | C09-N08-N07 | 5.99  | 109.78      | 103.94   |
| 4   | L     | 1004 | R5X  | C02-C03-C12 | -3.80 | 114.69      | 120.78   |
| 4   | A     | 1004 | R5X  | C06-N07-N08 | 3.71  | 127.42      | 121.08   |
| 4   | F     | 1004 | R5X  | C02-C03-C12 | -3.70 | 114.86      | 120.78   |
| 4   | H     | 1004 | R5X  | C02-C03-C12 | -3.66 | 114.91      | 120.78   |
| 4   | C     | 1004 | R5X  | C06-N07-N08 | 3.46  | 127.00      | 121.08   |
| 4   | C     | 1004 | R5X  | C02-C03-C12 | -3.38 | 115.37      | 120.78   |
| 4   | G     | 1004 | R5X  | C06-N07-N08 | 3.30  | 126.72      | 121.08   |
| 4   | G     | 1004 | R5X  | C02-C03-C12 | -3.24 | 115.59      | 120.78   |
| 4   | B     | 1004 | R5X  | C02-C03-C12 | -3.23 | 115.61      | 120.78   |
| 4   | B     | 1004 | R5X  | C06-N07-N08 | 3.15  | 126.46      | 121.08   |
| 4   | A     | 1004 | R5X  | C02-C03-C12 | -3.06 | 115.88      | 120.78   |
| 4   | L     | 1004 | R5X  | C04-C03-C12 | 3.01  | 125.61      | 120.78   |
| 4   | L     | 1004 | R5X  | C11-N07-N08 | -2.96 | 109.36      | 111.83   |
| 4   | F     | 1004 | R5X  | C11-N07-N08 | -2.95 | 109.36      | 111.83   |
| 4   | L     | 1004 | R5X  | C03-C12-N13 | 2.95  | 120.18      | 112.75   |
| 4   | J     | 1004 | R5X  | C02-C03-C12 | -2.94 | 116.06      | 120.78   |
| 4   | H     | 1004 | R5X  | C04-C03-C12 | 2.92  | 125.46      | 120.78   |
| 4   | F     | 1004 | R5X  | C04-C03-C12 | 2.86  | 125.38      | 120.78   |
| 4   | K     | 1004 | R5X  | C02-C03-C12 | -2.84 | 116.23      | 120.78   |
| 4   | D     | 1004 | R5X  | C02-C03-C12 | -2.84 | 116.23      | 120.78   |
| 4   | D     | 1004 | R5X  | C11-N07-N08 | -2.84 | 109.46      | 111.83   |
| 4   | H     | 1004 | R5X  | C11-N07-N08 | -2.81 | 109.48      | 111.83   |
| 4   | E     | 1004 | R5X  | C02-C03-C12 | -2.76 | 116.36      | 120.78   |
| 4   | J     | 1004 | R5X  | C11-N07-N08 | -2.73 | 109.54      | 111.83   |
| 4   | H     | 1004 | R5X  | C03-C12-N13 | 2.73  | 119.64      | 112.75   |
| 4   | G     | 1004 | R5X  | C04-C03-C12 | 2.68  | 125.08      | 120.78   |
| 4   | G     | 1004 | R5X  | C11-N07-N08 | -2.67 | 109.59      | 111.83   |
| 4   | A     | 1004 | R5X  | C06-N07-C11 | -2.64 | 122.64      | 128.39   |
| 4   | E     | 1004 | R5X  | C11-N07-N08 | -2.57 | 109.68      | 111.83   |
| 4   | B     | 1004 | R5X  | C11-N07-N08 | -2.55 | 109.70      | 111.83   |
| 4   | C     | 1004 | R5X  | C04-C03-C12 | 2.55  | 124.87      | 120.78   |
| 4   | B     | 1004 | R5X  | C04-C03-C12 | 2.52  | 124.82      | 120.78   |
| 4   | C     | 1004 | R5X  | C06-N07-C11 | -2.51 | 122.91      | 128.39   |
| 4   | F     | 1004 | R5X  | C03-C12-N13 | 2.51  | 119.08      | 112.75   |
| 4   | L     | 1004 | R5X  | C05-C06-N07 | 2.51  | 122.65      | 119.58   |
| 4   | B     | 1004 | R5X  | C03-C12-N13 | 2.39  | 118.77      | 112.75   |
| 4   | F     | 1004 | R5X  | C05-C06-N07 | 2.37  | 122.48      | 119.58   |
| 4   | I     | 1004 | R5X  | C06-N07-N08 | 2.36  | 125.10      | 121.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | G     | 1004 | R5X  | C03-C12-N13 | 2.35  | 118.69      | 112.75   |
| 4   | I     | 1004 | R5X  | C10-C09-N08 | -2.35 | 106.95      | 111.72   |
| 4   | K     | 1004 | R5X  | C10-C09-N08 | -2.35 | 106.95      | 111.72   |
| 4   | F     | 1004 | R5X  | C10-C09-N08 | -2.34 | 106.96      | 111.72   |
| 4   | J     | 1004 | R5X  | C10-C09-N08 | -2.34 | 106.96      | 111.72   |
| 4   | A     | 1004 | R5X  | C03-C12-N13 | 2.33  | 118.63      | 112.75   |
| 4   | L     | 1004 | R5X  | C10-C09-N08 | -2.33 | 106.99      | 111.72   |
| 4   | L     | 1004 | R5X  | C19-C18-N13 | -2.32 | 112.73      | 117.04   |
| 4   | K     | 1004 | R5X  | C11-N07-N08 | -2.32 | 109.89      | 111.83   |
| 4   | A     | 1004 | R5X  | C04-C03-C12 | 2.29  | 124.46      | 120.78   |
| 4   | H     | 1004 | R5X  | C10-C09-N08 | -2.29 | 107.06      | 111.72   |
| 4   | E     | 1004 | R5X  | C10-C09-N08 | -2.29 | 107.07      | 111.72   |
| 4   | L     | 1004 | R5X  | C05-C04-C03 | -2.28 | 118.91      | 121.18   |
| 4   | D     | 1004 | R5X  | C10-C09-N08 | -2.27 | 107.10      | 111.72   |
| 4   | A     | 1004 | R5X  | C11-N07-N08 | -2.26 | 109.94      | 111.83   |
| 4   | I     | 1004 | R5X  | C11-N07-N08 | -2.24 | 109.96      | 111.83   |
| 4   | C     | 1004 | R5X  | C03-C12-N13 | 2.21  | 118.33      | 112.75   |
| 4   | H     | 1004 | R5X  | C05-C06-N07 | 2.20  | 122.28      | 119.58   |
| 4   | F     | 1004 | R5X  | C05-C04-C03 | -2.19 | 119.00      | 121.18   |
| 4   | G     | 1004 | R5X  | C10-C09-N08 | -2.18 | 107.28      | 111.72   |
| 4   | B     | 1004 | R5X  | C10-C09-N08 | -2.17 | 107.31      | 111.72   |
| 4   | G     | 1004 | R5X  | C06-N07-C11 | -2.16 | 123.68      | 128.39   |
| 4   | C     | 1004 | R5X  | C05-C04-C03 | -2.15 | 119.04      | 121.18   |
| 4   | K     | 1004 | R5X  | C06-N07-N08 | 2.14  | 124.73      | 121.08   |
| 4   | K     | 1004 | R5X  | C05-C04-C03 | -2.11 | 119.08      | 121.18   |
| 4   | C     | 1004 | R5X  | C10-C09-N08 | -2.10 | 107.46      | 111.72   |
| 4   | B     | 1004 | R5X  | C06-N07-C11 | -2.09 | 123.83      | 128.39   |
| 4   | E     | 1004 | R5X  | C06-N07-N08 | 2.08  | 124.63      | 121.08   |
| 4   | C     | 1004 | R5X  | C11-N07-N08 | -2.08 | 110.09      | 111.83   |
| 4   | A     | 1004 | R5X  | C10-C09-N08 | -2.06 | 107.54      | 111.72   |
| 4   | G     | 1004 | R5X  | C05-C06-N07 | 2.02  | 122.05      | 119.58   |
| 4   | A     | 1004 | R5X  | C05-C04-C03 | -2.01 | 119.18      | 121.18   |
| 4   | L     | 1004 | R5X  | C12-N13-C18 | 2.00  | 126.10      | 121.66   |

There are no chirality outliers.

All (41) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | L     | 1005 | 1PE  | OH7-C16-C26-OH6 |
| 6   | H     | 1006 | 1PE  | OH4-C13-C23-OH3 |
| 6   | G     | 1005 | 1PE  | OH7-C16-C26-OH6 |
| 4   | I     | 1004 | R5X  | C14-C12-N13-C18 |

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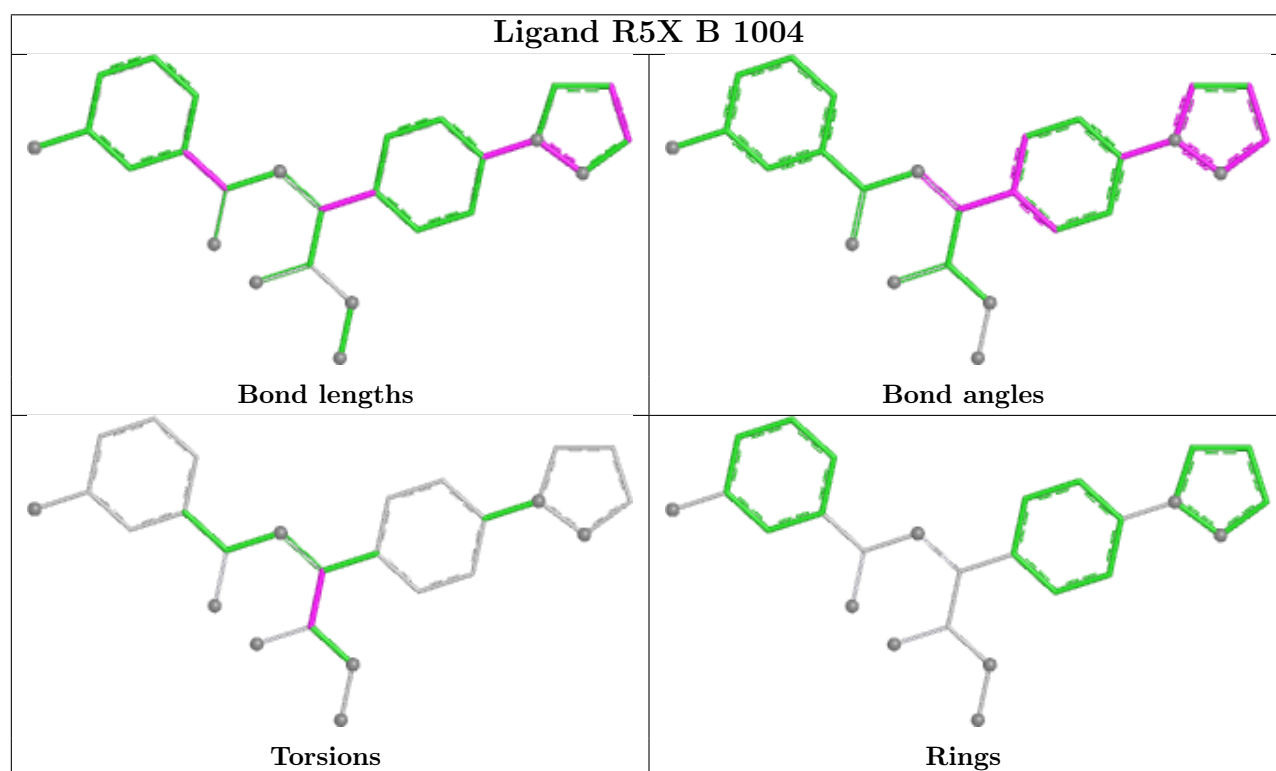
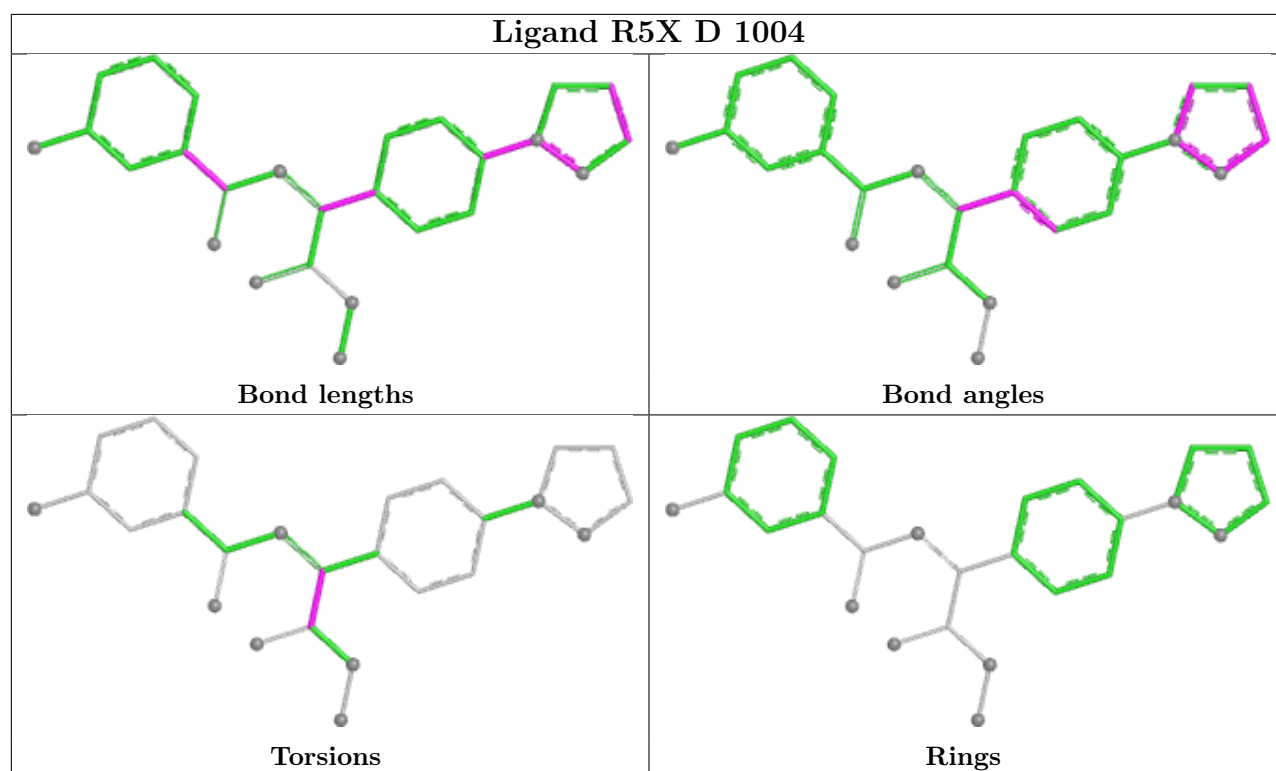
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | B     | 1005 | 1PE  | OH7-C16-C26-OH6 |
| 6   | G     | 1005 | 1PE  | C16-C26-OH6-C15 |
| 6   | G     | 1005 | 1PE  | C25-C15-OH6-C26 |
| 4   | L     | 1004 | R5X  | N13-C12-C14-O15 |
| 6   | I     | 1006 | 1PE  | OH4-C13-C23-OH3 |
| 6   | I     | 1006 | 1PE  | OH5-C14-C24-OH4 |
| 6   | E     | 1007 | 1PE  | OH6-C15-C25-OH5 |
| 4   | B     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | C     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | E     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | E     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | H     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | J     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | L     | 1004 | R5X  | N13-C12-C14-N16 |
| 6   | L     | 1005 | 1PE  | OH6-C15-C25-OH5 |
| 6   | G     | 1006 | 1PE  | OH5-C14-C24-OH4 |
| 4   | A     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | A     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | D     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | D     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | F     | 1004 | R5X  | N13-C12-C14-O15 |
| 4   | G     | 1004 | R5X  | N13-C12-C14-O15 |
| 6   | K     | 1006 | 1PE  | OH6-C15-C25-OH5 |
| 6   | G     | 1005 | 1PE  | OH5-C14-C24-OH4 |
| 6   | B     | 1006 | 1PE  | C23-C13-OH4-C24 |
| 6   | I     | 1006 | 1PE  | C14-C24-OH4-C13 |
| 4   | F     | 1004 | R5X  | C03-C12-C14-N16 |
| 4   | L     | 1004 | R5X  | C03-C12-C14-O15 |
| 4   | B     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | C     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | F     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | H     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | H     | 1004 | R5X  | C03-C12-C14-O15 |
| 4   | L     | 1004 | R5X  | C03-C12-C14-N16 |
| 4   | G     | 1004 | R5X  | N13-C12-C14-N16 |
| 4   | J     | 1004 | R5X  | N13-C12-C14-N16 |
| 6   | H     | 1006 | 1PE  | OH5-C14-C24-OH4 |

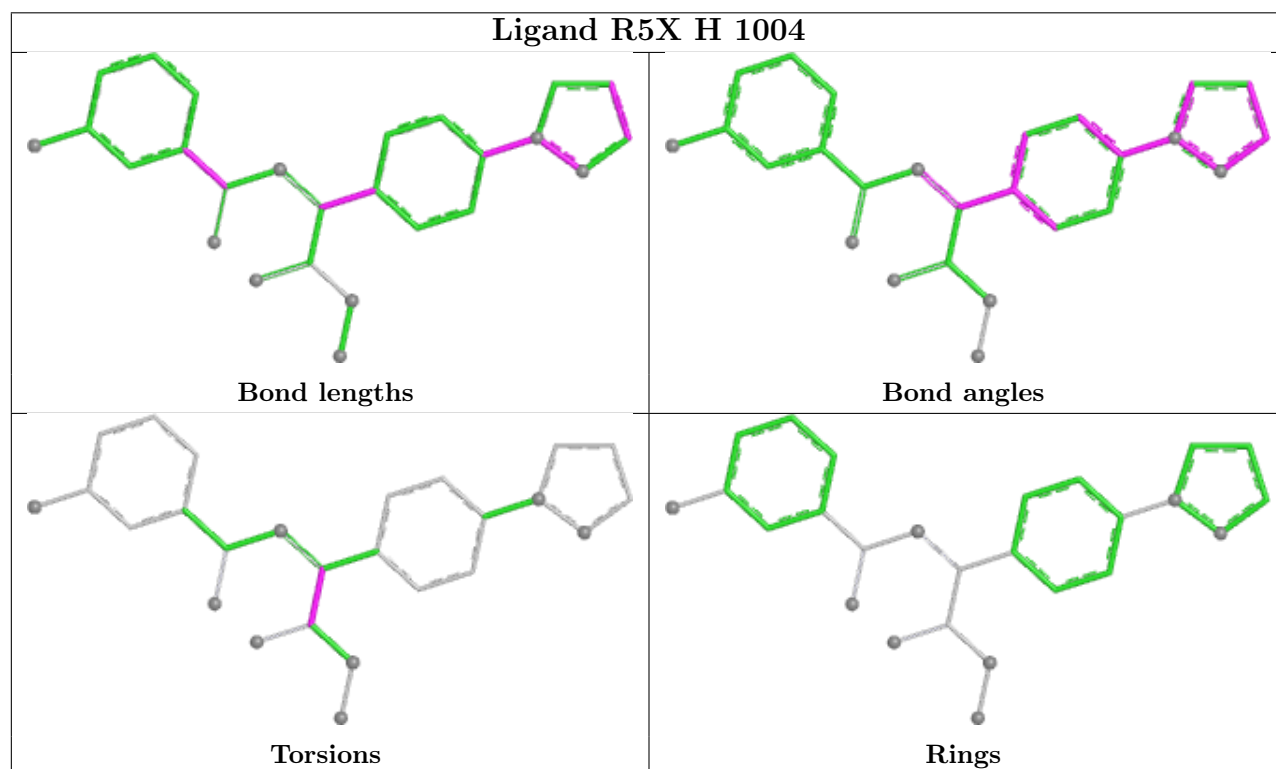
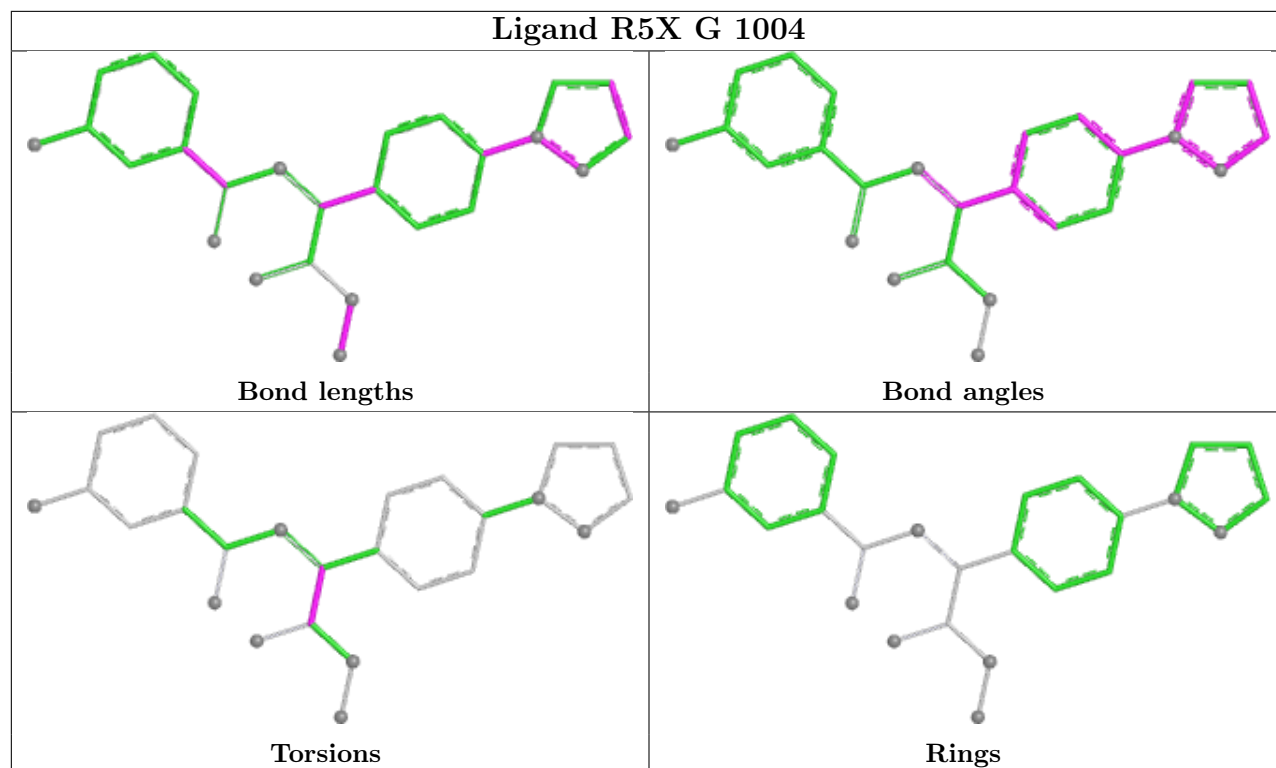
There are no ring outliers.

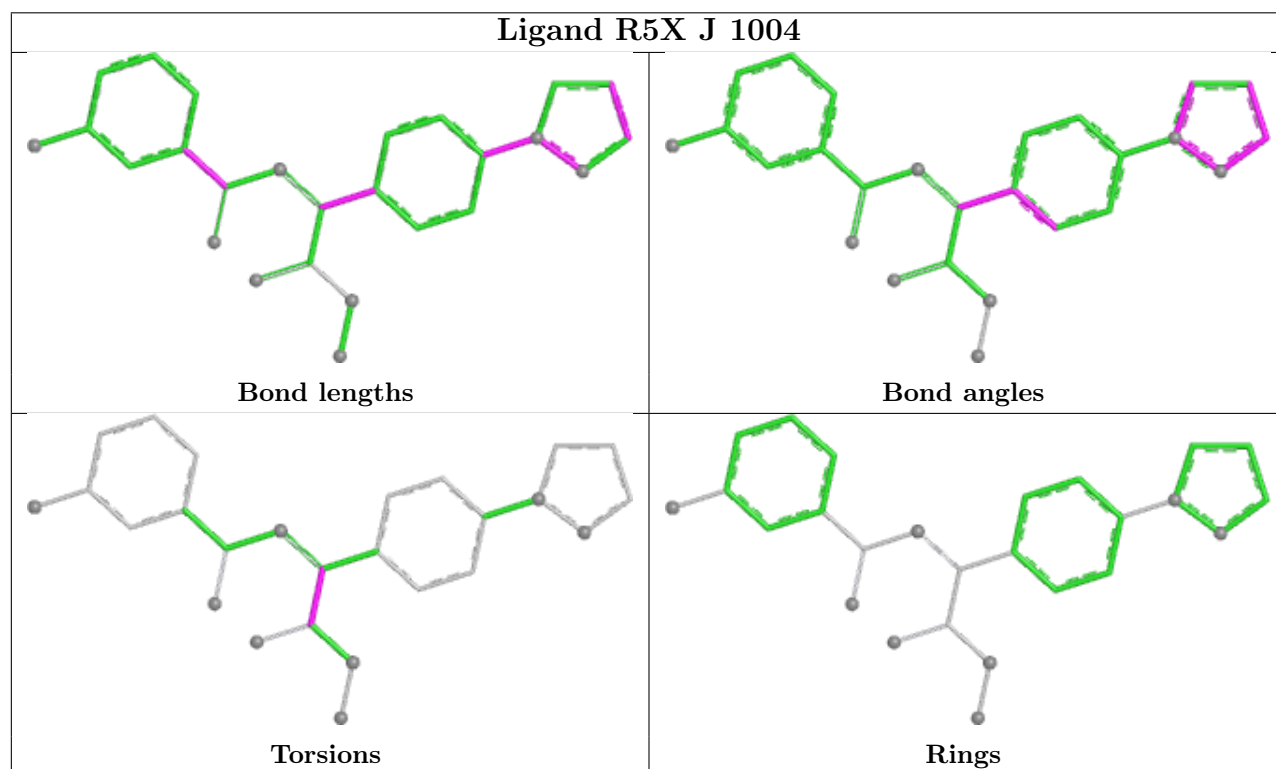
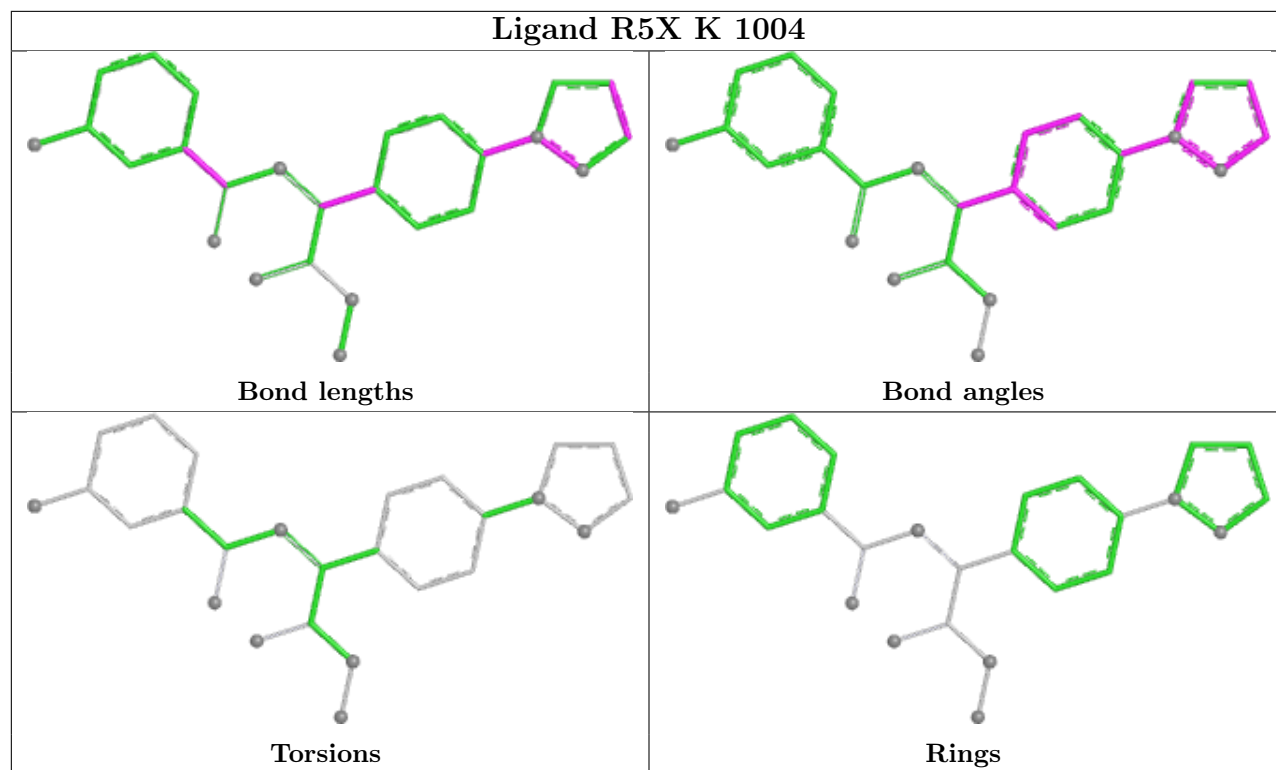
15 monomers are involved in 23 short contacts:

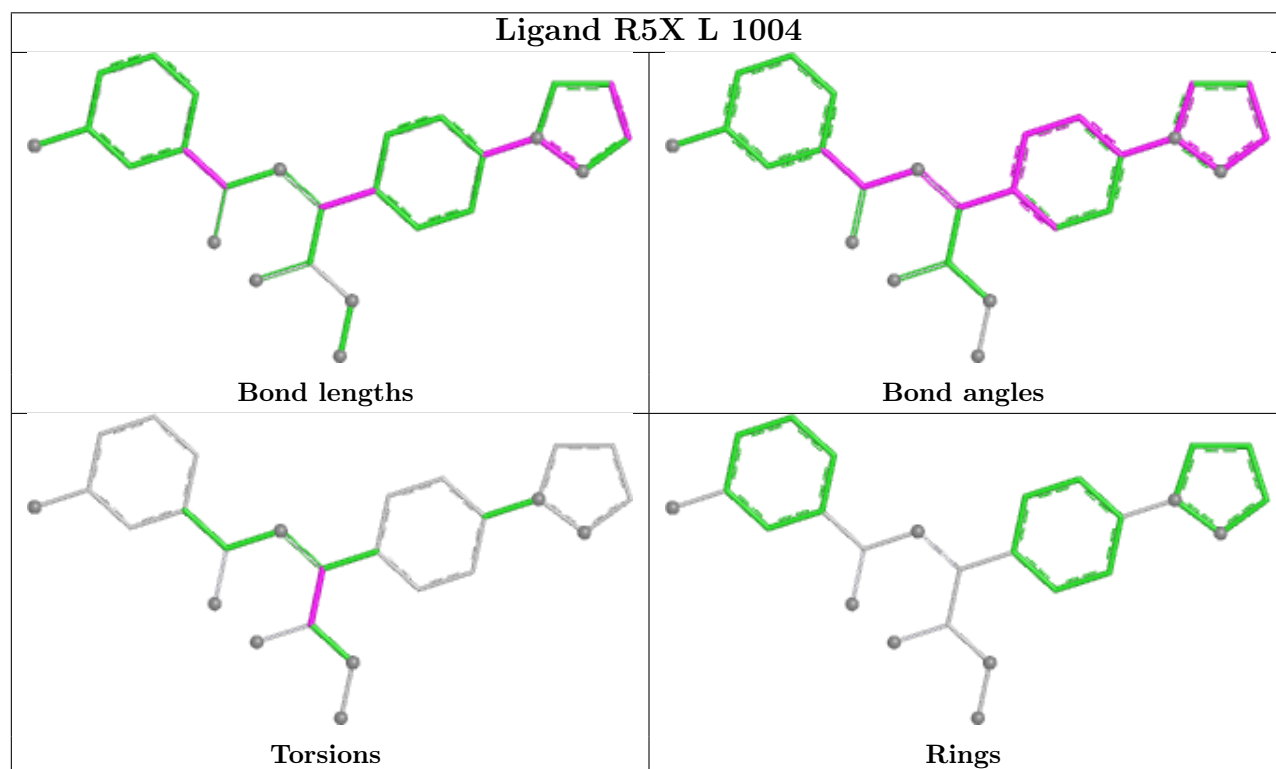
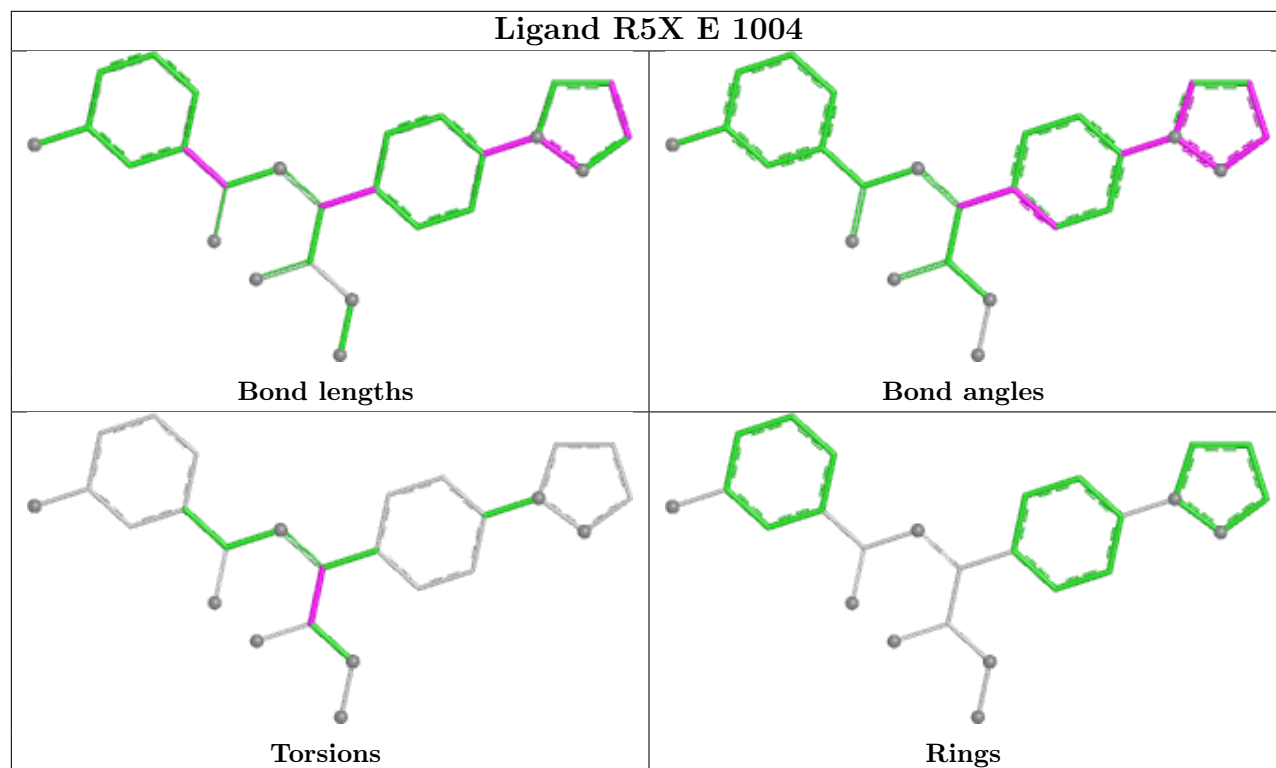
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | D     | 1004 | R5X  | 1       | 0            |
| 6   | G     | 1005 | 1PE  | 1       | 0            |
| 4   | B     | 1004 | R5X  | 1       | 0            |
| 6   | F     | 1005 | 1PE  | 1       | 0            |
| 4   | K     | 1004 | R5X  | 2       | 0            |
| 4   | J     | 1004 | R5X  | 3       | 0            |
| 4   | E     | 1004 | R5X  | 1       | 0            |
| 4   | L     | 1004 | R5X  | 2       | 0            |
| 5   | A     | 1005 | SO4  | 2       | 0            |
| 4   | I     | 1004 | R5X  | 2       | 0            |
| 4   | F     | 1004 | R5X  | 1       | 0            |
| 6   | G     | 1006 | 1PE  | 1       | 0            |
| 4   | C     | 1004 | R5X  | 3       | 0            |
| 6   | B     | 1005 | 1PE  | 1       | 0            |
| 4   | A     | 1004 | R5X  | 1       | 0            |

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

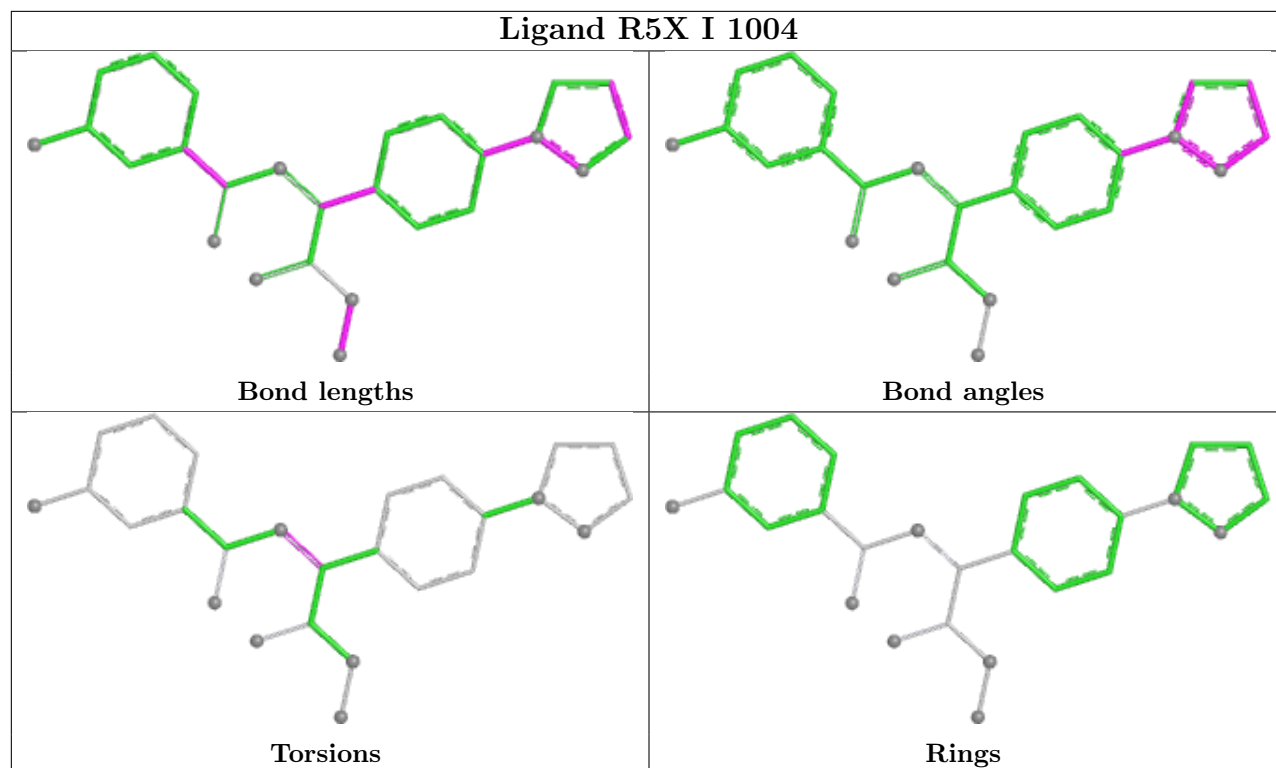




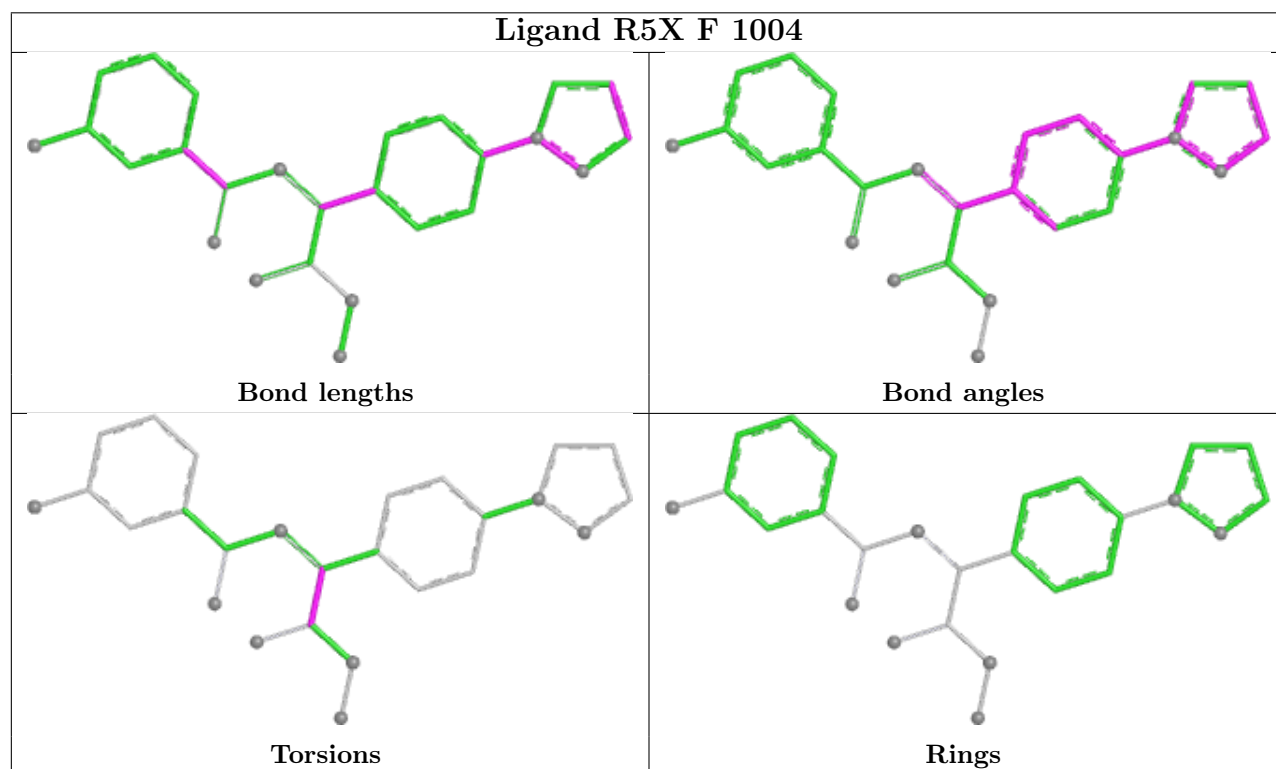


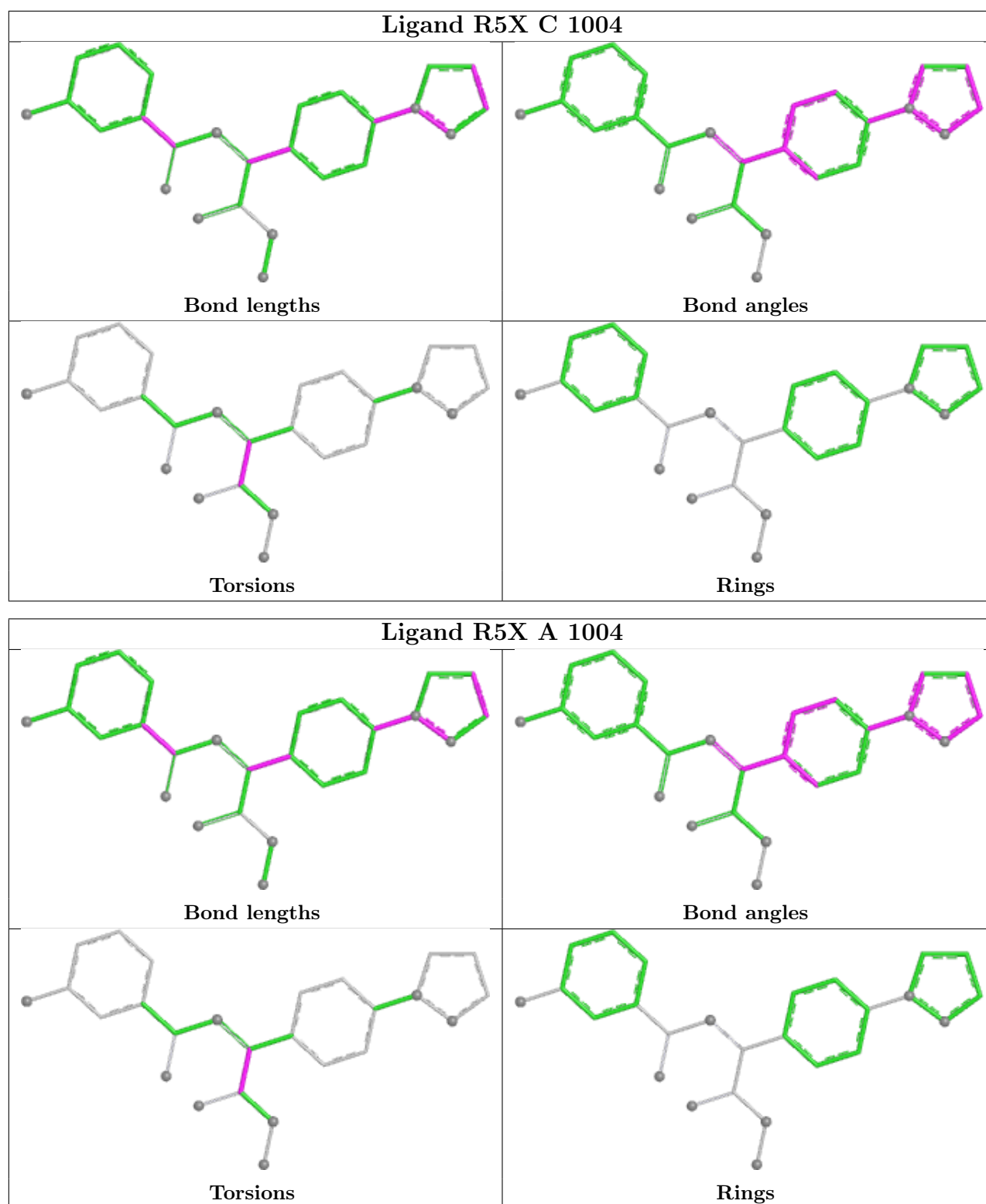


## Ligand R5X I 1004



## Ligand R5X F 1004





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 1   | A     | 515/528 (97%)   | -0.06  | 5 (0%) 79 76   | 14, 23, 43, 75        | 1 (0%) |
| 1   | B     | 511/528 (96%)   | 0.22   | 23 (4%) 38 33  | 15, 26, 62, 82        | 1 (0%) |
| 1   | C     | 518/528 (98%)   | 0.06   | 9 (1%) 69 65   | 15, 24, 53, 88        | 1 (0%) |
| 1   | D     | 514/528 (97%)   | -0.00  | 12 (2%) 61 57  | 16, 23, 45, 99        | 0      |
| 1   | E     | 510/528 (96%)   | -0.07  | 9 (1%) 67 64   | 16, 23, 39, 68        | 0      |
| 1   | F     | 509/528 (96%)   | 0.31   | 22 (4%) 40 35  | 16, 28, 55, 85        | 0      |
| 1   | G     | 517/528 (97%)   | -0.09  | 2 (0%) 88 86   | 18, 25, 45, 67        | 0      |
| 1   | H     | 515/528 (97%)   | 0.30   | 29 (5%) 30 26  | 17, 28, 64, 100       | 1 (0%) |
| 1   | I     | 516/528 (97%)   | 0.12   | 11 (2%) 63 59  | 17, 26, 53, 79        | 0      |
| 1   | J     | 511/528 (96%)   | 0.05   | 10 (1%) 65 61  | 19, 25, 45, 66        | 0      |
| 1   | K     | 509/528 (96%)   | 0.01   | 8 (1%) 70 67   | 20, 25, 41, 69        | 0      |
| 1   | L     | 510/528 (96%)   | 0.20   | 17 (3%) 49 45  | 20, 27, 52, 66        | 0      |
| All | All   | 6155/6336 (97%) | 0.09   | 157 (2%) 57 52 | 14, 25, 52, 100       | 4 (0%) |

All (157) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 603 | ASP  | 5.6  |
| 1   | F     | 363 | GLY  | 4.9  |
| 1   | F     | 161 | ASN  | 4.8  |
| 1   | E     | 439 | TYR  | 4.6  |
| 1   | B     | 123 | VAL  | 4.6  |
| 1   | F     | 439 | TYR  | 4.4  |
| 1   | I     | 400 | MET  | 4.3  |
| 1   | E     | 550 | SER  | 4.1  |
| 1   | F     | 365 | VAL  | 4.1  |
| 1   | H     | 549 | SER  | 4.0  |
| 1   | D     | 260 | ASN  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 217 | ASN  | 3.9  |
| 1   | H     | 260 | ASN  | 3.9  |
| 1   | B     | 255 | THR  | 3.9  |
| 1   | D     | 398 | PHE  | 3.8  |
| 1   | H     | 322 | ASN  | 3.7  |
| 1   | L     | 363 | GLY  | 3.7  |
| 1   | B     | 322 | ASN  | 3.6  |
| 1   | F     | 216 | ASP  | 3.6  |
| 1   | F     | 364 | ASP  | 3.6  |
| 1   | D     | 603 | ASP  | 3.6  |
| 1   | D     | 322 | ASN  | 3.5  |
| 1   | H     | 259 | VAL  | 3.5  |
| 1   | C     | 400 | MET  | 3.5  |
| 1   | L     | 161 | ASN  | 3.4  |
| 1   | L     | 272 | ASN  | 3.4  |
| 1   | L     | 439 | TYR  | 3.4  |
| 1   | H     | 398 | PHE  | 3.4  |
| 1   | E     | 255 | THR  | 3.4  |
| 1   | H     | 216 | ASP  | 3.4  |
| 1   | K     | 439 | TYR  | 3.3  |
| 1   | F     | 141 | PRO  | 3.3  |
| 1   | L     | 136 | GLY  | 3.3  |
| 1   | C     | 285 | ARG  | 3.3  |
| 1   | E     | 551 | VAL  | 3.3  |
| 1   | K     | 550 | SER  | 3.2  |
| 1   | J     | 439 | TYR  | 3.2  |
| 1   | J     | 398 | PHE  | 3.2  |
| 1   | C     | 439 | TYR  | 3.2  |
| 1   | C     | 195 | VAL  | 3.2  |
| 1   | B     | 182 | LYS  | 3.1  |
| 1   | I     | 568 | ASN  | 3.1  |
| 1   | F     | 550 | SER  | 3.1  |
| 1   | I     | 364 | ASP  | 3.1  |
| 1   | B     | 363 | GLY  | 3.1  |
| 1   | I     | 246 | TYR  | 3.0  |
| 1   | J     | 137 | LYS  | 3.0  |
| 1   | H     | 508 | GLU  | 3.0  |
| 1   | J     | 148 | VAL  | 3.0  |
| 1   | D     | 261 | MET  | 2.9  |
| 1   | A     | 197 | ASP  | 2.9  |
| 1   | H     | 197 | ASP  | 2.9  |
| 1   | B     | 549 | SER  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 195 | VAL  | 2.9  |
| 1   | J     | 419 | GLU  | 2.9  |
| 1   | C     | 603 | ASP  | 2.9  |
| 1   | F     | 335 | GLU  | 2.9  |
| 1   | H     | 400 | MET  | 2.9  |
| 1   | F     | 531 | ASN  | 2.9  |
| 1   | H     | 363 | GLY  | 2.9  |
| 1   | I     | 439 | TYR  | 2.9  |
| 1   | D     | 136 | GLY  | 2.9  |
| 1   | J     | 104 | ASN  | 2.8  |
| 1   | L     | 145 | SER  | 2.8  |
| 1   | D     | 255 | THR  | 2.8  |
| 1   | I     | 201 | ALA  | 2.8  |
| 1   | E     | 102 | GLU  | 2.8  |
| 1   | J     | 580 | SER  | 2.7  |
| 1   | E     | 395 | LEU  | 2.7  |
| 1   | B     | 193 | GLY  | 2.7  |
| 1   | D     | 137 | LYS  | 2.7  |
| 1   | D     | 125 | GLU  | 2.7  |
| 1   | E     | 398 | PHE  | 2.7  |
| 1   | H     | 193 | GLY  | 2.7  |
| 1   | L     | 153 | VAL  | 2.7  |
| 1   | H     | 261 | MET  | 2.7  |
| 1   | L     | 271 | ILE  | 2.7  |
| 1   | F     | 508 | GLU  | 2.7  |
| 1   | D     | 216 | ASP  | 2.6  |
| 1   | H     | 201 | ALA  | 2.6  |
| 1   | L     | 216 | ASP  | 2.6  |
| 1   | H     | 118 | LYS  | 2.6  |
| 1   | L     | 217 | ASN  | 2.5  |
| 1   | B     | 118 | LYS  | 2.5  |
| 1   | H     | 255 | THR  | 2.5  |
| 1   | A     | 363 | GLY  | 2.5  |
| 1   | I     | 603 | ASP  | 2.5  |
| 1   | A     | 258 | ASN  | 2.5  |
| 1   | H     | 135 | PRO  | 2.5  |
| 1   | H     | 117 | ILE  | 2.5  |
| 1   | K     | 549 | SER  | 2.5  |
| 1   | J     | 136 | GLY  | 2.4  |
| 1   | E     | 124 | GLU  | 2.4  |
| 1   | J     | 603 | ASP  | 2.4  |
| 1   | B     | 198 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 195 | VAL  | 2.4  |
| 1   | K     | 216 | ASP  | 2.4  |
| 1   | L     | 364 | ASP  | 2.4  |
| 1   | B     | 124 | GLU  | 2.4  |
| 1   | J     | 262 | GLU  | 2.4  |
| 1   | B     | 122 | ASN  | 2.4  |
| 1   | K     | 160 | GLU  | 2.4  |
| 1   | F     | 138 | GLU  | 2.3  |
| 1   | B     | 119 | GLY  | 2.3  |
| 1   | L     | 171 | THR  | 2.3  |
| 1   | I     | 332 | GLU  | 2.3  |
| 1   | H     | 196 | ALA  | 2.2  |
| 1   | K     | 572 | ALA  | 2.2  |
| 1   | H     | 137 | LYS  | 2.2  |
| 1   | F     | 159 | ASP  | 2.2  |
| 1   | D     | 262 | GLU  | 2.2  |
| 1   | C     | 602 | ASN  | 2.2  |
| 1   | B     | 136 | GLY  | 2.2  |
| 1   | B     | 102 | GLU  | 2.2  |
| 1   | H     | 102 | GLU  | 2.2  |
| 1   | F     | 165 | PHE  | 2.2  |
| 1   | B     | 201 | ALA  | 2.2  |
| 1   | B     | 272 | ASN  | 2.2  |
| 1   | C     | 119 | GLY  | 2.2  |
| 1   | E     | 86  | SER  | 2.2  |
| 1   | F     | 448 | SER  | 2.2  |
| 1   | L     | 146 | SER  | 2.2  |
| 1   | F     | 419 | GLU  | 2.2  |
| 1   | A     | 398 | PHE  | 2.2  |
| 1   | D     | 362 | LYS  | 2.2  |
| 1   | C     | 568 | ASN  | 2.1  |
| 1   | B     | 262 | GLU  | 2.1  |
| 1   | L     | 125 | GLU  | 2.1  |
| 1   | L     | 160 | GLU  | 2.1  |
| 1   | F     | 135 | PRO  | 2.1  |
| 1   | F     | 266 | HIS  | 2.1  |
| 1   | H     | 121 | CYS  | 2.1  |
| 1   | L     | 603 | ASP  | 2.1  |
| 1   | F     | 113 | GLN  | 2.1  |
| 1   | G     | 259 | VAL  | 2.1  |
| 1   | C     | 363 | GLY  | 2.1  |
| 1   | B     | 216 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 123 | VAL  | 2.1  |
| 1   | G     | 196 | ALA  | 2.1  |
| 1   | B     | 149 | ASN  | 2.1  |
| 1   | I     | 258 | ASN  | 2.1  |
| 1   | H     | 483 | ASP  | 2.1  |
| 1   | B     | 135 | PRO  | 2.1  |
| 1   | I     | 121 | CYS  | 2.1  |
| 1   | L     | 135 | PRO  | 2.1  |
| 1   | B     | 167 | VAL  | 2.0  |
| 1   | H     | 153 | VAL  | 2.0  |
| 1   | K     | 551 | VAL  | 2.0  |
| 1   | F     | 139 | ASN  | 2.0  |
| 1   | H     | 262 | GLU  | 2.0  |
| 1   | F     | 116 | ASP  | 2.0  |
| 1   | B     | 121 | CYS  | 2.0  |
| 1   | B     | 362 | LYS  | 2.0  |
| 1   | H     | 122 | ASN  | 2.0  |
| 1   | H     | 182 | LYS  | 2.0  |
| 1   | K     | 568 | ASN  | 2.0  |
| 1   | A     | 256 | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | SO4  | E     | 1008 | 5/5   | 0.72 | 0.29 | 87,87,88,88                 | 0     |
| 6   | 1PE  | B     | 1005 | 10/16 | 0.74 | 0.18 | 58,61,62,62                 | 0     |
| 6   | 1PE  | F     | 1006 | 9/16  | 0.75 | 0.18 | 39,39,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 6   | 1PE  | E     | 1007 | 10/16 | 0.76 | 0.19 | 56,59,61,61                 | 0     |
| 6   | 1PE  | F     | 1005 | 8/16  | 0.78 | 0.16 | 47,47,48,48                 | 0     |
| 5   | SO4  | F     | 1008 | 5/5   | 0.78 | 0.20 | 92,92,92,92                 | 0     |
| 6   | 1PE  | H     | 1006 | 10/16 | 0.80 | 0.18 | 39,42,47,47                 | 0     |
| 6   | 1PE  | F     | 1007 | 9/16  | 0.82 | 0.14 | 39,40,42,43                 | 0     |
| 6   | 1PE  | I     | 1005 | 10/16 | 0.82 | 0.15 | 38,42,43,43                 | 0     |
| 6   | 1PE  | G     | 1006 | 10/16 | 0.83 | 0.17 | 56,57,58,58                 | 0     |
| 6   | 1PE  | I     | 1006 | 11/16 | 0.84 | 0.16 | 33,38,42,43                 | 0     |
| 6   | 1PE  | J     | 1005 | 10/16 | 0.84 | 0.11 | 42,43,45,46                 | 0     |
| 4   | R5X  | I     | 1004 | 26/26 | 0.85 | 0.14 | 20,28,38,41                 | 0     |
| 6   | 1PE  | B     | 1006 | 9/16  | 0.86 | 0.17 | 35,38,47,48                 | 0     |
| 6   | 1PE  | L     | 1005 | 7/16  | 0.88 | 0.11 | 37,38,38,38                 | 0     |
| 4   | R5X  | A     | 1004 | 26/26 | 0.90 | 0.12 | 26,28,43,44                 | 0     |
| 5   | SO4  | A     | 1006 | 5/5   | 0.90 | 0.22 | 62,63,63,63                 | 0     |
| 4   | R5X  | L     | 1004 | 26/26 | 0.91 | 0.11 | 24,28,43,43                 | 0     |
| 4   | R5X  | F     | 1004 | 26/26 | 0.91 | 0.11 | 23,29,45,45                 | 0     |
| 6   | 1PE  | G     | 1005 | 13/16 | 0.91 | 0.12 | 38,39,45,45                 | 0     |
| 4   | R5X  | K     | 1004 | 26/26 | 0.92 | 0.13 | 31,36,48,48                 | 0     |
| 4   | R5X  | G     | 1004 | 26/26 | 0.92 | 0.09 | 24,27,38,39                 | 0     |
| 4   | R5X  | C     | 1004 | 26/26 | 0.92 | 0.10 | 21,31,35,35                 | 0     |
| 4   | R5X  | B     | 1004 | 26/26 | 0.93 | 0.11 | 22,28,36,36                 | 0     |
| 4   | R5X  | J     | 1004 | 26/26 | 0.93 | 0.10 | 25,34,44,44                 | 0     |
| 4   | R5X  | D     | 1004 | 26/26 | 0.93 | 0.10 | 26,30,43,43                 | 0     |
| 6   | 1PE  | K     | 1006 | 13/16 | 0.93 | 0.08 | 34,36,39,40                 | 0     |
| 4   | R5X  | H     | 1004 | 26/26 | 0.93 | 0.11 | 27,31,39,39                 | 0     |
| 3   | CO3  | A     | 1002 | 4/4   | 0.94 | 0.09 | 22,22,23,23                 | 0     |
| 4   | R5X  | E     | 1004 | 26/26 | 0.94 | 0.10 | 26,44,50,51                 | 0     |
| 6   | 1PE  | E     | 1006 | 10/16 | 0.94 | 0.08 | 27,28,29,30                 | 0     |
| 3   | CO3  | C     | 1002 | 4/4   | 0.95 | 0.07 | 19,21,21,22                 | 0     |
| 3   | CO3  | F     | 1002 | 4/4   | 0.95 | 0.07 | 15,18,18,19                 | 0     |
| 3   | CO3  | H     | 1002 | 4/4   | 0.95 | 0.09 | 22,23,23,24                 | 0     |
| 3   | CO3  | G     | 1002 | 4/4   | 0.96 | 0.07 | 23,23,23,24                 | 0     |
| 3   | CO3  | E     | 1002 | 4/4   | 0.96 | 0.07 | 22,23,24,24                 | 0     |
| 3   | CO3  | K     | 1002 | 4/4   | 0.96 | 0.09 | 29,29,29,30                 | 0     |
| 3   | CO3  | J     | 1002 | 4/4   | 0.97 | 0.07 | 20,20,20,20                 | 0     |
| 3   | CO3  | D     | 1002 | 4/4   | 0.97 | 0.09 | 17,18,18,19                 | 0     |
| 3   | CO3  | L     | 1002 | 4/4   | 0.97 | 0.07 | 19,20,24,25                 | 0     |
| 3   | CO3  | B     | 1002 | 4/4   | 0.98 | 0.08 | 19,19,19,20                 | 0     |
| 5   | SO4  | H     | 1005 | 5/5   | 0.98 | 0.07 | 16,20,20,21                 | 0     |
| 5   | SO4  | K     | 1005 | 5/5   | 0.98 | 0.06 | 23,24,25,25                 | 0     |
| 2   | ZN   | C     | 1003 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 2   | ZN   | D     | 1001 | 1/1   | 0.98 | 0.03 | 24,24,24,24                 | 0     |

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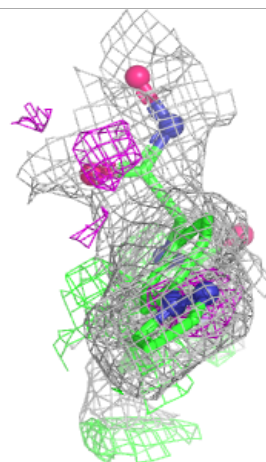
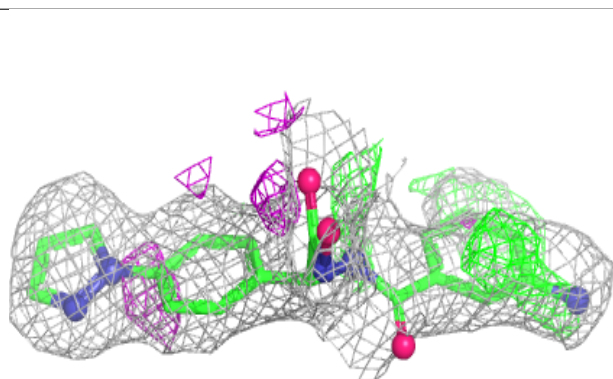
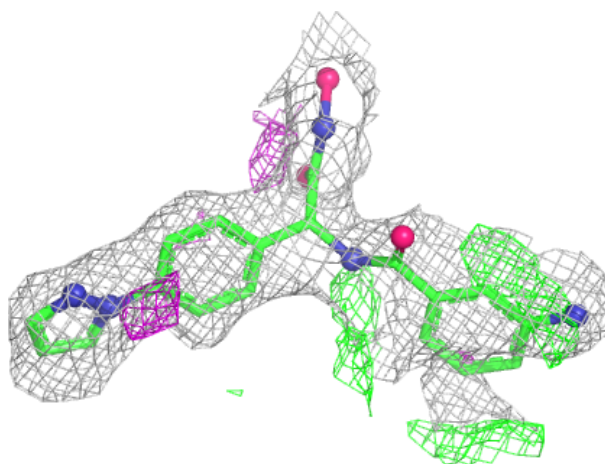
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | ZN   | B     | 1001 | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 2   | ZN   | G     | 1003 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 2   | ZN   | H     | 1001 | 1/1   | 0.99 | 0.03 | 30,30,30,30                 | 0     |
| 3   | CO3  | I     | 1002 | 4/4   | 0.99 | 0.04 | 21,21,22,23                 | 0     |
| 2   | ZN   | H     | 1003 | 1/1   | 0.99 | 0.02 | 34,34,34,34                 | 0     |
| 2   | ZN   | I     | 1001 | 1/1   | 0.99 | 0.02 | 32,32,32,32                 | 0     |
| 2   | ZN   | I     | 1003 | 1/1   | 0.99 | 0.03 | 29,29,29,29                 | 0     |
| 5   | SO4  | A     | 1005 | 5/5   | 0.99 | 0.05 | 14,17,19,20                 | 0     |
| 2   | ZN   | C     | 1001 | 1/1   | 0.99 | 0.02 | 28,28,28,28                 | 0     |
| 5   | SO4  | E     | 1005 | 5/5   | 0.99 | 0.05 | 22,22,22,23                 | 0     |
| 2   | ZN   | A     | 1003 | 1/1   | 0.99 | 0.02 | 23,23,23,23                 | 0     |
| 2   | ZN   | A     | 1001 | 1/1   | 0.99 | 0.03 | 27,27,27,27                 | 0     |
| 2   | ZN   | D     | 1003 | 1/1   | 0.99 | 0.02 | 28,28,28,28                 | 0     |
| 2   | ZN   | E     | 1003 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 2   | ZN   | G     | 1001 | 1/1   | 0.99 | 0.03 | 30,30,30,30                 | 0     |
| 2   | ZN   | K     | 1001 | 1/1   | 1.00 | 0.02 | 27,27,27,27                 | 0     |
| 2   | ZN   | K     | 1003 | 1/1   | 1.00 | 0.02 | 28,28,28,28                 | 0     |
| 2   | ZN   | L     | 1001 | 1/1   | 1.00 | 0.01 | 29,29,29,29                 | 0     |
| 2   | ZN   | L     | 1003 | 1/1   | 1.00 | 0.02 | 30,30,30,30                 | 0     |
| 2   | ZN   | F     | 1001 | 1/1   | 1.00 | 0.01 | 28,28,28,28                 | 0     |
| 2   | ZN   | F     | 1003 | 1/1   | 1.00 | 0.02 | 26,26,26,26                 | 0     |
| 2   | ZN   | E     | 1001 | 1/1   | 1.00 | 0.01 | 26,26,26,26                 | 0     |
| 2   | ZN   | B     | 1003 | 1/1   | 1.00 | 0.03 | 29,29,29,29                 | 0     |
| 2   | ZN   | J     | 1001 | 1/1   | 1.00 | 0.01 | 23,23,23,23                 | 0     |
| 2   | ZN   | J     | 1003 | 1/1   | 1.00 | 0.02 | 28,28,28,28                 | 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.

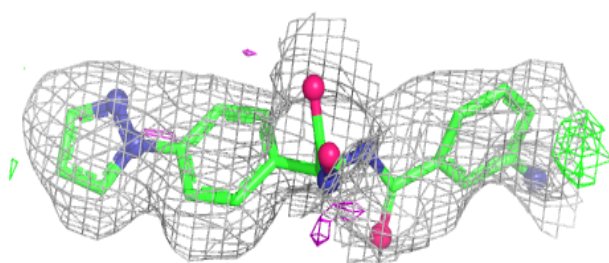
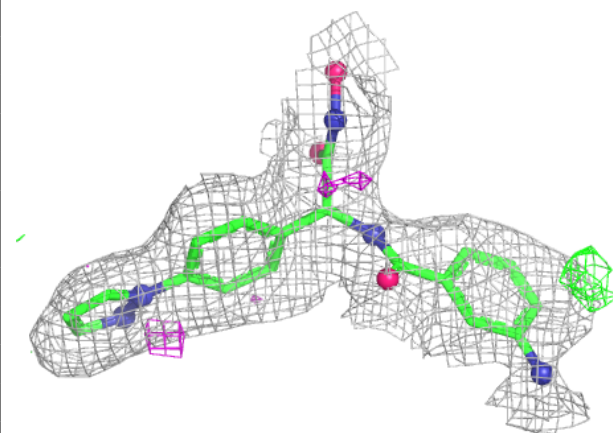
**Electron density around R5X I 1004:**

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



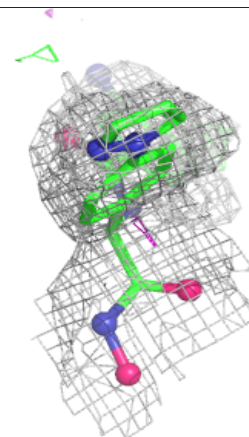
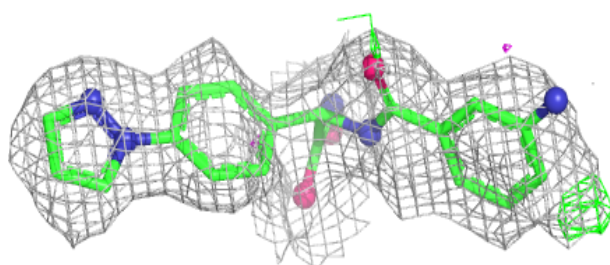
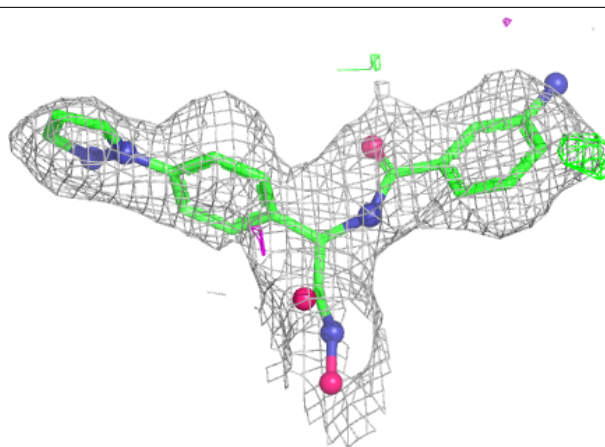
**Electron density around R5X A 1004:**

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

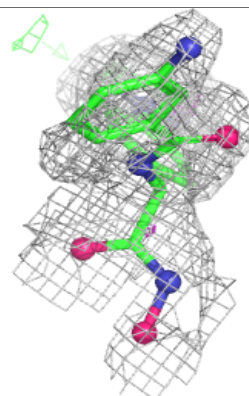
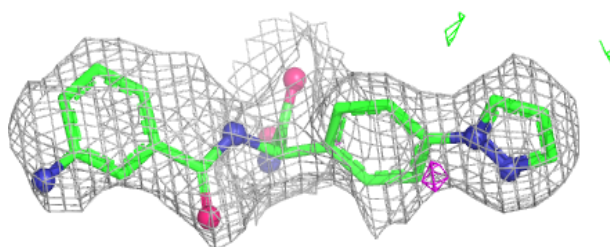
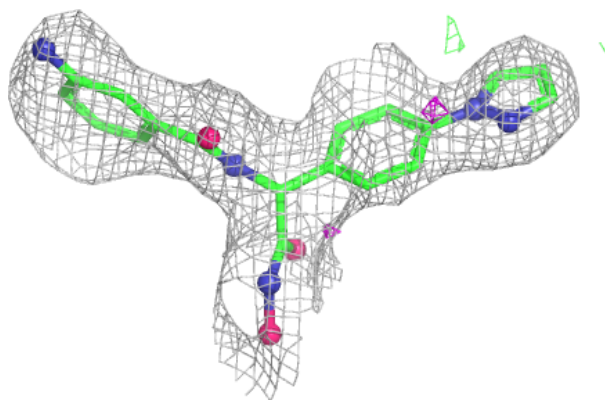


**Electron density around R5X L 1004:**

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

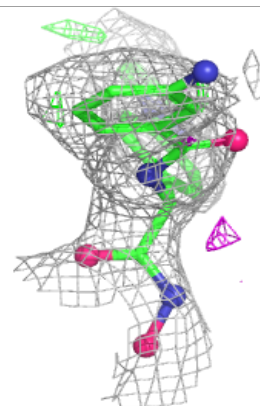
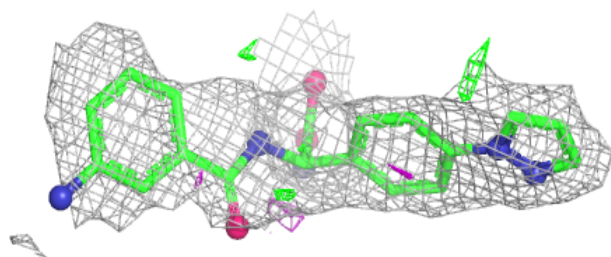
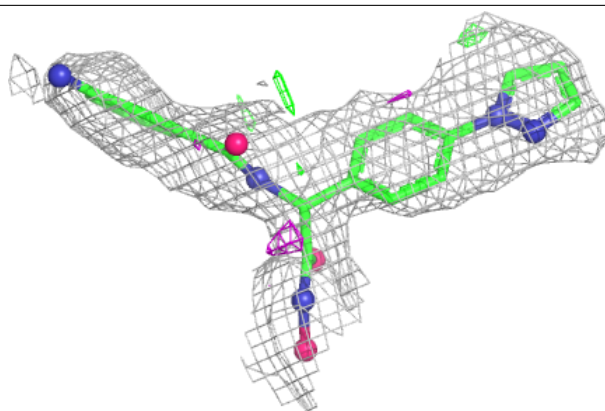
**Electron density around R5X F 1004:**

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

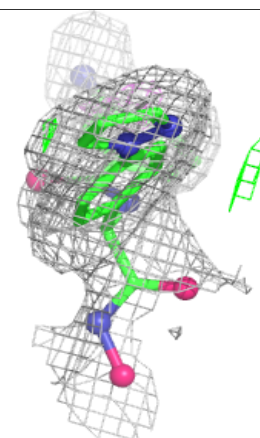
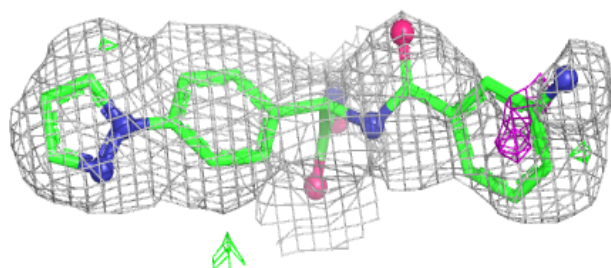
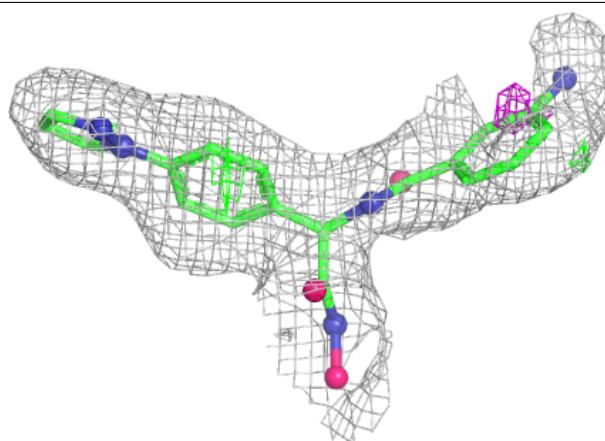


**Electron density around R5X K 1004:**

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

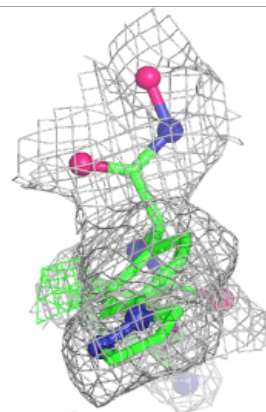
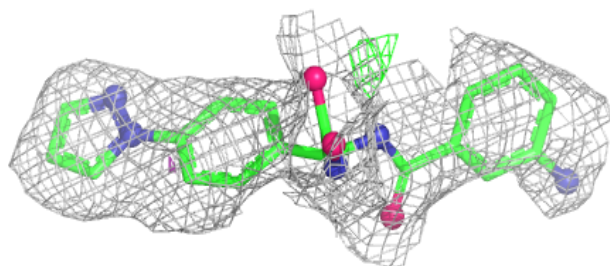
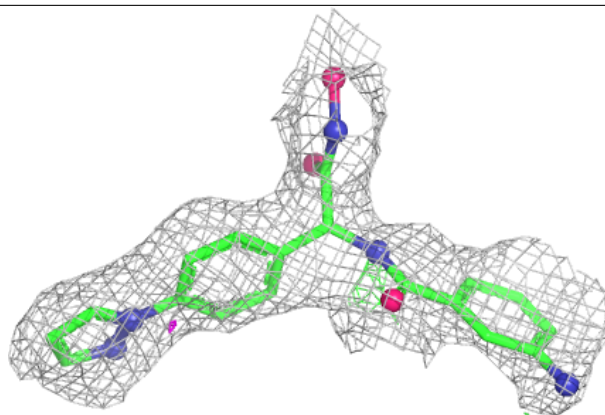
**Electron density around R5X G 1004:**

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

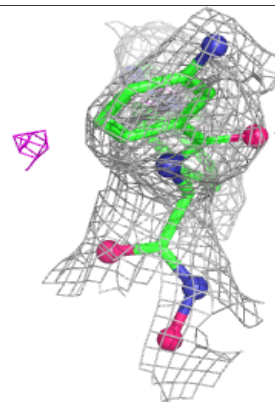
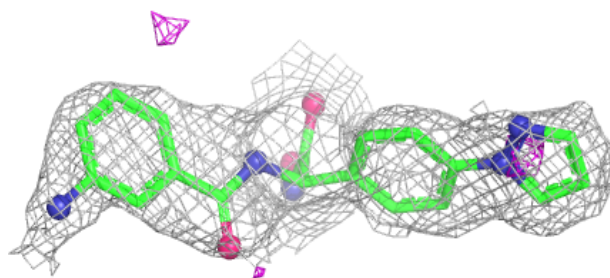
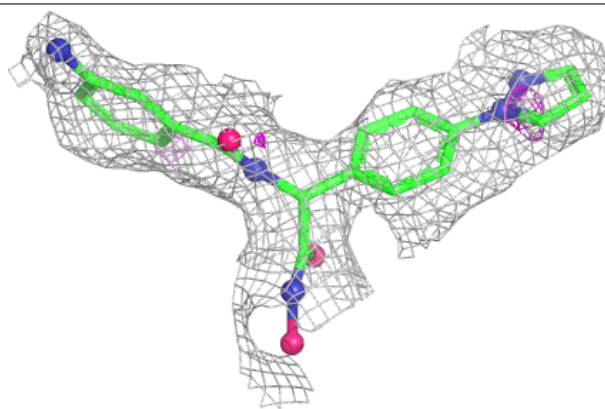


**Electron density around R5X C 1004:**

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

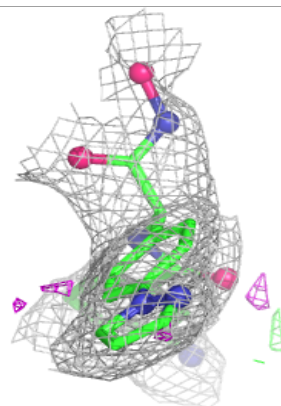
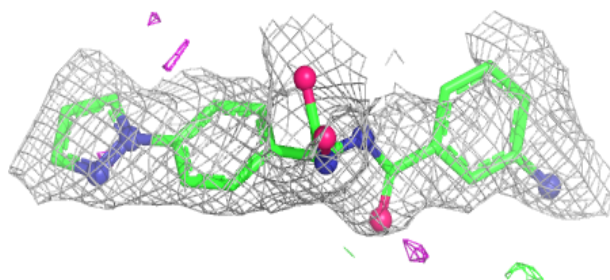
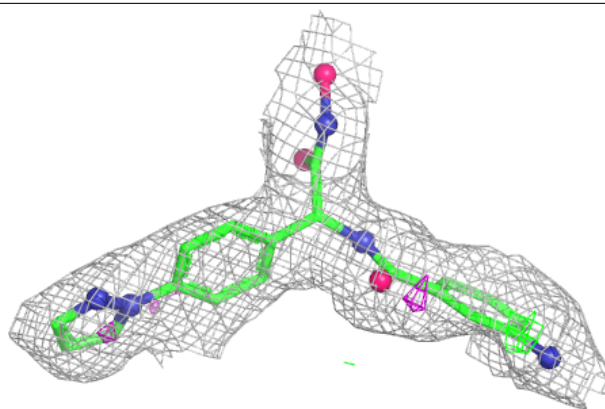
**Electron density around R5X B 1004:**

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

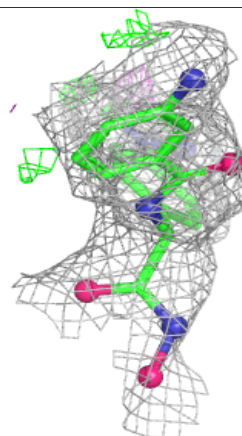
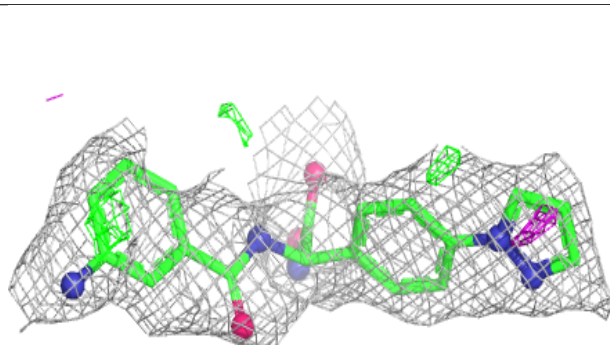
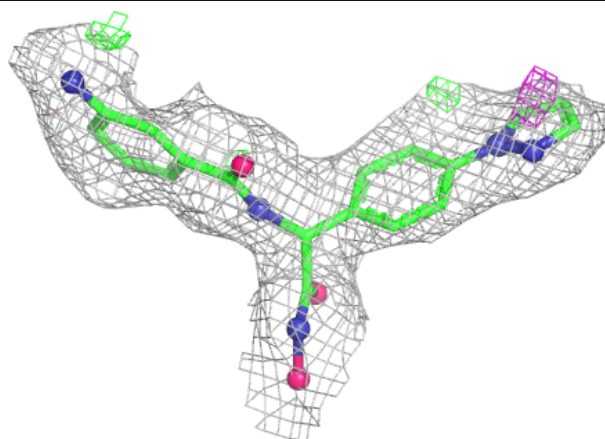


**Electron density around R5X J 1004:**

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

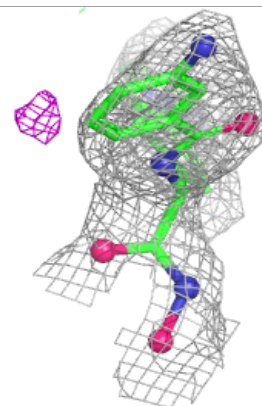
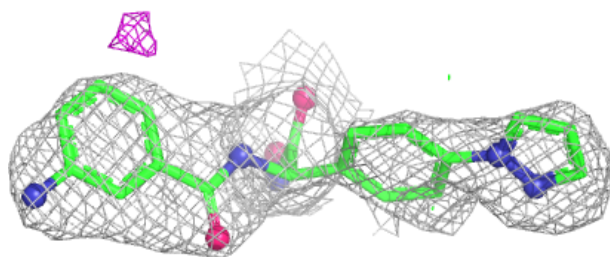
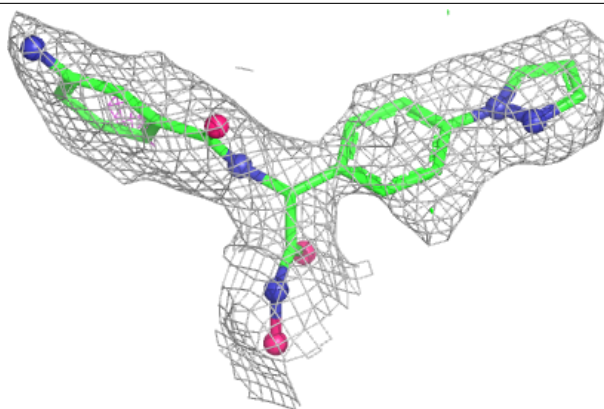
**Electron density around R5X D 1004:**

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

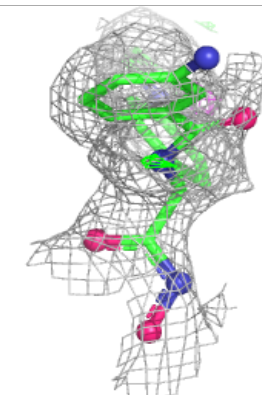
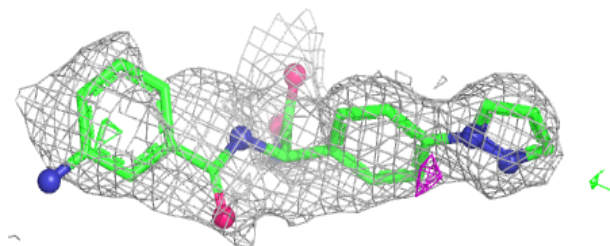
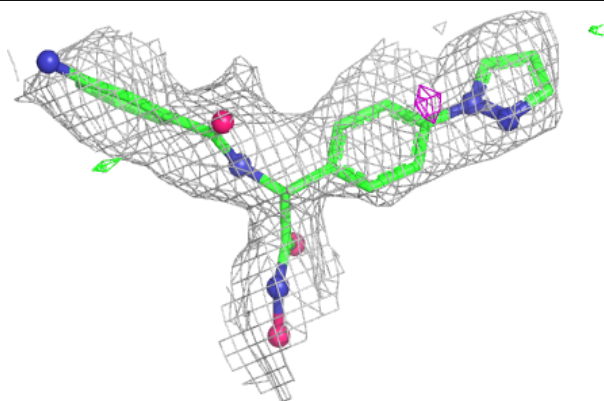


**Electron density around R5X H 1004:**

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

**Electron density around R5X E 1004:**

$2mF_o-DF_c$  (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.