



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:38 PM UTC

PDB ID : 3U8M / pdb\_00003u8m  
Title : Crystal structure of the acetylcholine binding protein (AChBP) from *Lymnaea stagnalis* in complex with NS3920 (1-(6-bromopyridin-3-yl)-1,4-diazepane)  
Authors : Rohde, L.A.H.; Ahring, P.K.; Jensen, M.L.; Nielsen, E.O.; Peters, D.; Helgstrand, C.; Krintel, C.; Harpsoe, K.; Gajhede, M.; Kastrup, J.S.; Balle, T.  
Deposited on : 2011-10-17  
Resolution : 2.70 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

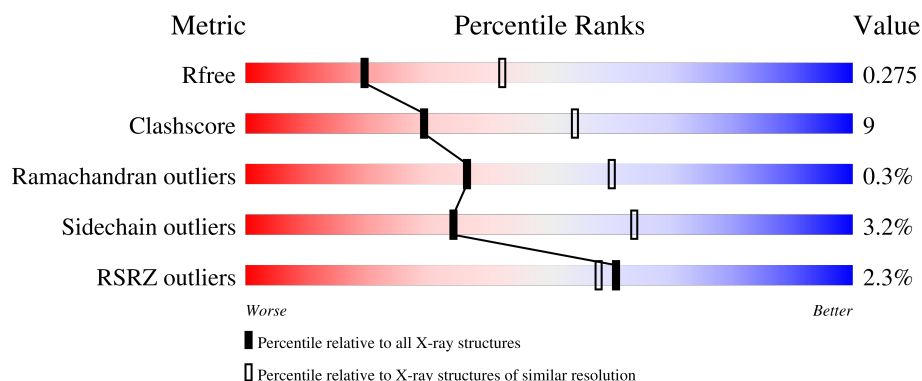
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

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     | 210    | <br>3% 84% 11% •    |
| 1   | B     | 210    | <br>2% 80% 14% • 5% |
| 1   | C     | 210    | <br>2% 83% 11% • •  |
| 1   | D     | 210    | <br>3% 76% 18% • •  |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | E     | 210    | <div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>  |
| 1   | F     | 210    | <div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> </div>   |
| 1   | G     | 210    | <div> <div>2%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>5%</div> </div> </div> |
| 1   | H     | 210    | <div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>  |
| 1   | I     | 210    | <div> <div>%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> </div>    |
| 1   | J     | 210    | <div> <div>%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>6%</div> </div> </div>  |
| 1   | K     | 210    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div></div> </div> </div>    |
| 1   | L     | 210    | <div> <div>3%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div></div> </div> </div>   |
| 1   | M     | 210    | <div> <div>3%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div> |
| 1   | N     | 210    | <div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div></div> </div> </div>    |
| 1   | O     | 210    | <div> <div>3%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div> |
| 1   | P     | 210    | <div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>5%</div> </div> </div> |
| 1   | Q     | 210    | <div> <div>3%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>5%</div> </div> </div> |
| 1   | R     | 210    | <div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>5%</div> </div> </div> |
| 1   | S     | 210    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>5%</div> </div> </div>  |
| 1   | T     | 210    | <div> <div>2%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>5%</div> </div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32783 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 Acetylcholine-binding protein.

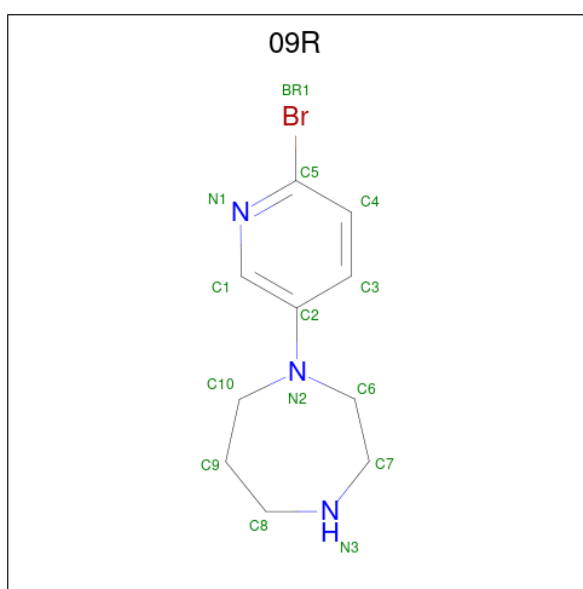
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 202      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1623  | 1017 | 279 | 322 | 5 |         |         |       |
| 1   | B     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 999  | 273 | 313 | 5 |         |         |       |
| 1   | C     | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1009 | 278 | 317 | 5 |         |         |       |
| 1   | D     | 202      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1617  | 1013 | 276 | 323 | 5 |         |         |       |
| 1   | E     | 196      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1575  | 992  | 270 | 308 | 5 |         |         |       |
| 1   | F     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1639  | 1025 | 282 | 327 | 5 |         |         |       |
| 1   | G     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 999  | 273 | 313 | 5 |         |         |       |
| 1   | H     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1584  | 996  | 272 | 311 | 5 |         |         |       |
| 1   | I     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1629  | 1019 | 281 | 324 | 5 |         |         |       |
| 1   | J     | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1608  | 1008 | 275 | 320 | 5 |         |         |       |
| 1   | K     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1632  | 1021 | 281 | 325 | 5 |         |         |       |
| 1   | L     | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1623  | 1016 | 280 | 322 | 5 |         |         |       |
| 1   | M     | 200      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1604  | 1007 | 274 | 318 | 5 |         |         |       |
| 1   | N     | 201      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1611  | 1010 | 275 | 320 | 6 |         |         |       |
| 1   | O     | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1580  | 994  | 271 | 310 | 5 |         |         |       |
| 1   | P     | 200      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1597  | 1003 | 274 | 315 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Q     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 999  | 273 | 313 | 5 |         |         |       |
| 1   | R     | 199      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1593  | 1001 | 273 | 314 | 5 |         |         |       |
| 1   | S     | 200      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1598  | 1003 | 274 | 316 | 5 |         |         |       |
| 1   | T     | 200      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1598  | 1003 | 274 | 316 | 5 |         |         |       |

- Molecule 2 is 1-(6-bromopyridin-3-yl)-1,4-diazepane (CCD ID: 09R) (formula: C<sub>10</sub>H<sub>14</sub>BrN<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 2   | A     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | B     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | C     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | D     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | E     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | F     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | G     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 2   | H     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | I     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | J     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | K     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | L     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | M     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | N     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | O     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | P     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | Q     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | R     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | S     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |
| 2   | T     | 1        | Total | Br | C  | N | 0       | 0       |
|     |       |          | 14    | 1  | 10 | 3 |         |         |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | T     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | B     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 4   | C     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 4   | E     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 4   | F     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | G     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | H     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 4   | I     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 4   | J     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | K     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | L     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | M     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 4   | N     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 4   | O     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 4   | P     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |

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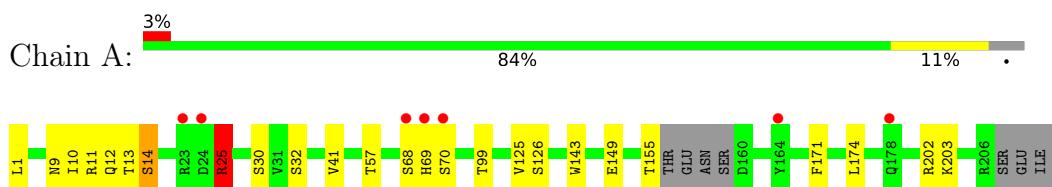
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | Q     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 4   | R     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | S     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | T     | 19       | Total<br>19 | O<br>19 | 0       | 0       |

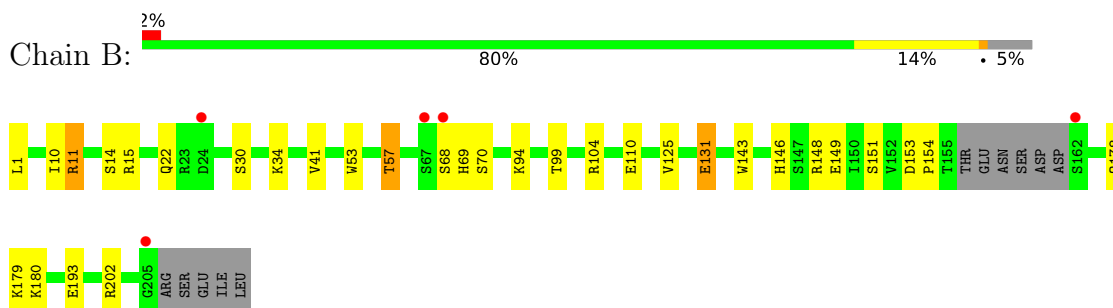
### 3 Residue-property plots [i](#)

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.

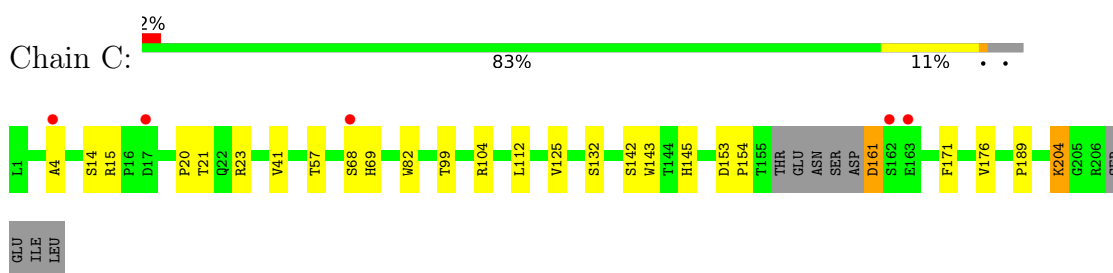
#### • Molecule 1: Acetylcholine-binding protein



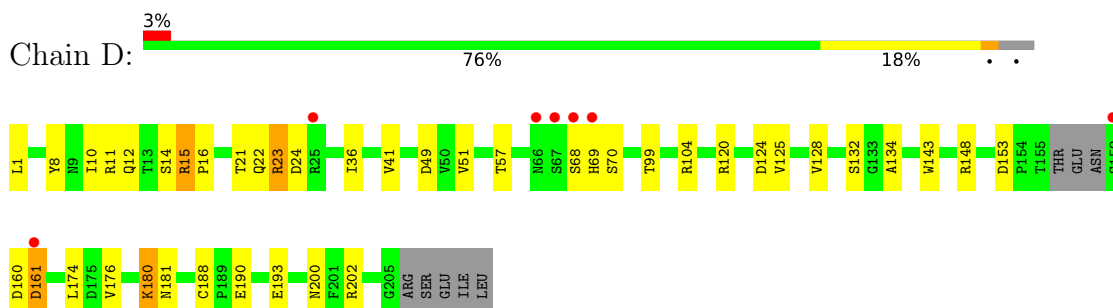
#### • Molecule 1: Acetylcholine-binding protein



#### • Molecule 1: Acetylcholine-binding protein

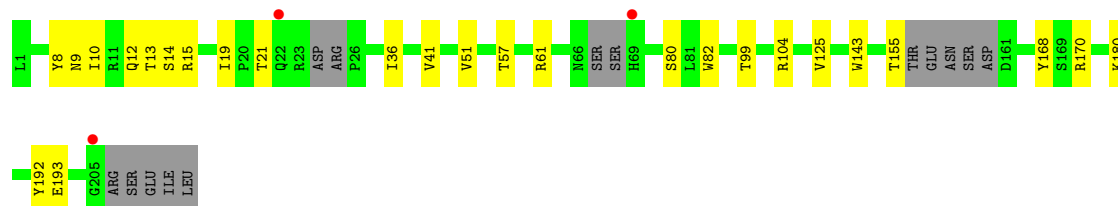


#### • Molecule 1: Acetylcholine-binding protein



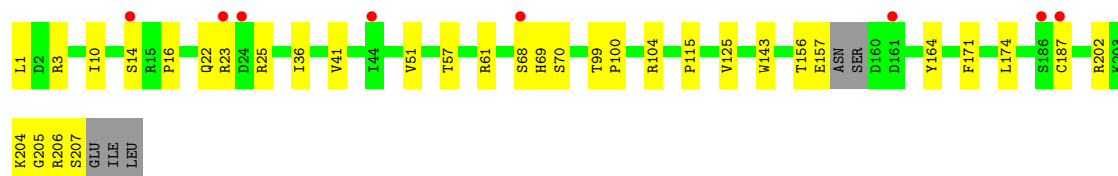
- Molecule 1: Acetylcholine-binding protein

Chain E: 



- Molecule 1: Acetylcholine-binding protein

Chain F: 



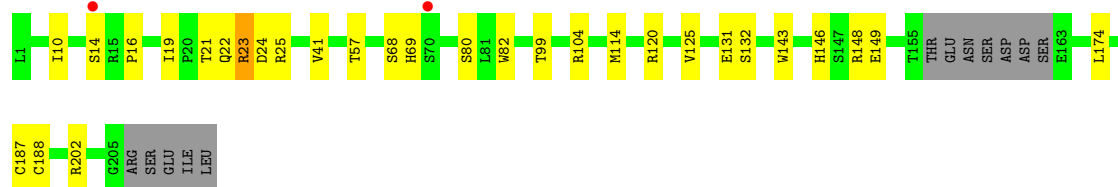
- Molecule 1: Acetylcholine-binding protein

Chain G: 



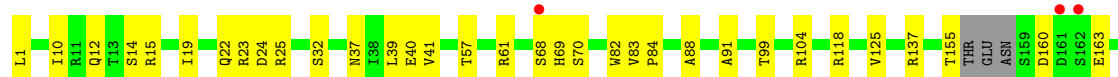
- Molecule 1: Acetylcholine-binding protein

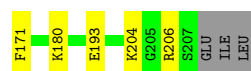
Chain H: 



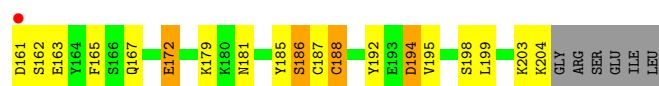
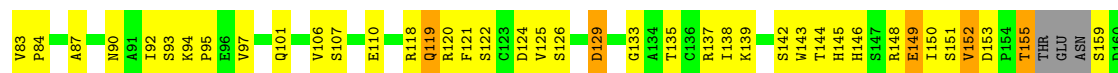
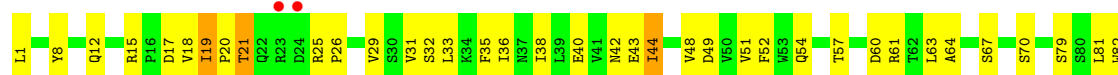
- Molecule 1: Acetylcholine-binding protein

Chain I: 

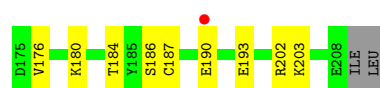
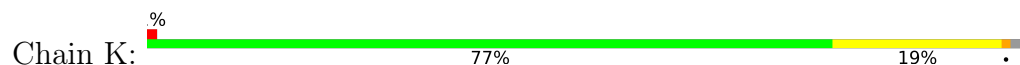




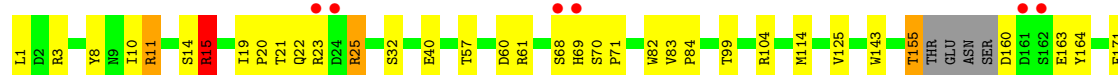
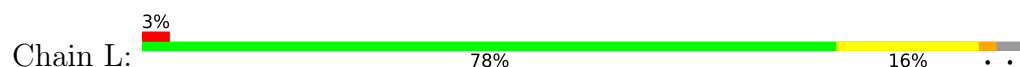
• Molecule 1: Acetylcholine-binding protein



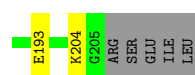
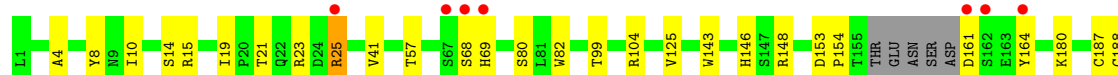
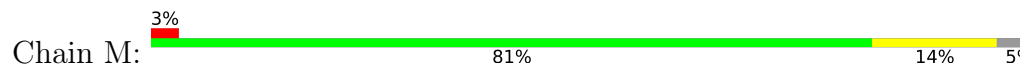
• Molecule 1: Acetylcholine-binding protein



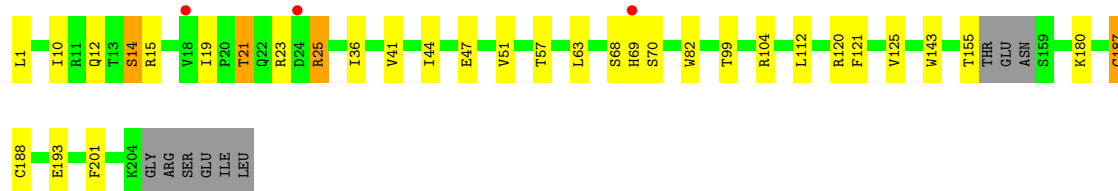
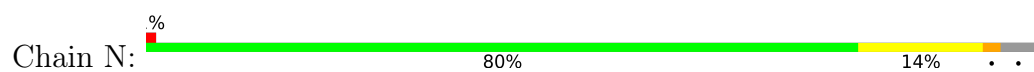
• Molecule 1: Acetylcholine-binding protein



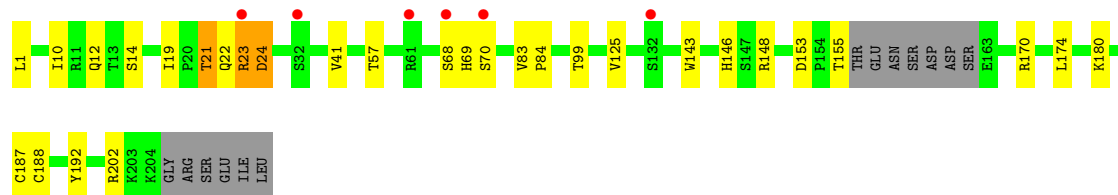
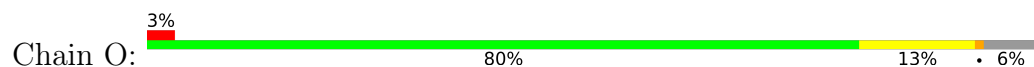
• Molecule 1: Acetylcholine-binding protein



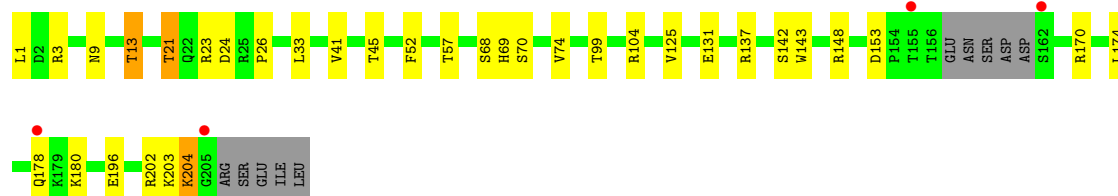
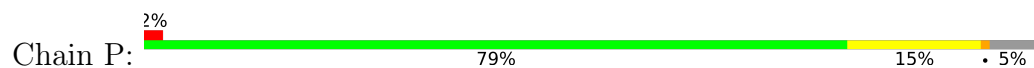
• Molecule 1: Acetylcholine-binding protein



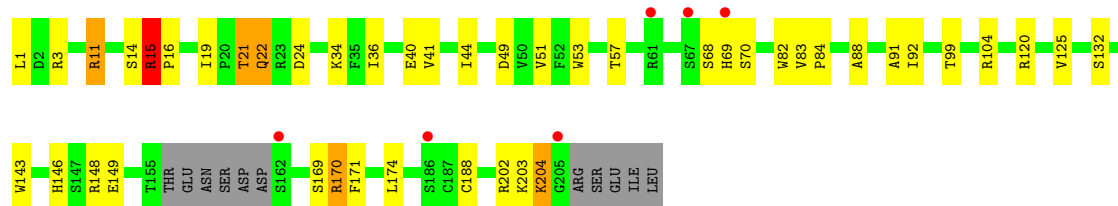
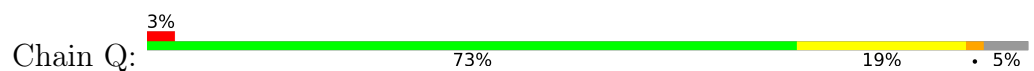
- Molecule 1: Acetylcholine-binding protein



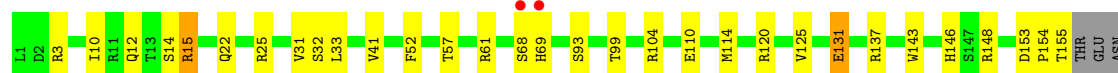
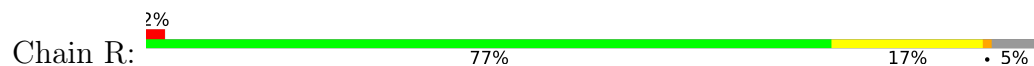
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

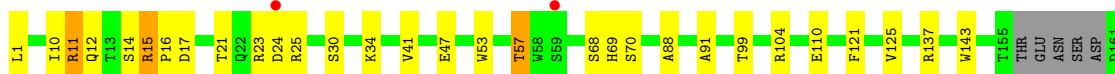
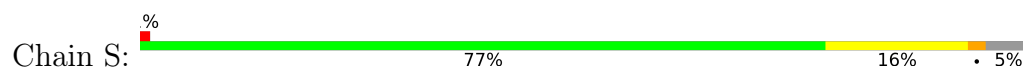


- Molecule 1: Acetylcholine-binding protein

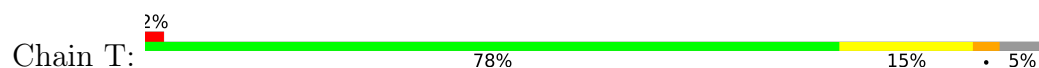




- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 233.06Å 268.45Å 73.26Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 30.01 – 2.70<br>30.01 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.8 (30.01-2.70)<br>97.7 (30.01-2.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | 0.11                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.00 (at 2.68Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.6.4_486                                            | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.275<br>0.214 , 0.275                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2514 reflections (1.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.870                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 43.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 32783                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 32.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 09R

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     | 0.52         | 0/1661      | 0.80        | 2/2264 (0.1%)   |
| 1   | B     | 0.53         | 0/1625      | 0.80        | 0/2216          |
| 1   | C     | 0.54         | 0/1644      | 0.79        | 1/2241 (0.0%)   |
| 1   | D     | 0.54         | 0/1655      | 0.86        | 3/2258 (0.1%)   |
| 1   | E     | 0.54         | 0/1611      | 0.82        | 2/2193 (0.1%)   |
| 1   | F     | 0.53         | 0/1674      | 0.79        | 0/2282          |
| 1   | G     | 0.53         | 0/1625      | 0.84        | 4/2216 (0.2%)   |
| 1   | H     | 0.55         | 0/1619      | 0.81        | 0/2208          |
| 1   | I     | 0.50         | 0/1664      | 0.78        | 0/2268          |
| 1   | J     | 0.61         | 0/1643      | 1.00        | 7/2241 (0.3%)   |
| 1   | K     | 0.54         | 0/1667      | 0.84        | 0/2272          |
| 1   | L     | 0.54         | 0/1658      | 0.90        | 5/2260 (0.2%)   |
| 1   | M     | 0.52         | 0/1642      | 0.78        | 0/2239          |
| 1   | N     | 0.51         | 0/1649      | 0.86        | 2/2249 (0.1%)   |
| 1   | O     | 0.53         | 0/1615      | 0.82        | 0/2203          |
| 1   | P     | 0.52         | 0/1632      | 0.80        | 0/2226          |
| 1   | Q     | 0.56         | 0/1625      | 0.97        | 5/2216 (0.2%)   |
| 1   | R     | 0.52         | 0/1631      | 0.85        | 4/2224 (0.2%)   |
| 1   | S     | 0.50         | 0/1633      | 0.82        | 3/2227 (0.1%)   |
| 1   | T     | 0.51         | 0/1633      | 0.83        | 0/2227          |
| All | All   | 0.53         | 0/32806     | 0.84        | 38/44730 (0.1%) |

There are no bond length outliers.

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | Q     | 170 | ARG  | NE-CZ-NH2 | 11.88  | 129.89      | 119.20   |
| 1   | Q     | 170 | ARG  | NE-CZ-NH1 | -11.81 | 109.69      | 121.50   |
| 1   | L     | 25  | ARG  | CA-C-N    | 9.71   | 129.66      | 119.85   |
| 1   | L     | 25  | ARG  | C-N-CA    | 9.71   | 129.66      | 119.85   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Q     | 15  | ARG  | CA-C-N   | 9.67  | 129.30      | 119.82   |
| 1   | Q     | 15  | ARG  | C-N-CA   | 9.67  | 129.30      | 119.82   |
| 1   | R     | 15  | ARG  | CA-C-N   | 9.18  | 128.82      | 119.82   |
| 1   | R     | 15  | ARG  | C-N-CA   | 9.18  | 128.82      | 119.82   |
| 1   | N     | 15  | ARG  | CA-C-N   | 8.89  | 128.63      | 119.56   |
| 1   | N     | 15  | ARG  | C-N-CA   | 8.89  | 128.63      | 119.56   |
| 1   | Q     | 170 | ARG  | CD-NE-CZ | 8.21  | 135.90      | 124.40   |
| 1   | L     | 15  | ARG  | CA-C-N   | 8.17  | 127.90      | 119.56   |
| 1   | L     | 15  | ARG  | C-N-CA   | 8.17  | 127.90      | 119.56   |
| 1   | G     | 25  | ARG  | N-CA-C   | 6.71  | 118.16      | 109.64   |
| 1   | G     | 15  | ARG  | CA-C-N   | 6.67  | 126.29      | 119.56   |
| 1   | G     | 15  | ARG  | C-N-CA   | 6.67  | 126.29      | 119.56   |
| 1   | J     | 188 | CYS  | CA-C-N   | 6.61  | 126.06      | 118.85   |
| 1   | J     | 188 | CYS  | C-N-CA   | 6.61  | 126.06      | 118.85   |
| 1   | S     | 15  | ARG  | CA-C-N   | 6.03  | 125.58      | 119.19   |
| 1   | S     | 15  | ARG  | C-N-CA   | 6.03  | 125.58      | 119.19   |
| 1   | E     | 15  | ARG  | CA-C-N   | 5.84  | 125.38      | 119.19   |
| 1   | E     | 15  | ARG  | C-N-CA   | 5.84  | 125.38      | 119.19   |
| 1   | D     | 15  | ARG  | CA-C-N   | 5.74  | 125.36      | 119.56   |
| 1   | D     | 15  | ARG  | C-N-CA   | 5.74  | 125.36      | 119.56   |
| 1   | J     | 19  | ILE  | N-CA-C   | 5.54  | 113.40      | 108.63   |
| 1   | R     | 25  | ARG  | CA-C-N   | 5.48  | 125.42      | 119.78   |
| 1   | R     | 25  | ARG  | C-N-CA   | 5.48  | 125.42      | 119.78   |
| 1   | J     | 181 | ASN  | N-CA-C   | 5.43  | 118.12      | 110.14   |
| 1   | C     | 204 | LYS  | N-CA-C   | -5.38 | 102.93      | 110.35   |
| 1   | L     | 204 | LYS  | N-CA-C   | -5.36 | 103.40      | 110.43   |
| 1   | J     | 25  | ARG  | CA-C-N   | 5.30  | 125.59      | 119.92   |
| 1   | J     | 25  | ARG  | C-N-CA   | 5.30  | 125.59      | 119.92   |
| 1   | A     | 25  | ARG  | CA-C-N   | -5.25 | 114.58      | 120.14   |
| 1   | A     | 25  | ARG  | C-N-CA   | -5.25 | 114.58      | 120.14   |
| 1   | J     | 119 | GLN  | N-CA-C   | 5.22  | 117.18      | 108.99   |
| 1   | D     | 160 | ASP  | N-CA-C   | 5.17  | 117.67      | 109.24   |
| 1   | G     | 23  | ARG  | CB-CA-C  | -5.10 | 110.72      | 116.63   |
| 1   | S     | 204 | LYS  | N-CA-C   | 5.01  | 117.78      | 109.46   |

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     | 1623  | 0        | 1575     | 21      | 0            |
| 1   | B     | 1590  | 0        | 1548     | 33      | 0            |
| 1   | C     | 1609  | 0        | 1565     | 23      | 0            |
| 1   | D     | 1617  | 0        | 1565     | 34      | 0            |
| 1   | E     | 1575  | 0        | 1537     | 24      | 0            |
| 1   | F     | 1639  | 0        | 1587     | 27      | 0            |
| 1   | G     | 1590  | 0        | 1548     | 40      | 0            |
| 1   | H     | 1584  | 0        | 1543     | 22      | 0            |
| 1   | I     | 1629  | 0        | 1579     | 29      | 0            |
| 1   | J     | 1608  | 0        | 1558     | 68      | 0            |
| 1   | K     | 1632  | 0        | 1580     | 37      | 0            |
| 1   | L     | 1623  | 0        | 1574     | 41      | 0            |
| 1   | M     | 1604  | 0        | 1558     | 24      | 0            |
| 1   | N     | 1611  | 0        | 1563     | 30      | 0            |
| 1   | O     | 1580  | 0        | 1540     | 24      | 0            |
| 1   | P     | 1597  | 0        | 1555     | 30      | 0            |
| 1   | Q     | 1590  | 0        | 1548     | 33      | 0            |
| 1   | R     | 1593  | 0        | 1553     | 37      | 0            |
| 1   | S     | 1598  | 0        | 1552     | 29      | 0            |
| 1   | T     | 1598  | 0        | 1552     | 38      | 0            |
| 2   | A     | 14    | 0        | 14       | 1       | 0            |
| 2   | B     | 14    | 0        | 14       | 2       | 0            |
| 2   | C     | 14    | 0        | 14       | 1       | 0            |
| 2   | D     | 14    | 0        | 14       | 1       | 0            |
| 2   | E     | 14    | 0        | 14       | 1       | 0            |
| 2   | F     | 14    | 0        | 14       | 2       | 0            |
| 2   | G     | 14    | 0        | 14       | 3       | 0            |
| 2   | H     | 14    | 0        | 14       | 1       | 0            |
| 2   | I     | 14    | 0        | 14       | 0       | 0            |
| 2   | J     | 14    | 0        | 14       | 2       | 0            |
| 2   | K     | 14    | 0        | 14       | 0       | 0            |
| 2   | L     | 14    | 0        | 14       | 3       | 0            |
| 2   | M     | 14    | 0        | 14       | 2       | 0            |
| 2   | N     | 14    | 0        | 14       | 2       | 0            |
| 2   | O     | 14    | 0        | 14       | 3       | 0            |
| 2   | P     | 14    | 0        | 14       | 2       | 0            |
| 2   | Q     | 14    | 0        | 14       | 2       | 0            |
| 2   | R     | 14    | 0        | 14       | 1       | 0            |
| 2   | S     | 14    | 0        | 14       | 2       | 0            |
| 2   | T     | 14    | 0        | 14       | 4       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | D     | 15    | 0        | 0        | 0       | 0            |
| 3   | F     | 10    | 0        | 0        | 1       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 5     | 0        | 0        | 0       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |
| 3   | K     | 5     | 0        | 0        | 0       | 0            |
| 3   | L     | 10    | 0        | 0        | 0       | 0            |
| 3   | N     | 5     | 0        | 0        | 0       | 0            |
| 3   | R     | 5     | 0        | 0        | 0       | 0            |
| 3   | T     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 23    | 0        | 0        | 1       | 0            |
| 4   | B     | 16    | 0        | 0        | 1       | 0            |
| 4   | C     | 20    | 0        | 0        | 2       | 0            |
| 4   | D     | 21    | 0        | 0        | 2       | 0            |
| 4   | E     | 15    | 0        | 0        | 1       | 0            |
| 4   | F     | 19    | 0        | 0        | 2       | 0            |
| 4   | G     | 14    | 0        | 0        | 2       | 0            |
| 4   | H     | 18    | 0        | 0        | 0       | 0            |
| 4   | I     | 15    | 0        | 0        | 1       | 0            |
| 4   | J     | 9     | 0        | 0        | 0       | 0            |
| 4   | K     | 19    | 0        | 0        | 0       | 0            |
| 4   | L     | 20    | 0        | 0        | 0       | 0            |
| 4   | M     | 11    | 0        | 0        | 0       | 0            |
| 4   | N     | 18    | 0        | 0        | 0       | 0            |
| 4   | O     | 12    | 0        | 0        | 0       | 0            |
| 4   | P     | 13    | 0        | 0        | 2       | 0            |
| 4   | Q     | 19    | 0        | 0        | 1       | 0            |
| 4   | R     | 13    | 0        | 0        | 0       | 0            |
| 4   | S     | 14    | 0        | 0        | 0       | 0            |
| 4   | T     | 19    | 0        | 0        | 1       | 0            |
| All | All   | 32783 | 0        | 31460    | 552     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (552) 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:170[B]:ARG:HG2 | 1:E:170[B]:ARG:HH11 | 1.00                     | 1.10              |
| 1:L:15:ARG:HG2     | 1:L:15:ARG:HH11     | 1.15                     | 1.07              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:25:ARG:HG3     | 1:A:25:ARG:HH11    | 1.19                     | 1.07              |
| 1:P:9:ASN:O        | 1:P:13:THR:HG22    | 1.58                     | 1.04              |
| 1:G:131:GLU:HG2    | 1:G:132:SER:H      | 1.23                     | 1.03              |
| 1:I:160:ASP:HB3    | 1:I:163:GLU:HB2    | 1.51                     | 0.93              |
| 1:H:10:ILE:O       | 1:H:14:SER:HB3     | 1.68                     | 0.93              |
| 1:R:22:GLN:HE22    | 1:R:61:ARG:HG2     | 1.33                     | 0.92              |
| 1:R:131:GLU:HG3    | 1:R:202:ARG:NH1    | 1.85                     | 0.92              |
| 1:T:148:ARG:HH11   | 1:T:148:ARG:HG2    | 1.32                     | 0.91              |
| 1:L:15:ARG:HH11    | 1:L:15:ARG:CG      | 1.82                     | 0.91              |
| 1:A:25:ARG:HH11    | 1:A:25:ARG:CG      | 1.84                     | 0.91              |
| 1:E:9:ASN:O        | 1:E:13:THR:HG22    | 1.70                     | 0.90              |
| 1:E:170[B]:ARG:HG2 | 1:E:170[B]:ARG:NH1 | 1.79                     | 0.87              |
| 1:R:22:GLN:NE2     | 1:R:61:ARG:HG2     | 1.90                     | 0.87              |
| 1:A:25:ARG:HG3     | 1:A:25:ARG:NH1     | 1.88                     | 0.85              |
| 1:L:15:ARG:NH2     | 1:M:8:TYR:HB2      | 1.90                     | 0.85              |
| 1:R:93:SER:HB2     | 1:R:120:ARG:HH21   | 1.42                     | 0.84              |
| 1:L:10:ILE:O       | 1:L:14:SER:HB2     | 1.78                     | 0.83              |
| 1:E:10:ILE:O       | 1:E:14:SER:HB3     | 1.80                     | 0.81              |
| 1:S:23:ARG:HB2     | 1:S:25:ARG:HG2     | 1.63                     | 0.81              |
| 1:Q:169:SER:O      | 1:Q:204:LYS:HE2    | 1.81                     | 0.80              |
| 1:L:15:ARG:HG2     | 1:L:15:ARG:NH1     | 1.91                     | 0.79              |
| 1:B:180:LYS:HD3    | 1:P:180:LYS:HD3    | 1.65                     | 0.79              |
| 1:N:23:ARG:HG3     | 1:N:23:ARG:O       | 1.80                     | 0.78              |
| 1:J:63:LEU:HD11    | 1:J:81:LEU:HD21    | 1.66                     | 0.76              |
| 1:A:10:ILE:O       | 1:A:14:SER:HB3     | 1.86                     | 0.76              |
| 1:B:180:LYS:HE2    | 1:P:153:ASP:OD2    | 1.87                     | 0.74              |
| 1:J:172:GLU:HG2    | 1:J:204:LYS:HG3    | 1.68                     | 0.74              |
| 1:L:15:ARG:HH21    | 1:M:8:TYR:HB2      | 1.50                     | 0.73              |
| 1:N:10:ILE:O       | 1:N:14:SER:HB3     | 1.88                     | 0.73              |
| 1:J:1:LEU:HB2      | 1:J:70:SER:OG      | 1.87                     | 0.73              |
| 1:O:12:GLN:HB3     | 1:R:12:GLN:HB3     | 1.72                     | 0.72              |
| 1:H:187:CYS:SG     | 1:H:188:CYS:N      | 2.63                     | 0.71              |
| 1:F:22:GLN:OE1     | 1:F:61:ARG:HG3     | 1.91                     | 0.71              |
| 1:J:172:GLU:HG2    | 1:J:204:LYS:CG     | 2.21                     | 0.71              |
| 1:K:143:TRP:CZ2    | 1:L:99:THR:HG21    | 2.26                     | 0.71              |
| 1:N:25:ARG:HH11    | 1:N:25:ARG:CG      | 2.04                     | 0.70              |
| 1:G:131:GLU:HG2    | 1:G:132:SER:N      | 2.03                     | 0.70              |
| 1:G:182:SER:HB3    | 1:K:184:THR:HG21   | 1.72                     | 0.70              |
| 1:D:161:ASP:HB3    | 1:D:176:VAL:HG23   | 1.73                     | 0.69              |
| 1:J:38:ILE:HG13    | 1:J:165:PHE:CZ     | 2.28                     | 0.69              |
| 1:R:131:GLU:HG3    | 1:R:202:ARG:HH12   | 1.55                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:15:ARG:NH2   | 1:L:8:TYR:HB2    | 2.07                     | 0.69              |
| 1:B:146:HIS:CE1  | 1:B:148:ARG:HB2  | 2.28                     | 0.68              |
| 1:M:143:TRP:CE2  | 1:N:99:THR:HG21  | 2.30                     | 0.67              |
| 1:H:120:ARG:HH12 | 1:I:118:ARG:HH12 | 1.41                     | 0.67              |
| 1:K:41:VAL:HG13  | 1:K:125:VAL:HG11 | 1.77                     | 0.67              |
| 1:G:131:GLU:CG   | 1:G:132:SER:H    | 2.02                     | 0.67              |
| 1:D:41:VAL:HG13  | 1:D:125:VAL:HG11 | 1.75                     | 0.67              |
| 1:G:182:SER:CB   | 1:K:184:THR:HG21 | 2.26                     | 0.66              |
| 1:K:143:TRP:CE2  | 1:L:99:THR:HG21  | 2.30                     | 0.66              |
| 1:G:41:VAL:HG13  | 1:G:125:VAL:HG11 | 1.78                     | 0.66              |
| 1:R:93:SER:CB    | 1:R:120:ARG:HH21 | 2.08                     | 0.66              |
| 1:F:1:LEU:HB2    | 1:F:70:SER:OG    | 1.95                     | 0.66              |
| 1:I:1:LEU:HB2    | 1:I:70:SER:OG    | 1.95                     | 0.65              |
| 1:R:143:TRP:CE2  | 1:S:99:THR:HG21  | 2.32                     | 0.65              |
| 1:F:115:PRO:HA   | 4:F:225:HOH:O    | 1.97                     | 0.65              |
| 1:R:143:TRP:CZ2  | 1:S:99:THR:HG21  | 2.32                     | 0.65              |
| 1:T:40:GLU:HB3   | 1:T:49:ASP:HB2   | 1.78                     | 0.65              |
| 1:M:143:TRP:CZ2  | 1:N:99:THR:HG21  | 2.32                     | 0.64              |
| 1:J:36:ILE:HB    | 1:J:51:VAL:HG12  | 1.78                     | 0.64              |
| 1:K:21:THR:HG23  | 1:K:21:THR:O     | 1.96                     | 0.64              |
| 1:Q:11:ARG:HG3   | 1:Q:11:ARG:HH11  | 1.61                     | 0.64              |
| 1:L:186:SER:HB2  | 1:M:164:TYR:OH   | 1.97                     | 0.64              |
| 1:P:143:TRP:CE2  | 1:Q:99:THR:HG21  | 2.31                     | 0.64              |
| 1:F:3:ARG:NH1    | 1:J:21:THR:HG21  | 2.13                     | 0.64              |
| 1:K:25:ARG:HB2   | 1:K:26:PRO:HD2   | 1.80                     | 0.64              |
| 1:Q:15:ARG:N     | 1:Q:16:PRO:HD3   | 2.13                     | 0.64              |
| 1:J:92:ILE:HG13  | 1:J:120:ARG:HB3  | 1.81                     | 0.63              |
| 1:J:64:ALA:HA    | 1:J:107:SER:O    | 1.98                     | 0.63              |
| 1:S:1:LEU:HB2    | 1:S:70:SER:OG    | 1.98                     | 0.62              |
| 1:A:99:THR:HG21  | 1:E:143:TRP:CE2  | 2.34                     | 0.62              |
| 1:D:15:ARG:HH12  | 1:E:8:TYR:HB2    | 1.64                     | 0.62              |
| 1:T:1:LEU:HB2    | 1:T:70:SER:OG    | 2.00                     | 0.62              |
| 1:G:23:ARG:HH22  | 1:L:68:SER:HA    | 1.65                     | 0.62              |
| 1:H:10:ILE:O     | 1:H:14:SER:CB    | 2.47                     | 0.62              |
| 1:J:152:VAL:HG23 | 1:J:195:VAL:HG23 | 1.80                     | 0.61              |
| 1:K:99:THR:HG21  | 1:O:143:TRP:CE2  | 2.34                     | 0.61              |
| 1:F:41:VAL:HG13  | 1:F:125:VAL:HG11 | 1.81                     | 0.61              |
| 1:A:9:ASN:O      | 1:A:13:THR:HG22  | 2.00                     | 0.61              |
| 1:B:180:LYS:NZ   | 1:B:193:GLU:OE1  | 2.33                     | 0.61              |
| 1:C:23:ARG:HH21  | 1:G:69:HIS:HE1   | 1.48                     | 0.61              |
| 1:P:21:THR:HG21  | 1:Q:3:ARG:NH1    | 2.15                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:41:VAL:HG13 | 1:B:125:VAL:HG11 | 1.82                     | 0.61              |
| 1:B:153:ASP:OD2 | 1:P:180:LYS:HE2  | 2.00                     | 0.61              |
| 1:F:14:SER:O    | 1:F:16:PRO:HD3   | 2.01                     | 0.60              |
| 1:D:190:GLU:HB2 | 4:D:232:HOH:O    | 2.01                     | 0.60              |
| 1:P:143:TRP:CZ2 | 1:Q:99:THR:HG21  | 2.36                     | 0.60              |
| 1:J:38:ILE:HG13 | 1:J:165:PHE:HZ   | 1.67                     | 0.60              |
| 1:O:192:TYR:CG  | 2:O:211:09R:H121 | 2.37                     | 0.60              |
| 1:D:1:LEU:HB2   | 1:D:70:SER:OG    | 2.01                     | 0.60              |
| 1:N:23:ARG:O    | 1:N:23:ARG:CG    | 2.50                     | 0.60              |
| 1:Q:143:TRP:CE2 | 1:R:99:THR:HG21  | 2.37                     | 0.60              |
| 1:H:143:TRP:CE2 | 1:I:99:THR:HG21  | 2.37                     | 0.59              |
| 1:N:25:ARG:HH11 | 1:N:25:ARG:HG2   | 1.65                     | 0.59              |
| 1:D:41:VAL:CG1  | 1:D:125:VAL:HG11 | 2.32                     | 0.59              |
| 1:J:49:ASP:OD1  | 1:J:120:ARG:HG3  | 2.02                     | 0.59              |
| 1:S:41:VAL:HG13 | 1:S:125:VAL:HG11 | 1.84                     | 0.59              |
| 1:B:94:LYS:HG2  | 4:C:217:HOH:O    | 2.02                     | 0.59              |
| 1:C:171:PHE:O   | 1:C:204:LYS:HE3  | 2.02                     | 0.59              |
| 1:R:32:SER:HB2  | 1:R:155:THR:HG22 | 1.83                     | 0.59              |
| 1:K:99:THR:HG21 | 1:O:143:TRP:CZ2  | 2.38                     | 0.58              |
| 1:P:99:THR:HG21 | 1:T:143:TRP:CE2  | 2.38                     | 0.58              |
| 1:J:26:PRO:HB3  | 1:J:148:ARG:O    | 2.04                     | 0.58              |
| 1:C:189:PRO:HD2 | 4:C:227:HOH:O    | 2.03                     | 0.58              |
| 1:Q:1:LEU:HB2   | 1:Q:70:SER:OG    | 2.03                     | 0.58              |
| 1:Q:11:ARG:HH11 | 1:Q:11:ARG:CG    | 2.15                     | 0.58              |
| 1:P:143:TRP:O   | 2:P:211:09R:H5   | 2.03                     | 0.58              |
| 1:A:99:THR:HG21 | 1:E:143:TRP:CZ2  | 2.38                     | 0.58              |
| 1:H:143:TRP:CZ2 | 1:I:99:THR:HG21  | 2.39                     | 0.58              |
| 1:I:22:GLN:HE21 | 1:I:61:ARG:HG2   | 1.67                     | 0.58              |
| 1:J:42:ASN:OD1  | 1:J:44:ILE:HB    | 2.04                     | 0.58              |
| 1:J:129:ASP:OD2 | 1:J:203:LYS:HD3  | 2.04                     | 0.58              |
| 1:J:43:GLU:OE2  | 1:J:126:SER:HA   | 2.04                     | 0.58              |
| 1:G:26:PRO:HB3  | 1:G:148:ARG:O    | 2.04                     | 0.57              |
| 1:E:9:ASN:O     | 1:E:13:THR:CG2   | 2.48                     | 0.57              |
| 1:L:1:LEU:HB2   | 1:L:70:SER:OG    | 2.04                     | 0.57              |
| 1:Q:41:VAL:HG13 | 1:Q:125:VAL:HG11 | 1.86                     | 0.57              |
| 1:T:148:ARG:HG2 | 1:T:148:ARG:NH1  | 2.09                     | 0.57              |
| 1:H:19:ILE:HG13 | 1:H:82:TRP:CZ2   | 2.40                     | 0.57              |
| 1:N:180:LYS:NZ  | 1:N:193:GLU:OE1  | 2.38                     | 0.56              |
| 1:C:143:TRP:CZ2 | 1:D:99:THR:HG21  | 2.40                     | 0.56              |
| 1:E:180:LYS:NZ  | 1:E:193:GLU:OE1  | 2.39                     | 0.56              |
| 1:S:1:LEU:HB2   | 1:S:70:SER:HG    | 1.69                     | 0.56              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:S:143:TRP:CZ2     | 1:T:99:THR:HG21   | 2.41                     | 0.56              |
| 1:B:180:LYS:CE      | 1:P:153:ASP:OD2   | 2.53                     | 0.56              |
| 1:K:15:ARG:HH22     | 1:L:8:TYR:HB2     | 1.69                     | 0.56              |
| 1:P:99:THR:HG21     | 1:T:143:TRP:CZ2   | 2.40                     | 0.56              |
| 1:F:171:PHE:O       | 1:F:204:LYS:HD2   | 2.05                     | 0.56              |
| 1:G:131:GLU:CG      | 1:G:132:SER:N     | 2.68                     | 0.55              |
| 1:K:10:ILE:O        | 1:K:14:SER:HB3    | 2.06                     | 0.55              |
| 1:A:12:GLN:HB3      | 1:I:12:GLN:HB3    | 1.88                     | 0.55              |
| 1:C:143:TRP:CE2     | 1:D:99:THR:HG21   | 2.41                     | 0.55              |
| 1:J:162:SER:O       | 1:J:163:GLU:C     | 2.49                     | 0.55              |
| 1:L:180:LYS:NZ      | 1:L:193:GLU:OE1   | 2.40                     | 0.55              |
| 1:M:23:ARG:CZ       | 1:T:69:HIS:CE1    | 2.89                     | 0.55              |
| 1:L:19:ILE:HG13     | 1:L:82:TRP:CZ2    | 2.42                     | 0.55              |
| 1:G:148:ARG:HD3     | 1:K:190:GLU:OE2   | 2.07                     | 0.55              |
| 1:B:179:LYS:HE3     | 1:P:178:GLN:O     | 2.07                     | 0.55              |
| 1:S:17:ASP:O        | 1:T:7:LEU:HD13    | 2.06                     | 0.55              |
| 1:D:143:TRP:CZ2     | 1:E:99:THR:HG21   | 2.42                     | 0.55              |
| 1:K:14:SER:O        | 1:K:16:PRO:HD3    | 2.07                     | 0.55              |
| 1:F:10:ILE:O        | 1:F:14:SER:HB3    | 2.07                     | 0.54              |
| 1:P:9:ASN:O         | 1:P:13:THR:CG2    | 2.46                     | 0.54              |
| 1:D:124:ASP:HB2     | 1:E:168:TYR:CE1   | 2.41                     | 0.54              |
| 1:F:99:THR:HG21     | 1:J:143:TRP:CE2   | 2.42                     | 0.54              |
| 1:F:104:ARG:NE      | 4:F:219:HOH:O     | 2.40                     | 0.54              |
| 1:I:206:ARG:HG3     | 1:I:206:ARG:HH11  | 1.72                     | 0.54              |
| 1:K:125:VAL:HG12    | 1:K:125:VAL:O     | 2.07                     | 0.54              |
| 1:E:170[B]:ARG:HH11 | 1:E:170[B]:ARG:CG | 1.93                     | 0.54              |
| 1:O:187:CYS:SG      | 1:O:188:CYS:N     | 2.81                     | 0.54              |
| 1:B:131:GLU:HG3     | 1:B:202:ARG:NH1   | 2.23                     | 0.54              |
| 1:J:152:VAL:CG2     | 1:J:195:VAL:HG23  | 2.38                     | 0.54              |
| 1:G:143:TRP:CZ2     | 1:H:99:THR:HG21   | 2.43                     | 0.54              |
| 1:F:205:GLY:C       | 1:F:207:SER:H     | 2.16                     | 0.53              |
| 1:N:143:TRP:CE2     | 1:O:99:THR:HG21   | 2.44                     | 0.53              |
| 1:S:174:LEU:HD11    | 1:S:202:ARG:HD3   | 1.90                     | 0.53              |
| 1:T:7:LEU:O         | 1:T:11:ARG:HB2    | 2.09                     | 0.53              |
| 1:S:143:TRP:CE2     | 1:T:99:THR:HG21   | 2.44                     | 0.53              |
| 1:J:139:LYS:HE3     | 1:J:194:ASP:OD2   | 2.09                     | 0.53              |
| 1:H:146:HIS:CE1     | 1:H:148:ARG:HB2   | 2.43                     | 0.53              |
| 1:J:194:ASP:OD1     | 1:J:194:ASP:C     | 2.52                     | 0.53              |
| 1:T:47:GLU:OE1      | 1:T:120:ARG:NH1   | 2.42                     | 0.53              |
| 1:E:14:SER:HB2      | 1:E:80:SER:O      | 2.08                     | 0.53              |
| 1:P:74:VAL:HA       | 4:P:305:HOH:O     | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:TRP:CE2  | 1:B:99:THR:HG21  | 2.44                     | 0.53              |
| 2:A:211:09R:BR1  | 1:B:104:ARG:HB2  | 2.64                     | 0.53              |
| 1:D:143:TRP:CE2  | 1:E:99:THR:HG21  | 2.44                     | 0.53              |
| 1:L:10:ILE:O     | 1:L:14:SER:CB    | 2.55                     | 0.53              |
| 1:B:143:TRP:CE2  | 1:C:99:THR:HG21  | 2.44                     | 0.52              |
| 1:D:49:ASP:HA    | 1:D:120:ARG:HG3  | 1.91                     | 0.52              |
| 1:I:41:VAL:HG13  | 1:I:125:VAL:HG11 | 1.92                     | 0.52              |
| 1:G:32:SER:HB2   | 1:G:155:THR:HB   | 1.92                     | 0.52              |
| 1:I:171:PHE:O    | 1:I:204:LYS:HD2  | 2.08                     | 0.52              |
| 1:G:41:VAL:HG13  | 1:G:125:VAL:CG1  | 2.38                     | 0.52              |
| 1:J:142:SER:OG   | 1:J:145:HIS:HB2  | 2.10                     | 0.52              |
| 1:Q:143:TRP:CZ2  | 1:R:99:THR:HG21  | 2.44                     | 0.52              |
| 1:L:22:GLN:NE2   | 1:L:61:ARG:HG2   | 2.25                     | 0.52              |
| 1:C:15:ARG:HE    | 1:D:11:ARG:NH2   | 2.08                     | 0.52              |
| 1:D:148:ARG:NH2  | 1:D:190:GLU:OE2  | 2.42                     | 0.52              |
| 1:K:104:ARG:HB2  | 2:O:211:09R:BR1  | 2.65                     | 0.52              |
| 1:S:143:TRP:CE3  | 2:S:211:09R:H7   | 2.45                     | 0.52              |
| 1:A:30:SER:HB3   | 1:A:155:THR:CG2  | 2.40                     | 0.52              |
| 1:M:14:SER:HB2   | 1:M:80:SER:O     | 2.10                     | 0.52              |
| 1:G:22:GLN:O     | 1:G:22:GLN:HG2   | 2.10                     | 0.51              |
| 1:J:15:ARG:NH1   | 1:J:18:VAL:HG21  | 2.25                     | 0.51              |
| 1:K:186:SER:H    | 1:L:164:TYR:HH   | 1.55                     | 0.51              |
| 1:G:143:TRP:CE2  | 1:H:99:THR:HG21  | 2.45                     | 0.51              |
| 1:J:33:LEU:HD22  | 1:J:52:PHE:CD2   | 2.45                     | 0.51              |
| 1:Q:171:PHE:CE2  | 1:Q:203:LYS:HG2  | 2.45                     | 0.51              |
| 1:A:32:SER:HB2   | 1:A:155:THR:OG1  | 2.10                     | 0.51              |
| 1:L:32:SER:HB2   | 1:L:155:THR:HB   | 1.91                     | 0.51              |
| 1:K:174:LEU:HD11 | 1:K:202:ARG:HD3  | 1.93                     | 0.51              |
| 1:B:143:TRP:CZ2  | 1:C:99:THR:HG21  | 2.46                     | 0.51              |
| 1:D:14:SER:O     | 1:D:16:PRO:HD3   | 2.11                     | 0.51              |
| 1:G:171:PHE:O    | 1:G:204:LYS:HD2  | 2.11                     | 0.51              |
| 1:L:15:ARG:NH2   | 1:M:4:ALA:O      | 2.43                     | 0.51              |
| 1:R:22:GLN:NE2   | 1:R:61:ARG:CG    | 2.66                     | 0.51              |
| 1:C:20:PRO:HD3   | 1:C:82:TRP:CD2   | 2.46                     | 0.51              |
| 1:A:1:LEU:HB2    | 1:A:70:SER:OG    | 2.11                     | 0.50              |
| 1:T:125:VAL:HG12 | 1:T:125:VAL:O    | 2.11                     | 0.50              |
| 1:I:37:ASN:HB2   | 4:I:228:HOH:O    | 2.11                     | 0.50              |
| 1:A:41:VAL:HG13  | 1:A:125:VAL:HG11 | 1.93                     | 0.50              |
| 1:D:15:ARG:HH22  | 1:E:8:TYR:HB2    | 1.76                     | 0.50              |
| 1:I:1:LEU:HB2    | 1:I:70:SER:HG    | 1.75                     | 0.50              |
| 1:F:174:LEU:HD11 | 1:F:202:ARG:HD3  | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:15:ARG:HG3   | 1:C:15:ARG:HH11  | 1.76                     | 0.50              |
| 1:J:90:ASN:HD21  | 1:J:138:ILE:HA   | 1.76                     | 0.50              |
| 1:L:143:TRP:CE2  | 1:M:99:THR:HG21  | 2.46                     | 0.50              |
| 1:O:1:LEU:HB2    | 1:O:70:SER:OG    | 2.12                     | 0.50              |
| 1:F:104:ARG:HH22 | 1:J:149:GLU:CD   | 2.19                     | 0.50              |
| 1:M:14:SER:O     | 1:M:15:ARG:HB2   | 2.11                     | 0.50              |
| 1:M:41:VAL:HG13  | 1:M:125:VAL:HG11 | 1.93                     | 0.50              |
| 1:N:1:LEU:HB2    | 1:N:70:SER:OG    | 2.10                     | 0.50              |
| 1:E:12:GLN:HB3   | 1:J:12:GLN:HB3   | 1.92                     | 0.50              |
| 1:K:15:ARG:NH1   | 1:L:11:ARG:HH12  | 2.09                     | 0.50              |
| 1:T:143:TRP:CE3  | 2:T:211:09R:H7   | 2.47                     | 0.50              |
| 1:G:182:SER:OG   | 1:K:184:THR:HG21 | 2.12                     | 0.50              |
| 1:R:15:ARG:HH21  | 1:S:11:ARG:NH1   | 2.10                     | 0.50              |
| 1:J:32:SER:HB2   | 1:J:155:THR:OG1  | 2.12                     | 0.50              |
| 1:N:21:THR:O     | 1:N:21:THR:CG2   | 2.60                     | 0.49              |
| 1:O:24:ASP:CG    | 1:O:24:ASP:O     | 2.54                     | 0.49              |
| 1:T:148:ARG:HH11 | 1:T:148:ARG:CG   | 2.15                     | 0.49              |
| 1:B:153:ASP:OD2  | 1:P:180:LYS:CE   | 2.60                     | 0.49              |
| 1:J:167:GLN:O    | 1:J:204:LYS:NZ   | 2.45                     | 0.49              |
| 1:R:32:SER:HB2   | 1:R:155:THR:CG2  | 2.42                     | 0.49              |
| 1:R:93:SER:CB    | 1:R:120:ARG:NH2  | 2.74                     | 0.49              |
| 1:T:13:THR:HG23  | 1:T:14:SER:N     | 2.27                     | 0.49              |
| 1:J:137:ARG:HG3  | 1:J:198:SER:OG   | 2.12                     | 0.49              |
| 1:J:161:ASP:C    | 1:J:163:GLU:H    | 2.19                     | 0.49              |
| 1:M:68:SER:O     | 1:M:69:HIS:HD2   | 1.94                     | 0.49              |
| 1:M:146:HIS:CE1  | 1:M:148:ARG:HB2  | 2.47                     | 0.49              |
| 1:O:21:THR:O     | 1:O:21:THR:HG22  | 2.11                     | 0.49              |
| 1:Q:92:ILE:HD11  | 1:Q:120:ARG:HG2  | 1.94                     | 0.49              |
| 2:D:211:09R:BR1  | 1:E:104:ARG:HB2  | 2.68                     | 0.49              |
| 1:N:143:TRP:CZ2  | 1:O:99:THR:HG21  | 2.47                     | 0.49              |
| 1:A:30:SER:HB3   | 1:A:155:THR:HG23 | 1.95                     | 0.49              |
| 1:F:164:TYR:OH   | 1:J:186:SER:HB3  | 2.12                     | 0.49              |
| 1:R:146:HIS:CE1  | 1:R:148:ARG:HB2  | 2.48                     | 0.49              |
| 1:A:143:TRP:CZ2  | 1:B:99:THR:HG21  | 2.48                     | 0.49              |
| 1:T:41:VAL:HG13  | 1:T:125:VAL:HG11 | 1.94                     | 0.49              |
| 1:K:1:LEU:HB2    | 1:K:70:SER:OG    | 2.12                     | 0.49              |
| 1:J:38:ILE:HG13  | 1:J:165:PHE:CE1  | 2.47                     | 0.49              |
| 1:O:21:THR:HG23  | 1:O:24:ASP:HA    | 1.95                     | 0.49              |
| 1:C:23:ARG:HH21  | 1:G:69:HIS:CE1   | 2.29                     | 0.49              |
| 1:J:143:TRP:CZ3  | 2:J:211:09R:H7   | 2.48                     | 0.49              |
| 1:B:146:HIS:CE1  | 1:B:149:GLU:HG3  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:125:VAL:HG12 | 1:E:125:VAL:O    | 2.12                     | 0.48              |
| 1:O:10:ILE:O     | 1:O:14:SER:HB3   | 2.13                     | 0.48              |
| 1:J:19:ILE:HG13  | 1:J:82:TRP:CZ2   | 2.48                     | 0.48              |
| 1:M:23:ARG:CZ    | 1:T:69:HIS:HE1   | 2.26                     | 0.48              |
| 2:P:211:09R:BR1  | 1:Q:104:ARG:HB2  | 2.68                     | 0.48              |
| 1:C:41:VAL:HG13  | 1:C:125:VAL:HG11 | 1.95                     | 0.48              |
| 1:G:83:VAL:CG1   | 4:G:219:HOH:O    | 2.61                     | 0.48              |
| 1:I:24:ASP:O     | 1:I:25:ARG:HD3   | 2.14                     | 0.48              |
| 1:M:10:ILE:O     | 1:M:14:SER:HB3   | 2.13                     | 0.48              |
| 1:F:143:TRP:CE2  | 1:G:99:THR:HG21  | 2.49                     | 0.48              |
| 1:G:55:GLN:HE22  | 1:G:155:THR:HG21 | 1.77                     | 0.48              |
| 1:G:182:SER:HB3  | 1:K:184:THR:CG2  | 2.42                     | 0.48              |
| 1:J:144:THR:HG22 | 2:J:211:09R:C5   | 2.43                     | 0.48              |
| 1:D:41:VAL:HG13  | 1:D:125:VAL:CG1  | 2.43                     | 0.48              |
| 1:H:14:SER:O     | 1:H:16:PRO:HD3   | 2.13                     | 0.48              |
| 1:P:41:VAL:HG13  | 1:P:125:VAL:HG11 | 1.96                     | 0.48              |
| 1:Q:21:THR:HG21  | 1:R:3:ARG:NH1    | 2.29                     | 0.48              |
| 1:A:171:PHE:CE2  | 1:A:203:LYS:HG2  | 2.48                     | 0.48              |
| 1:J:161:ASP:C    | 1:J:163:GLU:N    | 2.72                     | 0.48              |
| 1:P:137:ARG:HD2  | 1:P:196:GLU:CD   | 2.39                     | 0.48              |
| 1:Q:15:ARG:HD2   | 1:Q:15:ARG:HA    | 1.58                     | 0.48              |
| 1:T:36:ILE:HB    | 1:T:51:VAL:HG12  | 1.95                     | 0.48              |
| 1:N:19:ILE:HG13  | 1:N:82:TRP:CZ2   | 2.47                     | 0.48              |
| 1:N:25:ARG:HG2   | 1:N:25:ARG:NH1   | 2.25                     | 0.48              |
| 1:R:41:VAL:HG21  | 1:R:201:PHE:HE2  | 1.79                     | 0.48              |
| 1:T:154:PRO:O    | 1:T:155:THR:HB   | 2.12                     | 0.48              |
| 1:D:36:ILE:HB    | 1:D:51:VAL:HG12  | 1.96                     | 0.48              |
| 2:G:211:09R:BR1  | 1:H:104:ARG:HB2  | 2.69                     | 0.47              |
| 1:B:1:LEU:HB2    | 1:B:70:SER:OG    | 2.14                     | 0.47              |
| 1:R:137:ARG:HD2  | 1:R:196:GLU:OE1  | 2.15                     | 0.47              |
| 1:B:131:GLU:O    | 1:B:202:ARG:NH1  | 2.40                     | 0.47              |
| 3:F:213:SO4:O1   | 1:G:71:PRO:HA    | 2.14                     | 0.47              |
| 1:J:29:VAL:O     | 1:J:152:VAL:HA   | 2.14                     | 0.47              |
| 1:L:68:SER:O     | 1:L:69:HIS:HD2   | 1.97                     | 0.47              |
| 1:K:36:ILE:HB    | 1:K:51:VAL:HG12  | 1.96                     | 0.47              |
| 1:N:41:VAL:HG13  | 1:N:125:VAL:HG11 | 1.95                     | 0.47              |
| 1:I:206:ARG:HG3  | 1:I:206:ARG:NH1  | 2.29                     | 0.47              |
| 1:K:187:CYS:SG   | 1:L:114:MET:HE1  | 2.54                     | 0.47              |
| 1:M:187:CYS:SG   | 1:M:188:CYS:N    | 2.87                     | 0.47              |
| 1:O:19:ILE:C     | 1:O:21:THR:H     | 2.23                     | 0.47              |
| 1:T:40:GLU:HB3   | 1:T:49:ASP:CB    | 2.42                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:10:ILE:O     | 1:B:14:SER:HB3   | 2.15                     | 0.47              |
| 1:B:11:ARG:NH2   | 4:B:215:HOH:O    | 2.48                     | 0.47              |
| 1:J:93:SER:HB3   | 1:J:120:ARG:HH21 | 1.80                     | 0.47              |
| 1:M:180:LYS:NZ   | 1:M:193:GLU:OE1  | 2.47                     | 0.47              |
| 1:S:41:VAL:CG1   | 1:S:125:VAL:HG11 | 2.45                     | 0.47              |
| 1:K:160:ASP:HB3  | 1:K:163:GLU:HB2  | 1.96                     | 0.47              |
| 1:P:174:LEU:HD11 | 1:P:202:ARG:HD3  | 1.96                     | 0.47              |
| 1:S:125:VAL:HG12 | 1:S:125:VAL:O    | 2.15                     | 0.47              |
| 1:B:30:SER:HB2   | 1:B:57:THR:HG22  | 1.97                     | 0.47              |
| 1:Q:149:GLU:CD   | 1:R:104:ARG:HH22 | 2.23                     | 0.47              |
| 1:N:143:TRP:CE2  | 2:N:211:09R:H5   | 2.50                     | 0.47              |
| 1:T:115:PRO:HA   | 4:T:360:HOH:O    | 2.14                     | 0.46              |
| 1:P:170:ARG:O    | 1:P:204:LYS:HB2  | 2.14                     | 0.46              |
| 1:D:68:SER:O     | 1:D:69:HIS:HD2   | 1.99                     | 0.46              |
| 1:F:41:VAL:CG1   | 1:F:125:VAL:HG11 | 2.46                     | 0.46              |
| 1:N:41:VAL:HG21  | 1:N:201:PHE:HE2  | 1.80                     | 0.46              |
| 1:O:174:LEU:HD11 | 1:O:202:ARG:HD3  | 1.96                     | 0.46              |
| 1:Q:36:ILE:HB    | 1:Q:51:VAL:HG12  | 1.97                     | 0.46              |
| 1:K:41:VAL:CG1   | 1:K:125:VAL:HG11 | 2.44                     | 0.46              |
| 1:B:151:SER:HB2  | 1:B:193:GLU:OE1  | 2.16                     | 0.46              |
| 1:Q:68:SER:O     | 1:Q:69:HIS:HD2   | 1.98                     | 0.46              |
| 1:G:26:PRO:HB3   | 1:G:148:ARG:C    | 2.40                     | 0.46              |
| 1:H:125:VAL:HG12 | 1:H:125:VAL:O    | 2.16                     | 0.46              |
| 1:P:125:VAL:HG12 | 1:P:125:VAL:O    | 2.16                     | 0.46              |
| 1:R:68:SER:O     | 1:R:69:HIS:HD2   | 1.99                     | 0.46              |
| 1:A:125:VAL:HG12 | 1:A:125:VAL:O    | 2.16                     | 0.46              |
| 1:E:192:TYR:CG   | 2:E:211:09R:H121 | 2.51                     | 0.46              |
| 1:R:33:LEU:HD22  | 1:R:52:PHE:CD2   | 2.51                     | 0.46              |
| 1:F:143:TRP:CD2  | 2:F:211:09R:H7   | 2.51                     | 0.46              |
| 1:J:26:PRO:HB3   | 1:J:148:ARG:C    | 2.40                     | 0.46              |
| 1:J:51:VAL:HG22  | 1:J:118:ARG:HB2  | 1.98                     | 0.46              |
| 1:B:41:VAL:CG1   | 1:B:125:VAL:HG11 | 2.46                     | 0.46              |
| 1:G:1:LEU:HB2    | 1:G:70:SER:OG    | 2.16                     | 0.46              |
| 1:H:174:LEU:HD11 | 1:H:202:ARG:HD3  | 1.98                     | 0.46              |
| 1:I:19:ILE:HG13  | 1:I:82:TRP:CZ2   | 2.51                     | 0.46              |
| 1:K:180:LYS:NZ   | 1:K:193:GLU:OE1  | 2.49                     | 0.46              |
| 1:G:23:ARG:HB3   | 1:G:24:ASP:H     | 1.54                     | 0.45              |
| 1:P:137:ARG:HD2  | 1:P:196:GLU:OE1  | 2.17                     | 0.45              |
| 1:S:24:ASP:C     | 1:S:25:ARG:HG2   | 2.41                     | 0.45              |
| 1:D:125:VAL:HG12 | 1:D:125:VAL:O    | 2.17                     | 0.45              |
| 1:O:146:HIS:CE1  | 1:O:148:ARG:HB2  | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:93:SER:HB3   | 1:R:120:ARG:NE   | 2.31                     | 0.45              |
| 1:C:161:ASP:HB3  | 1:C:176:VAL:CG2  | 2.47                     | 0.45              |
| 1:J:83:VAL:HG12  | 1:J:84:PRO:HD2   | 1.99                     | 0.45              |
| 1:K:32:SER:HB2   | 1:K:155:THR:HG22 | 1.98                     | 0.45              |
| 1:K:186:SER:N    | 1:L:164:TYR:OH   | 2.36                     | 0.45              |
| 1:F:36:ILE:HB    | 1:F:51:VAL:HG12  | 1.98                     | 0.45              |
| 1:G:10:ILE:O     | 1:G:14:SER:HB3   | 2.17                     | 0.45              |
| 1:D:161:ASP:HB3  | 1:D:176:VAL:CG2  | 2.45                     | 0.45              |
| 1:D:174:LEU:HD11 | 1:D:202:ARG:HD3  | 1.98                     | 0.45              |
| 1:J:35:PHE:CE1   | 1:J:199:LEU:HD22 | 2.51                     | 0.45              |
| 1:N:12:GLN:HB3   | 1:S:12:GLN:HB3   | 1.99                     | 0.45              |
| 1:Q:41:VAL:CG1   | 1:Q:125:VAL:HG11 | 2.47                     | 0.45              |
| 1:R:41:VAL:HG13  | 1:R:125:VAL:HG11 | 1.98                     | 0.45              |
| 2:R:211:09R:BR1  | 1:S:104:ARG:HB2  | 2.72                     | 0.45              |
| 1:C:23:ARG:NH2   | 1:G:69:HIS:HE1   | 2.14                     | 0.45              |
| 1:H:146:HIS:HE1  | 1:H:148:ARG:HB2  | 1.82                     | 0.45              |
| 1:I:23:ARG:HG3   | 1:I:23:ARG:HH11  | 1.81                     | 0.45              |
| 1:R:202:ARG:HG3  | 1:R:203:LYS:O    | 2.16                     | 0.45              |
| 1:B:68:SER:O     | 1:B:69:HIS:HD2   | 2.00                     | 0.45              |
| 1:B:146:HIS:ND1  | 1:B:148:ARG:HB2  | 2.31                     | 0.45              |
| 1:I:68:SER:O     | 1:I:69:HIS:HD2   | 2.00                     | 0.45              |
| 1:J:97:VAL:CB    | 1:J:101:GLN:HE21 | 2.29                     | 0.45              |
| 1:J:125:VAL:HG12 | 1:J:125:VAL:O    | 2.17                     | 0.45              |
| 1:J:97:VAL:HB    | 1:J:101:GLN:HE21 | 1.82                     | 0.45              |
| 1:P:33:LEU:HD22  | 1:P:52:PHE:CD2   | 2.52                     | 0.45              |
| 1:B:153:ASP:OD2  | 1:B:180:LYS:HD2  | 2.17                     | 0.44              |
| 1:C:68:SER:O     | 1:C:69:HIS:HD2   | 2.00                     | 0.44              |
| 1:C:125:VAL:HG12 | 1:C:125:VAL:O    | 2.18                     | 0.44              |
| 2:L:211:09R:H5   | 2:L:211:09R:H1   | 1.70                     | 0.44              |
| 1:N:68:SER:O     | 1:N:69:HIS:HD2   | 2.00                     | 0.44              |
| 1:O:22:GLN:O     | 1:O:23:ARG:C     | 2.60                     | 0.44              |
| 1:O:41:VAL:HG13  | 1:O:125:VAL:HG11 | 1.99                     | 0.44              |
| 1:R:110:GLU:HA   | 1:R:110:GLU:OE2  | 2.17                     | 0.44              |
| 1:F:125:VAL:HG12 | 1:F:125:VAL:O    | 2.17                     | 0.44              |
| 1:J:20:PRO:HB3   | 1:J:60:ASP:CG    | 2.42                     | 0.44              |
| 1:D:22:GLN:O     | 1:D:23:ARG:C     | 2.60                     | 0.44              |
| 1:F:68:SER:O     | 1:F:69:HIS:HD2   | 2.00                     | 0.44              |
| 1:J:81:LEU:HD23  | 1:J:81:LEU:HA    | 1.83                     | 0.44              |
| 1:S:23:ARG:HB2   | 1:S:25:ARG:CG    | 2.39                     | 0.44              |
| 1:F:143:TRP:CZ2  | 1:G:99:THR:HG21  | 2.52                     | 0.44              |
| 1:P:3:ARG:NH1    | 1:T:21:THR:HG21  | 2.33                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:10:ILE:O      | 1:I:14:SER:CB    | 2.64                     | 0.44              |
| 1:K:161:ASP:OD2   | 1:K:176:VAL:HB   | 2.18                     | 0.44              |
| 1:R:125:VAL:HG12  | 1:R:125:VAL:O    | 2.18                     | 0.44              |
| 1:S:180:LYS:NZ    | 1:S:193:GLU:OE1  | 2.51                     | 0.44              |
| 1:S:187:CYS:SG    | 1:S:188:CYS:N    | 2.90                     | 0.44              |
| 1:B:125:VAL:O     | 1:B:125:VAL:HG12 | 2.17                     | 0.44              |
| 1:C:15:ARG:HG3    | 1:C:15:ARG:NH1   | 2.32                     | 0.44              |
| 1:I:39:LEU:C      | 1:I:40:GLU:HG3   | 2.41                     | 0.44              |
| 1:J:172:GLU:HG2   | 1:J:204:LYS:HG2  | 1.98                     | 0.44              |
| 1:L:3:ARG:HG3     | 1:L:71:PRO:HG2   | 2.00                     | 0.44              |
| 1:M:125:VAL:HG12  | 1:M:125:VAL:O    | 2.18                     | 0.44              |
| 1:O:83:VAL:HG13   | 1:O:84:PRO:HD2   | 2.00                     | 0.44              |
| 1:P:26:PRO:HB3    | 1:P:148:ARG:C    | 2.43                     | 0.44              |
| 1:G:41:VAL:CG1    | 1:G:125:VAL:HG11 | 2.46                     | 0.44              |
| 1:G:125:VAL:HG12  | 1:G:125:VAL:O    | 2.18                     | 0.44              |
| 1:I:23:ARG:HG3    | 1:I:23:ARG:NH1   | 2.33                     | 0.44              |
| 1:L:143:TRP:CZ2   | 1:M:99:THR:HG21  | 2.52                     | 0.44              |
| 1:D:180:LYS:HE2   | 1:D:193:GLU:OE1  | 2.18                     | 0.44              |
| 1:E:41:VAL:HG13   | 1:E:125:VAL:HG11 | 2.00                     | 0.44              |
| 1:H:68:SER:O      | 1:H:69:HIS:HD2   | 2.00                     | 0.44              |
| 1:F:156:THR:HG22  | 1:F:157:GLU:O    | 2.18                     | 0.44              |
| 2:G:211:09R:H6    | 2:G:211:09R:H12  | 1.71                     | 0.44              |
| 1:J:187:CYS:SG    | 1:J:188:CYS:N    | 2.90                     | 0.44              |
| 1:K:41:VAL:HG13   | 1:K:125:VAL:CG1  | 2.46                     | 0.44              |
| 1:N:36:ILE:HB     | 1:N:51:VAL:HG12  | 2.00                     | 0.44              |
| 1:N:187[B]:CYS:SG | 1:N:188:CYS:N    | 2.91                     | 0.44              |
| 1:R:93:SER:CB     | 1:R:120:ARG:HE   | 2.30                     | 0.44              |
| 1:T:203:LYS:HE3   | 1:T:203:LYS:HB2  | 1.76                     | 0.44              |
| 1:A:68:SER:O      | 1:A:69:HIS:HD2   | 2.01                     | 0.43              |
| 1:B:69:HIS:CE1    | 1:H:23:ARG:NH1   | 2.86                     | 0.43              |
| 1:N:25:ARG:CG     | 1:N:25:ARG:NH1   | 2.71                     | 0.43              |
| 1:Q:40:GLU:HB2    | 1:Q:49:ASP:HB2   | 2.00                     | 0.43              |
| 1:F:41:VAL:HG13   | 1:F:125:VAL:CG1  | 2.47                     | 0.43              |
| 1:F:100:PRO:HD3   | 1:J:87:ALA:HB2   | 2.00                     | 0.43              |
| 1:J:63:LEU:CD1    | 1:J:81:LEU:HD21  | 2.45                     | 0.43              |
| 1:L:1:LEU:HB2     | 1:L:70:SER:HG    | 1.83                     | 0.43              |
| 1:T:13:THR:CG2    | 1:T:14:SER:N     | 2.81                     | 0.43              |
| 1:D:128:VAL:O     | 1:D:202:ARG:HA   | 2.19                     | 0.43              |
| 1:J:19:ILE:HD11   | 1:J:150:ILE:HG13 | 1.98                     | 0.43              |
| 1:L:23:ARG:NH2    | 1:L:25:ARG:HH22  | 2.16                     | 0.43              |
| 1:N:143:TRP:NE1   | 2:N:211:09R:H1   | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:137:ARG:HD2  | 1:S:196:GLU:CD   | 2.44                     | 0.43              |
| 1:L:15:ARG:CG    | 1:L:15:ARG:NH1   | 2.53                     | 0.43              |
| 1:N:23:ARG:C     | 1:N:25:ARG:N     | 2.76                     | 0.43              |
| 1:P:68:SER:O     | 1:P:69:HIS:HD2   | 2.02                     | 0.43              |
| 1:Q:22:GLN:O     | 1:Q:22:GLN:HG3   | 2.18                     | 0.43              |
| 1:A:149:GLU:CD   | 1:B:104:ARG:HH22 | 2.27                     | 0.43              |
| 1:D:10:ILE:O     | 1:D:14:SER:HB3   | 2.19                     | 0.43              |
| 1:J:119:GLN:HB3  | 1:J:121:PHE:CE2  | 2.54                     | 0.43              |
| 1:Q:125:VAL:HG12 | 1:Q:125:VAL:O    | 2.17                     | 0.43              |
| 1:Q:174:LEU:HD11 | 1:Q:202:ARG:HD3  | 2.00                     | 0.43              |
| 1:T:23:ARG:O     | 1:T:25:ARG:N     | 2.52                     | 0.43              |
| 1:B:34:LYS:HB2   | 1:B:53:TRP:HB2   | 2.01                     | 0.43              |
| 1:R:131:GLU:O    | 1:R:202:ARG:NH1  | 2.51                     | 0.43              |
| 1:T:174:LEU:HD11 | 1:T:202:ARG:HD3  | 2.01                     | 0.43              |
| 1:F:171:PHE:C    | 1:F:204:LYS:HD2  | 2.44                     | 0.43              |
| 1:M:21:THR:HG23  | 1:M:25:ARG:O     | 2.19                     | 0.43              |
| 1:Q:34:LYS:HB2   | 1:Q:53:TRP:HB2   | 2.00                     | 0.43              |
| 1:R:10:ILE:O     | 1:R:14:SER:HB2   | 2.19                     | 0.43              |
| 1:T:143:TRP:CZ3  | 2:T:211:09R:H7   | 2.53                     | 0.43              |
| 1:G:187:CYS:SG   | 1:G:188:CYS:N    | 2.91                     | 0.43              |
| 1:H:14:SER:HB2   | 1:H:80:SER:O     | 2.18                     | 0.43              |
| 1:I:83:VAL:HG13  | 1:I:84:PRO:HD2   | 2.00                     | 0.43              |
| 2:F:211:09R:H11  | 2:F:211:09R:H2   | 1.74                     | 0.43              |
| 1:K:149:GLU:CD   | 1:L:104:ARG:HH22 | 2.27                     | 0.43              |
| 1:D:188:CYS:HB3  | 4:D:232:HOH:O    | 2.18                     | 0.42              |
| 1:K:21:THR:O     | 1:K:21:THR:CG2   | 2.67                     | 0.42              |
| 1:O:125:VAL:HG12 | 1:O:125:VAL:O    | 2.18                     | 0.42              |
| 1:T:180:LYS:NZ   | 1:T:193:GLU:OE1  | 2.51                     | 0.42              |
| 1:G:68:SER:O     | 1:G:69:HIS:HD2   | 2.02                     | 0.42              |
| 1:L:160:ASP:CG   | 1:L:163:GLU:HB2  | 2.44                     | 0.42              |
| 2:L:211:09R:BR1  | 1:M:104:ARG:HB2  | 2.74                     | 0.42              |
| 1:T:68:SER:O     | 1:T:69:HIS:HD2   | 2.02                     | 0.42              |
| 1:I:125:VAL:HG12 | 1:I:125:VAL:O    | 2.18                     | 0.42              |
| 1:N:44:ILE:HG22  | 1:O:170:ARG:HD3  | 2.01                     | 0.42              |
| 1:S:41:VAL:HG13  | 1:S:125:VAL:CG1  | 2.49                     | 0.42              |
| 1:T:51:VAL:HG22  | 1:T:118:ARG:HB2  | 2.01                     | 0.42              |
| 1:D:8:TYR:O      | 1:D:12:GLN:HG2   | 2.20                     | 0.42              |
| 1:J:192:TYR:N    | 1:J:192:TYR:CD1  | 2.88                     | 0.42              |
| 1:L:20:PRO:HB3   | 1:L:60:ASP:CG    | 2.45                     | 0.42              |
| 1:N:125:VAL:HG12 | 1:N:125:VAL:O    | 2.18                     | 0.42              |
| 1:Q:188:CYS:HB2  | 4:Q:213:HOH:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:88:ALA:HB3   | 1:S:91:ALA:HB2   | 2.02                     | 0.42              |
| 2:C:211:09R:BR1  | 1:D:104:ARG:HB2  | 2.75                     | 0.42              |
| 1:S:30:SER:HB2   | 1:S:57:THR:HG22  | 2.02                     | 0.42              |
| 1:S:68:SER:O     | 1:S:69:HIS:HD2   | 2.02                     | 0.42              |
| 2:S:211:09R:H5   | 2:S:211:09R:H1   | 1.82                     | 0.42              |
| 1:J:106:VAL:HB   | 1:J:110:GLU:HB2  | 2.01                     | 0.42              |
| 1:K:25:ARG:CB    | 1:K:26:PRO:HD2   | 2.48                     | 0.42              |
| 1:K:68:SER:O     | 1:K:69:HIS:HD2   | 2.03                     | 0.42              |
| 1:Q:146:HIS:CE1  | 1:Q:148:ARG:HB2  | 2.54                     | 0.42              |
| 1:O:1:LEU:HB2    | 1:O:70:SER:HG    | 1.85                     | 0.42              |
| 1:A:174:LEU:HD11 | 1:A:202:ARG:HD3  | 2.02                     | 0.42              |
| 1:G:137:ARG:HG3  | 1:G:198:SER:OG   | 2.20                     | 0.42              |
| 1:J:19:ILE:O     | 1:J:19:ILE:HG23  | 2.19                     | 0.42              |
| 1:M:19:ILE:HG13  | 1:M:82:TRP:CZ2   | 2.55                     | 0.42              |
| 1:Q:88:ALA:HB3   | 1:Q:91:ALA:HB2   | 2.02                     | 0.42              |
| 1:D:15:ARG:HH22  | 1:E:8:TYR:CA     | 2.33                     | 0.42              |
| 1:I:15:ARG:HH12  | 1:J:8:TYR:HD1    | 1.65                     | 0.42              |
| 1:I:32:SER:HB2   | 1:I:155:THR:CG2  | 2.50                     | 0.42              |
| 1:L:171:PHE:O    | 1:L:204:LYS:HD2  | 2.19                     | 0.42              |
| 2:M:211:09R:BR1  | 1:N:104:ARG:HB2  | 2.75                     | 0.42              |
| 1:N:14:SER:HB2   | 1:N:63:LEU:CD2   | 2.50                     | 0.42              |
| 1:B:154:PRO:HB3  | 1:B:178:GLN:OE1  | 2.20                     | 0.42              |
| 1:L:23:ARG:CZ    | 1:L:25:ARG:HH22  | 2.33                     | 0.42              |
| 1:P:45:THR:HA    | 1:Q:170:ARG:HD2  | 2.01                     | 0.42              |
| 1:B:15:ARG:NH1   | 1:C:4:ALA:HB1    | 2.35                     | 0.41              |
| 2:B:211:09R:H3   | 1:C:112:LEU:HD23 | 2.02                     | 0.41              |
| 1:F:99:THR:HG21  | 1:J:143:TRP:CZ2  | 2.55                     | 0.41              |
| 1:J:92:ILE:CG1   | 1:J:120:ARG:HB3  | 2.48                     | 0.41              |
| 1:O:153:ASP:OD2  | 1:O:180:LYS:HD2  | 2.21                     | 0.41              |
| 1:Q:19:ILE:HG13  | 1:Q:82:TRP:CZ2   | 2.55                     | 0.41              |
| 1:Q:83:VAL:HG13  | 1:Q:84:PRO:HD2   | 2.03                     | 0.41              |
| 1:S:10:ILE:O     | 1:S:14:SER:HB3   | 2.20                     | 0.41              |
| 1:S:34:LYS:HB2   | 1:S:53:TRP:HB2   | 2.02                     | 0.41              |
| 1:D:41:VAL:CG1   | 1:D:125:VAL:CG1  | 2.99                     | 0.41              |
| 1:H:149:GLU:CD   | 1:I:104:ARG:HH22 | 2.28                     | 0.41              |
| 1:O:68:SER:O     | 1:O:69:HIS:HD2   | 2.02                     | 0.41              |
| 1:T:154:PRO:O    | 1:T:155:THR:CB   | 2.68                     | 0.41              |
| 1:E:61:ARG:HG2   | 4:E:216:HOH:O    | 2.20                     | 0.41              |
| 1:S:47:GLU:HA    | 1:S:121:PHE:O    | 2.21                     | 0.41              |
| 1:H:21:THR:HG23  | 1:H:25:ARG:O     | 2.21                     | 0.41              |
| 1:I:22:GLN:HE21  | 1:I:61:ARG:CG    | 2.33                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:180:LYS:NZ   | 1:I:193:GLU:OE1  | 2.54                     | 0.41              |
| 1:K:22:GLN:O     | 1:K:24:ASP:N     | 2.53                     | 0.41              |
| 1:P:104:ARG:HH22 | 1:T:149:GLU:CD   | 2.29                     | 0.41              |
| 1:Q:11:ARG:HG3   | 1:Q:11:ARG:NH1   | 2.33                     | 0.41              |
| 1:R:137:ARG:HD2  | 1:R:196:GLU:CD   | 2.46                     | 0.41              |
| 1:G:143:TRP:CE2  | 2:G:211:09R:H5   | 2.56                     | 0.41              |
| 2:H:211:09R:BR1  | 1:I:104:ARG:HB2  | 2.75                     | 0.41              |
| 1:K:88:ALA:HB1   | 1:K:121:PHE:HE1  | 1.86                     | 0.41              |
| 1:M:153:ASP:HA   | 1:M:154:PRO:HD3  | 1.94                     | 0.41              |
| 1:R:203:LYS:HG2  | 1:R:204:LYS:O    | 2.20                     | 0.41              |
| 1:T:143:TRP:O    | 2:T:211:09R:N3   | 2.54                     | 0.41              |
| 1:C:153:ASP:HA   | 1:C:154:PRO:HD3  | 1.91                     | 0.41              |
| 1:G:187:CYS:SG   | 1:H:114:MET:HE1  | 2.61                     | 0.41              |
| 1:G:193:GLU:O    | 4:G:213:HOH:O    | 2.22                     | 0.41              |
| 1:I:88:ALA:HB3   | 1:I:91:ALA:HB2   | 2.03                     | 0.41              |
| 1:J:17:ASP:OD1   | 1:J:17:ASP:N     | 2.53                     | 0.41              |
| 1:L:20:PRO:HD3   | 1:L:82:TRP:CD2   | 2.56                     | 0.41              |
| 1:L:125:VAL:O    | 1:L:125:VAL:HG12 | 2.19                     | 0.41              |
| 1:P:142:SER:HB3  | 4:P:319:HOH:O    | 2.19                     | 0.41              |
| 2:Q:211:09R:BR1  | 1:R:104:ARG:HB2  | 2.76                     | 0.41              |
| 2:Q:211:09R:H4   | 1:R:114:MET:HE3  | 2.01                     | 0.41              |
| 1:C:142:SER:OG   | 1:C:145:HIS:HB2  | 2.21                     | 0.41              |
| 1:D:134:ALA:O    | 1:D:200:ASN:HA   | 2.21                     | 0.41              |
| 1:E:19:ILE:HG13  | 1:E:82:TRP:CZ2   | 2.56                     | 0.41              |
| 1:G:134:ALA:O    | 1:G:200:ASN:HA   | 2.21                     | 0.41              |
| 1:G:180:LYS:NZ   | 1:G:193:GLU:OE1  | 2.54                     | 0.41              |
| 1:H:41:VAL:HG13  | 1:H:125:VAL:HG11 | 2.03                     | 0.41              |
| 1:J:94:LYS:HB2   | 1:J:95:PRO:HD2   | 2.03                     | 0.41              |
| 1:L:22:GLN:NE2   | 1:L:61:ARG:CG    | 2.82                     | 0.41              |
| 1:N:47:GLU:HA    | 1:N:121:PHE:O    | 2.21                     | 0.41              |
| 1:P:104:ARG:HB2  | 2:T:211:09R:BR1  | 2.75                     | 0.41              |
| 1:Q:44:ILE:HG22  | 1:R:170:ARG:HD3  | 2.03                     | 0.41              |
| 1:S:15:ARG:HA    | 1:S:16:PRO:HD3   | 1.85                     | 0.41              |
| 1:A:126:SER:HB3  | 4:A:216:HOH:O    | 2.21                     | 0.41              |
| 1:J:185:TYR:O    | 1:J:186:SER:C    | 2.63                     | 0.41              |
| 1:E:36:ILE:HB    | 1:E:51:VAL:HG12  | 2.03                     | 0.40              |
| 1:L:143:TRP:CZ3  | 2:L:211:09R:H7   | 2.56                     | 0.40              |
| 1:T:47:GLU:HA    | 1:T:121:PHE:O    | 2.21                     | 0.40              |
| 1:J:93:SER:HB3   | 1:J:120:ARG:NH2  | 2.36                     | 0.40              |
| 1:J:124:ASP:HB3  | 1:J:135:THR:O    | 2.21                     | 0.40              |
| 1:J:146:HIS:CE1  | 1:J:148:ARG:HB2  | 2.57                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:67:SER:HA   | 1:J:70:SER:HB2   | 2.04                     | 0.40              |
| 1:O:143:TRP:O   | 2:O:211:09R:H5   | 2.21                     | 0.40              |
| 1:T:23:ARG:C    | 1:T:25:ARG:N     | 2.79                     | 0.40              |
| 1:T:153:ASP:HA  | 1:T:154:PRO:HD3  | 1.93                     | 0.40              |
| 1:C:161:ASP:HB3 | 1:C:176:VAL:HG23 | 2.03                     | 0.40              |
| 1:J:29:VAL:CG2  | 1:J:84:PRO:HG3   | 2.52                     | 0.40              |
| 1:L:83:VAL:HG13 | 1:L:84:PRO:HD2   | 2.03                     | 0.40              |
| 1:L:206:ARG:CZ  | 1:L:206:ARG:HB2  | 2.51                     | 0.40              |
| 1:P:1:LEU:HB2   | 1:P:70:SER:OG    | 2.21                     | 0.40              |
| 1:R:153:ASP:HA  | 1:R:154:PRO:HD3  | 1.95                     | 0.40              |
| 2:B:211:09R:BR1 | 1:C:104:ARG:HB2  | 2.77                     | 0.40              |
| 1:F:205:GLY:O   | 1:F:207:SER:N    | 2.53                     | 0.40              |
| 1:M:146:HIS:HE1 | 1:M:148:ARG:HB2  | 1.86                     | 0.40              |
| 2:M:211:09R:H3  | 1:N:112:LEU:HD23 | 2.03                     | 0.40              |
| 1:T:23:ARG:HA   | 1:T:23:ARG:HD3   | 1.78                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | A     | 199/210 (95%) | 196 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | B     | 195/210 (93%) | 193 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | C     | 197/210 (94%) | 195 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | D     | 199/210 (95%) | 195 (98%)  | 3 (2%)  | 1 (0%)   | 24          | 48  |
| 1   | E     | 189/210 (90%) | 188 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | F     | 201/210 (96%) | 194 (96%)  | 6 (3%)  | 1 (0%)   | 24          | 48  |
| 1   | G     | 195/210 (93%) | 192 (98%)  | 2 (1%)  | 1 (0%)   | 24          | 48  |
| 1   | H     | 194/210 (92%) | 192 (99%)  | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | I     | 200/210 (95%)   | 198 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | J     | 197/210 (94%)   | 182 (92%)  | 12 (6%) | 3 (2%)   | 8           | 22  |
| 1   | K     | 200/210 (95%)   | 194 (97%)  | 4 (2%)  | 2 (1%)   | 12          | 32  |
| 1   | L     | 199/210 (95%)   | 197 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | M     | 197/210 (94%)   | 192 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | N     | 198/210 (94%)   | 194 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | O     | 193/210 (92%)   | 188 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | P     | 196/210 (93%)   | 192 (98%)  | 3 (2%)  | 1 (0%)   | 24          | 48  |
| 1   | Q     | 195/210 (93%)   | 189 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | R     | 196/210 (93%)   | 190 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | S     | 196/210 (93%)   | 191 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | T     | 196/210 (93%)   | 191 (97%)  | 4 (2%)  | 1 (0%)   | 24          | 48  |
| All | All   | 3932/4200 (94%) | 3843 (98%) | 79 (2%) | 10 (0%)  | 36          | 60  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 23  | ARG  |
| 1   | T     | 24  | ASP  |
| 1   | D     | 23  | ARG  |
| 1   | F     | 206 | ARG  |
| 1   | G     | 131 | GLU  |
| 1   | J     | 44  | ILE  |
| 1   | J     | 133 | GLY  |
| 1   | K     | 22  | GLN  |
| 1   | P     | 23  | ARG  |
| 1   | J     | 186 | SER  |

### 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     | 189/196 (96%)   | 185 (98%)  | 4 (2%)   | 47          | 75 |
| 1   | B     | 185/196 (94%)   | 180 (97%)  | 5 (3%)   | 39          | 69 |
| 1   | C     | 187/196 (95%)   | 182 (97%)  | 5 (3%)   | 39          | 69 |
| 1   | D     | 189/196 (96%)   | 182 (96%)  | 7 (4%)   | 30          | 59 |
| 1   | E     | 183/196 (93%)   | 180 (98%)  | 3 (2%)   | 55          | 80 |
| 1   | F     | 191/196 (97%)   | 187 (98%)  | 4 (2%)   | 47          | 75 |
| 1   | G     | 185/196 (94%)   | 180 (97%)  | 5 (3%)   | 39          | 69 |
| 1   | H     | 184/196 (94%)   | 178 (97%)  | 6 (3%)   | 33          | 63 |
| 1   | I     | 190/196 (97%)   | 188 (99%)  | 2 (1%)   | 65          | 85 |
| 1   | J     | 188/196 (96%)   | 169 (90%)  | 19 (10%) | 7           | 18 |
| 1   | K     | 190/196 (97%)   | 185 (97%)  | 5 (3%)   | 40          | 70 |
| 1   | L     | 189/196 (96%)   | 182 (96%)  | 7 (4%)   | 30          | 59 |
| 1   | M     | 187/196 (95%)   | 183 (98%)  | 4 (2%)   | 47          | 75 |
| 1   | N     | 189/196 (96%)   | 181 (96%)  | 8 (4%)   | 26          | 55 |
| 1   | O     | 184/196 (94%)   | 179 (97%)  | 5 (3%)   | 39          | 69 |
| 1   | P     | 186/196 (95%)   | 179 (96%)  | 7 (4%)   | 29          | 58 |
| 1   | Q     | 185/196 (94%)   | 176 (95%)  | 9 (5%)   | 22          | 49 |
| 1   | R     | 186/196 (95%)   | 183 (98%)  | 3 (2%)   | 55          | 80 |
| 1   | S     | 186/196 (95%)   | 181 (97%)  | 5 (3%)   | 39          | 69 |
| 1   | T     | 186/196 (95%)   | 178 (96%)  | 8 (4%)   | 26          | 54 |
| All | All   | 3739/3920 (95%) | 3618 (97%) | 121 (3%) | 34          | 64 |

All (121) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ARG  |
| 1   | A     | 14  | SER  |
| 1   | A     | 25  | ARG  |
| 1   | A     | 57  | THR  |
| 1   | B     | 11  | ARG  |
| 1   | B     | 22  | GLN  |
| 1   | B     | 57  | THR  |
| 1   | B     | 110 | GLU  |
| 1   | B     | 131 | GLU  |
| 1   | C     | 14  | SER  |
| 1   | C     | 21  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 57  | THR  |
| 1   | C     | 132 | SER  |
| 1   | C     | 161 | ASP  |
| 1   | D     | 21  | THR  |
| 1   | D     | 24  | ASP  |
| 1   | D     | 57  | THR  |
| 1   | D     | 132 | SER  |
| 1   | D     | 161 | ASP  |
| 1   | D     | 180 | LYS  |
| 1   | D     | 181 | ASN  |
| 1   | E     | 21  | THR  |
| 1   | E     | 57  | THR  |
| 1   | E     | 155 | THR  |
| 1   | F     | 23  | ARG  |
| 1   | F     | 25  | ARG  |
| 1   | F     | 57  | THR  |
| 1   | F     | 187 | CYS  |
| 1   | G     | 13  | THR  |
| 1   | G     | 57  | THR  |
| 1   | G     | 131 | GLU  |
| 1   | G     | 132 | SER  |
| 1   | G     | 155 | THR  |
| 1   | H     | 22  | GLN  |
| 1   | H     | 23  | ARG  |
| 1   | H     | 24  | ASP  |
| 1   | H     | 57  | THR  |
| 1   | H     | 131 | GLU  |
| 1   | H     | 132 | SER  |
| 1   | I     | 57  | THR  |
| 1   | I     | 137 | ARG  |
| 1   | J     | 21  | THR  |
| 1   | J     | 31  | VAL  |
| 1   | J     | 40  | GLU  |
| 1   | J     | 48  | VAL  |
| 1   | J     | 54  | GLN  |
| 1   | J     | 57  | THR  |
| 1   | J     | 61  | ARG  |
| 1   | J     | 79  | SER  |
| 1   | J     | 122 | SER  |
| 1   | J     | 129 | ASP  |
| 1   | J     | 149 | GLU  |
| 1   | J     | 151 | SER  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | J     | 152    | VAL  |
| 1   | J     | 153    | ASP  |
| 1   | J     | 155    | THR  |
| 1   | J     | 159    | SER  |
| 1   | J     | 172    | GLU  |
| 1   | J     | 179    | LYS  |
| 1   | J     | 194    | ASP  |
| 1   | K     | 25     | ARG  |
| 1   | K     | 57     | THR  |
| 1   | K     | 110    | GLU  |
| 1   | K     | 132    | SER  |
| 1   | K     | 203    | LYS  |
| 1   | L     | 11     | ARG  |
| 1   | L     | 15     | ARG  |
| 1   | L     | 21     | THR  |
| 1   | L     | 40     | GLU  |
| 1   | L     | 57     | THR  |
| 1   | L     | 155    | THR  |
| 1   | L     | 206    | ARG  |
| 1   | M     | 25     | ARG  |
| 1   | M     | 57     | THR  |
| 1   | M     | 161    | ASP  |
| 1   | M     | 204    | LYS  |
| 1   | N     | 14     | SER  |
| 1   | N     | 21     | THR  |
| 1   | N     | 25     | ARG  |
| 1   | N     | 57     | THR  |
| 1   | N     | 120    | ARG  |
| 1   | N     | 155    | THR  |
| 1   | N     | 187[A] | CYS  |
| 1   | N     | 187[B] | CYS  |
| 1   | O     | 21     | THR  |
| 1   | O     | 23     | ARG  |
| 1   | O     | 24     | ASP  |
| 1   | O     | 57     | THR  |
| 1   | O     | 155    | THR  |
| 1   | P     | 13     | THR  |
| 1   | P     | 21     | THR  |
| 1   | P     | 24     | ASP  |
| 1   | P     | 57     | THR  |
| 1   | P     | 131    | GLU  |
| 1   | P     | 203    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 204 | LYS  |
| 1   | Q     | 11  | ARG  |
| 1   | Q     | 14  | SER  |
| 1   | Q     | 15  | ARG  |
| 1   | Q     | 21  | THR  |
| 1   | Q     | 22  | GLN  |
| 1   | Q     | 24  | ASP  |
| 1   | Q     | 57  | THR  |
| 1   | Q     | 132 | SER  |
| 1   | Q     | 204 | LYS  |
| 1   | R     | 31  | VAL  |
| 1   | R     | 57  | THR  |
| 1   | R     | 131 | GLU  |
| 1   | S     | 11  | ARG  |
| 1   | S     | 21  | THR  |
| 1   | S     | 57  | THR  |
| 1   | S     | 110 | GLU  |
| 1   | S     | 187 | CYS  |
| 1   | T     | 21  | THR  |
| 1   | T     | 23  | ARG  |
| 1   | T     | 24  | ASP  |
| 1   | T     | 57  | THR  |
| 1   | T     | 120 | ARG  |
| 1   | T     | 148 | ARG  |
| 1   | T     | 155 | THR  |
| 1   | T     | 204 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | GLN  |
| 1   | B     | 55  | GLN  |
| 1   | B     | 119 | GLN  |
| 1   | C     | 69  | HIS  |
| 1   | D     | 69  | HIS  |
| 1   | D     | 119 | GLN  |
| 1   | D     | 200 | ASN  |
| 1   | F     | 69  | HIS  |
| 1   | F     | 119 | GLN  |
| 1   | F     | 200 | ASN  |
| 1   | G     | 55  | GLN  |
| 1   | G     | 69  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 119 | GLN  |
| 1   | G     | 200 | ASN  |
| 1   | H     | 69  | HIS  |
| 1   | I     | 22  | GLN  |
| 1   | I     | 119 | GLN  |
| 1   | J     | 55  | GLN  |
| 1   | J     | 69  | HIS  |
| 1   | J     | 101 | GLN  |
| 1   | K     | 9   | ASN  |
| 1   | K     | 22  | GLN  |
| 1   | K     | 69  | HIS  |
| 1   | K     | 200 | ASN  |
| 1   | L     | 9   | ASN  |
| 1   | L     | 22  | GLN  |
| 1   | L     | 69  | HIS  |
| 1   | M     | 69  | HIS  |
| 1   | M     | 200 | ASN  |
| 1   | N     | 69  | HIS  |
| 1   | O     | 69  | HIS  |
| 1   | P     | 22  | GLN  |
| 1   | P     | 69  | HIS  |
| 1   | Q     | 69  | HIS  |
| 1   | Q     | 200 | ASN  |
| 1   | R     | 9   | ASN  |
| 1   | R     | 22  | GLN  |
| 1   | R     | 69  | HIS  |
| 1   | S     | 22  | GLN  |
| 1   | S     | 69  | HIS  |
| 1   | S     | 119 | GLN  |
| 1   | S     | 200 | ASN  |
| 1   | T     | 200 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

37 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | F     | 212 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.18 | 0           |
| 3   | SO4  | N     | 212 | -    | 4,4,4        | 0.27 | 0           | 6,6,6       | 0.16 | 0           |
| 2   | 09R  | M     | 211 | -    | 14,15,15     | 3.32 | 2 (14%)     | 14,19,19    | 1.45 | 2 (14%)     |
| 2   | 09R  | K     | 211 | -    | 14,15,15     | 3.37 | 2 (14%)     | 14,19,19    | 1.58 | 2 (14%)     |
| 2   | 09R  | C     | 211 | -    | 14,15,15     | 3.50 | 2 (14%)     | 14,19,19    | 1.12 | 0           |
| 3   | SO4  | D     | 212 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.22 | 0           |
| 3   | SO4  | B     | 213 | -    | 4,4,4        | 0.27 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | 09R  | A     | 211 | -    | 14,15,15     | 3.53 | 4 (28%)     | 14,19,19    | 2.96 | 8 (57%)     |
| 2   | 09R  | N     | 211 | -    | 14,15,15     | 3.35 | 2 (14%)     | 14,19,19    | 2.04 | 5 (35%)     |
| 3   | SO4  | F     | 213 | -    | 4,4,4        | 0.27 | 0           | 6,6,6       | 0.20 | 0           |
| 2   | 09R  | D     | 211 | -    | 14,15,15     | 3.41 | 2 (14%)     | 14,19,19    | 1.63 | 2 (14%)     |
| 2   | 09R  | L     | 211 | -    | 14,15,15     | 3.46 | 2 (14%)     | 14,19,19    | 1.77 | 3 (21%)     |
| 3   | SO4  | D     | 214 | -    | 4,4,4        | 0.27 | 0           | 6,6,6       | 0.40 | 0           |
| 2   | 09R  | G     | 211 | -    | 14,15,15     | 3.49 | 3 (21%)     | 14,19,19    | 1.46 | 2 (14%)     |
| 3   | SO4  | K     | 212 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.22 | 0           |
| 2   | 09R  | S     | 211 | -    | 14,15,15     | 3.30 | 2 (14%)     | 14,19,19    | 1.53 | 2 (14%)     |
| 3   | SO4  | D     | 213 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.11 | 0           |
| 3   | SO4  | R     | 212 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.44 | 0           |
| 2   | 09R  | H     | 211 | -    | 14,15,15     | 3.38 | 4 (28%)     | 14,19,19    | 1.87 | 4 (28%)     |
| 2   | 09R  | P     | 211 | -    | 14,15,15     | 3.38 | 2 (14%)     | 14,19,19    | 1.70 | 1 (7%)      |
| 2   | 09R  | B     | 211 | -    | 14,15,15     | 3.48 | 1 (7%)      | 14,19,19    | 1.32 | 2 (14%)     |
| 2   | 09R  | Q     | 211 | -    | 14,15,15     | 3.28 | 3 (21%)     | 14,19,19    | 1.58 | 4 (28%)     |
| 2   | 09R  | T     | 211 | -    | 14,15,15     | 3.35 | 1 (7%)      | 14,19,19    | 1.63 | 4 (28%)     |
| 3   | SO4  | L     | 213 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.18 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 09R  | R     | 211 | -    | 14,15,15     | 3.36 | 2 (14%)  | 14,19,19    | 1.53 | 3 (21%)  |
| 2   | 09R  | J     | 211 | -    | 14,15,15     | 3.11 | 2 (14%)  | 14,19,19    | 1.96 | 4 (28%)  |
| 3   | SO4  | L     | 212 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.25 | 0        |
| 2   | 09R  | E     | 211 | -    | 14,15,15     | 3.78 | 1 (7%)   | 14,19,19    | 1.05 | 1 (7%)   |
| 2   | 09R  | F     | 211 | -    | 14,15,15     | 3.27 | 1 (7%)   | 14,19,19    | 2.02 | 5 (35%)  |
| 2   | 09R  | O     | 211 | -    | 14,15,15     | 3.32 | 1 (7%)   | 14,19,19    | 1.59 | 2 (14%)  |
| 3   | SO4  | I     | 212 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.07 | 0        |
| 3   | SO4  | J     | 212 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.21 | 0        |
| 3   | SO4  | A     | 212 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.15 | 0        |
| 3   | SO4  | B     | 212 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.20 | 0        |
| 3   | SO4  | H     | 212 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.29 | 0        |
| 3   | SO4  | T     | 212 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.24 | 0        |
| 2   | 09R  | I     | 211 | -    | 14,15,15     | 3.42 | 3 (21%)  | 14,19,19    | 1.28 | 1 (7%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | 09R  | M     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | K     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | C     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | A     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | N     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | D     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | L     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | G     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | S     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | H     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | P     | 211 | -    | -       | 2/4/13/13 | 0/2/2/2 |
| 2   | 09R  | B     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | Q     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | T     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | R     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | J     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | E     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | F     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |
| 2   | 09R  | O     | 211 | -    | -       | 2/4/13/13 | 0/2/2/2 |
| 2   | 09R  | I     | 211 | -    | -       | 0/4/13/13 | 0/2/2/2 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | E     | 211 | 09R  | BR1-C5 | -13.63 | 1.70        | 1.90     |
| 2   | B     | 211 | 09R  | BR1-C5 | -12.45 | 1.72        | 1.90     |
| 2   | C     | 211 | 09R  | BR1-C5 | -12.42 | 1.72        | 1.90     |
| 2   | L     | 211 | 09R  | BR1-C5 | -12.38 | 1.72        | 1.90     |
| 2   | G     | 211 | 09R  | BR1-C5 | -12.19 | 1.72        | 1.90     |
| 2   | D     | 211 | 09R  | BR1-C5 | -12.07 | 1.73        | 1.90     |
| 2   | I     | 211 | 09R  | BR1-C5 | -11.98 | 1.73        | 1.90     |
| 2   | P     | 211 | 09R  | BR1-C5 | -11.93 | 1.73        | 1.90     |
| 2   | A     | 211 | 09R  | BR1-C5 | -11.92 | 1.73        | 1.90     |
| 2   | T     | 211 | 09R  | BR1-C5 | -11.87 | 1.73        | 1.90     |
| 2   | K     | 211 | 09R  | BR1-C5 | -11.81 | 1.73        | 1.90     |
| 2   | R     | 211 | 09R  | BR1-C5 | -11.77 | 1.73        | 1.90     |
| 2   | M     | 211 | 09R  | BR1-C5 | -11.75 | 1.73        | 1.90     |
| 2   | O     | 211 | 09R  | BR1-C5 | -11.73 | 1.73        | 1.90     |
| 2   | S     | 211 | 09R  | BR1-C5 | -11.65 | 1.73        | 1.90     |
| 2   | N     | 211 | 09R  | BR1-C5 | -11.62 | 1.73        | 1.90     |
| 2   | F     | 211 | 09R  | BR1-C5 | -11.53 | 1.73        | 1.90     |
| 2   | H     | 211 | 09R  | BR1-C5 | -11.51 | 1.73        | 1.90     |
| 2   | Q     | 211 | 09R  | BR1-C5 | -11.33 | 1.74        | 1.90     |
| 2   | J     | 211 | 09R  | BR1-C5 | -10.79 | 1.75        | 1.90     |
| 2   | A     | 211 | 09R  | C3-C2  | 2.93   | 1.44        | 1.39     |
| 2   | A     | 211 | 09R  | C4-C5  | 2.72   | 1.42        | 1.38     |
| 2   | N     | 211 | 09R  | C1-C2  | 2.51   | 1.43        | 1.38     |
| 2   | H     | 211 | 09R  | C4-C5  | 2.48   | 1.42        | 1.38     |
| 2   | Q     | 211 | 09R  | C1-C2  | 2.45   | 1.43        | 1.38     |
| 2   | P     | 211 | 09R  | C1-C2  | 2.44   | 1.43        | 1.38     |
| 2   | R     | 211 | 09R  | C1-C2  | 2.38   | 1.42        | 1.38     |
| 2   | G     | 211 | 09R  | C4-C5  | 2.34   | 1.42        | 1.38     |
| 2   | H     | 211 | 09R  | C3-C2  | 2.34   | 1.43        | 1.39     |
| 2   | S     | 211 | 09R  | C1-C2  | 2.28   | 1.42        | 1.38     |
| 2   | I     | 211 | 09R  | C4-C5  | 2.27   | 1.41        | 1.38     |
| 2   | I     | 211 | 09R  | C1-C2  | 2.27   | 1.42        | 1.38     |
| 2   | Q     | 211 | 09R  | C3-C2  | 2.26   | 1.43        | 1.39     |
| 2   | G     | 211 | 09R  | C1-C2  | 2.16   | 1.42        | 1.38     |
| 2   | D     | 211 | 09R  | C4-C5  | 2.13   | 1.41        | 1.38     |
| 2   | J     | 211 | 09R  | C4-C5  | 2.12   | 1.41        | 1.38     |
| 2   | L     | 211 | 09R  | C4-C5  | 2.12   | 1.41        | 1.38     |
| 2   | C     | 211 | 09R  | C4-C5  | 2.12   | 1.41        | 1.38     |
| 2   | K     | 211 | 09R  | C4-C5  | 2.11   | 1.41        | 1.38     |
| 2   | A     | 211 | 09R  | C4-C3  | 2.09   | 1.42        | 1.38     |
| 2   | H     | 211 | 09R  | C1-C2  | 2.06   | 1.42        | 1.38     |
| 2   | M     | 211 | 09R  | C1-C2  | 2.04   | 1.42        | 1.38     |

All (57) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A     | 211 | 09R  | BR1-C5-C4 | 5.97  | 124.77      | 118.69   |
| 2   | F     | 211 | 09R  | C3-C4-C5  | 4.58  | 120.47      | 117.41   |
| 2   | P     | 211 | 09R  | C3-C4-C5  | 4.47  | 120.40      | 117.41   |
| 2   | A     | 211 | 09R  | C9-C10-N2 | 4.34  | 121.20      | 113.63   |
| 2   | A     | 211 | 09R  | C1-N1-C5  | 4.12  | 119.38      | 116.58   |
| 2   | A     | 211 | 09R  | C3-C2-N2  | 4.10  | 127.09      | 121.39   |
| 2   | H     | 211 | 09R  | C1-N1-C5  | 3.88  | 119.21      | 116.58   |
| 2   | J     | 211 | 09R  | C1-N1-C5  | 3.83  | 119.18      | 116.58   |
| 2   | Q     | 211 | 09R  | C1-N1-C5  | 3.67  | 119.07      | 116.58   |
| 2   | H     | 211 | 09R  | BR1-C5-C4 | 3.64  | 122.39      | 118.69   |
| 2   | F     | 211 | 09R  | C1-N1-C5  | 3.62  | 119.04      | 116.58   |
| 2   | N     | 211 | 09R  | C1-N1-C5  | 3.61  | 119.03      | 116.58   |
| 2   | O     | 211 | 09R  | C1-N1-C5  | 3.59  | 119.01      | 116.58   |
| 2   | N     | 211 | 09R  | C3-C4-C5  | 3.58  | 119.80      | 117.41   |
| 2   | R     | 211 | 09R  | C3-C4-C5  | 3.56  | 119.79      | 117.41   |
| 2   | S     | 211 | 09R  | C3-C4-C5  | 3.54  | 119.77      | 117.41   |
| 2   | T     | 211 | 09R  | C1-N1-C5  | 3.47  | 118.93      | 116.58   |
| 2   | D     | 211 | 09R  | C3-C4-C5  | 3.34  | 119.64      | 117.41   |
| 2   | J     | 211 | 09R  | C3-C4-C5  | 3.31  | 119.62      | 117.41   |
| 2   | T     | 211 | 09R  | C3-C4-C5  | 3.13  | 119.50      | 117.41   |
| 2   | L     | 211 | 09R  | BR1-C5-C4 | 3.12  | 121.87      | 118.69   |
| 2   | G     | 211 | 09R  | C7-C6-N2  | -3.09 | 107.63      | 113.11   |
| 2   | K     | 211 | 09R  | C3-C4-C5  | 3.03  | 119.43      | 117.41   |
| 2   | N     | 211 | 09R  | BR1-C5-N1 | 3.03  | 119.84      | 116.32   |
| 2   | I     | 211 | 09R  | C3-C4-C5  | 3.02  | 119.43      | 117.41   |
| 2   | M     | 211 | 09R  | C3-C4-C5  | 2.90  | 119.35      | 117.41   |
| 2   | A     | 211 | 09R  | C1-C2-N2  | -2.86 | 117.46      | 121.80   |
| 2   | Q     | 211 | 09R  | C3-C4-C5  | 2.79  | 119.27      | 117.41   |
| 2   | J     | 211 | 09R  | C4-C5-N1  | -2.73 | 120.67      | 124.83   |
| 2   | H     | 211 | 09R  | C3-C4-C5  | 2.70  | 119.22      | 117.41   |
| 2   | M     | 211 | 09R  | C1-N1-C5  | 2.70  | 118.41      | 116.58   |
| 2   | J     | 211 | 09R  | C9-C10-N2 | 2.67  | 118.30      | 113.63   |
| 2   | F     | 211 | 09R  | C4-C5-N1  | -2.64 | 120.81      | 124.83   |
| 2   | L     | 211 | 09R  | C3-C4-C5  | 2.64  | 119.17      | 117.41   |
| 2   | G     | 211 | 09R  | C3-C4-C5  | 2.56  | 119.12      | 117.41   |
| 2   | N     | 211 | 09R  | C7-C6-N2  | -2.54 | 108.61      | 113.11   |
| 2   | N     | 211 | 09R  | C4-C5-N1  | -2.51 | 121.02      | 124.83   |
| 2   | A     | 211 | 09R  | C3-C4-C5  | 2.46  | 119.05      | 117.41   |
| 2   | S     | 211 | 09R  | C1-N1-C5  | 2.46  | 118.25      | 116.58   |
| 2   | B     | 211 | 09R  | BR1-C5-C4 | 2.41  | 121.15      | 118.69   |
| 2   | O     | 211 | 09R  | C9-C10-N2 | 2.41  | 117.83      | 113.63   |
| 2   | E     | 211 | 09R  | C7-C6-N2  | -2.40 | 108.86      | 113.11   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | Q     | 211 | 09R  | BR1-C5-N1 | 2.40  | 119.11      | 116.32   |
| 2   | D     | 211 | 09R  | BR1-C5-C4 | 2.38  | 121.12      | 118.69   |
| 2   | F     | 211 | 09R  | BR1-C5-N1 | 2.36  | 119.06      | 116.32   |
| 2   | A     | 211 | 09R  | BR1-C5-N1 | -2.36 | 113.57      | 116.32   |
| 2   | T     | 211 | 09R  | BR1-C5-C4 | 2.22  | 120.95      | 118.69   |
| 2   | R     | 211 | 09R  | C1-N1-C5  | 2.18  | 118.06      | 116.58   |
| 2   | L     | 211 | 09R  | C1-N1-C5  | 2.17  | 118.05      | 116.58   |
| 2   | H     | 211 | 09R  | C4-C5-N1  | -2.17 | 121.53      | 124.83   |
| 2   | K     | 211 | 09R  | C1-N1-C5  | 2.16  | 118.04      | 116.58   |
| 2   | A     | 211 | 09R  | C4-C5-N1  | -2.11 | 121.62      | 124.83   |
| 2   | B     | 211 | 09R  | C3-C2-N2  | 2.10  | 124.31      | 121.39   |
| 2   | T     | 211 | 09R  | C4-C5-N1  | -2.09 | 121.65      | 124.83   |
| 2   | Q     | 211 | 09R  | C4-C5-N1  | -2.07 | 121.68      | 124.83   |
| 2   | F     | 211 | 09R  | C9-C10-N2 | 2.06  | 117.23      | 113.63   |
| 2   | R     | 211 | 09R  | BR1-C5-N1 | 2.04  | 118.69      | 116.32   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | O     | 211 | 09R  | C1-C2-N2-C6 |
| 2   | O     | 211 | 09R  | C3-C2-N2-C6 |
| 2   | P     | 211 | 09R  | C1-C2-N2-C6 |
| 2   | P     | 211 | 09R  | C3-C2-N2-C6 |

There are no ring outliers.

19 monomers are involved in 36 short contacts:

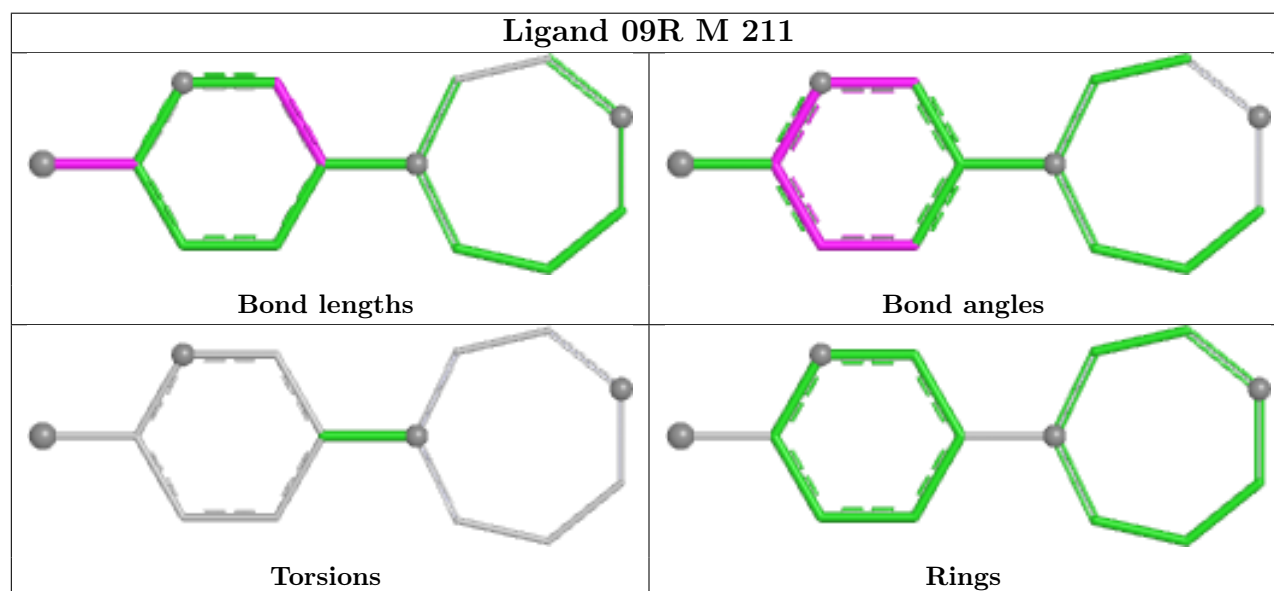
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | M     | 211 | 09R  | 2       | 0            |
| 2   | C     | 211 | 09R  | 1       | 0            |
| 2   | A     | 211 | 09R  | 1       | 0            |
| 2   | N     | 211 | 09R  | 2       | 0            |
| 3   | F     | 213 | SO4  | 1       | 0            |
| 2   | D     | 211 | 09R  | 1       | 0            |
| 2   | L     | 211 | 09R  | 3       | 0            |
| 2   | G     | 211 | 09R  | 3       | 0            |
| 2   | S     | 211 | 09R  | 2       | 0            |
| 2   | H     | 211 | 09R  | 1       | 0            |
| 2   | P     | 211 | 09R  | 2       | 0            |
| 2   | B     | 211 | 09R  | 2       | 0            |

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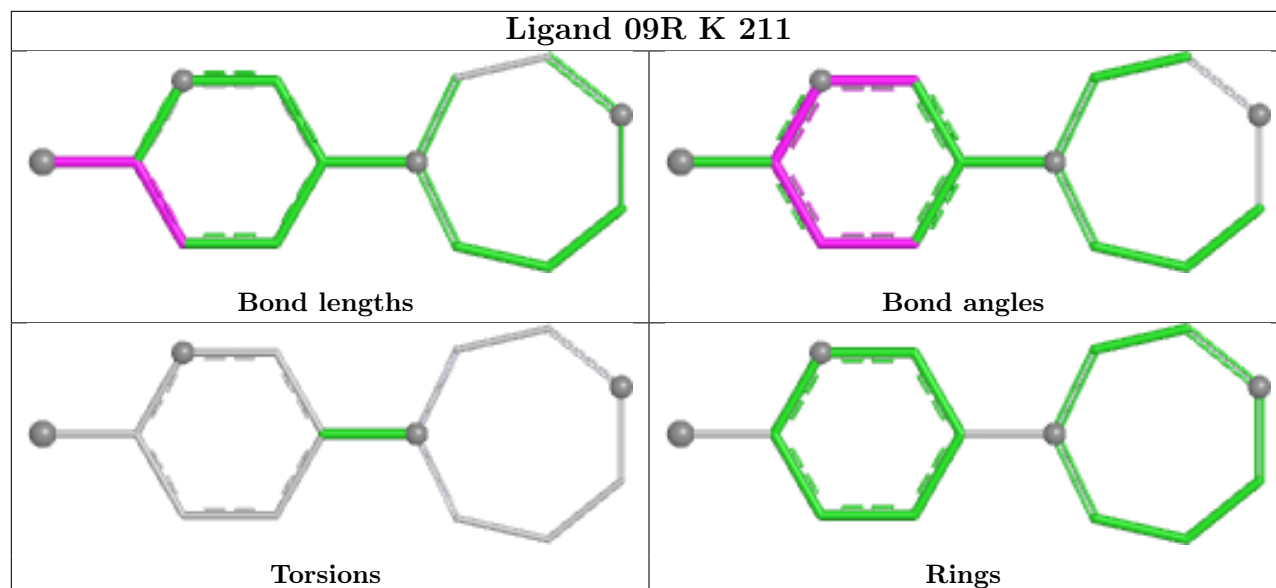
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | Q     | 211 | 09R  | 2       | 0            |
| 2   | T     | 211 | 09R  | 4       | 0            |
| 2   | R     | 211 | 09R  | 1       | 0            |
| 2   | J     | 211 | 09R  | 2       | 0            |
| 2   | E     | 211 | 09R  | 1       | 0            |
| 2   | F     | 211 | 09R  | 2       | 0            |
| 2   | O     | 211 | 09R  | 3       | 0            |

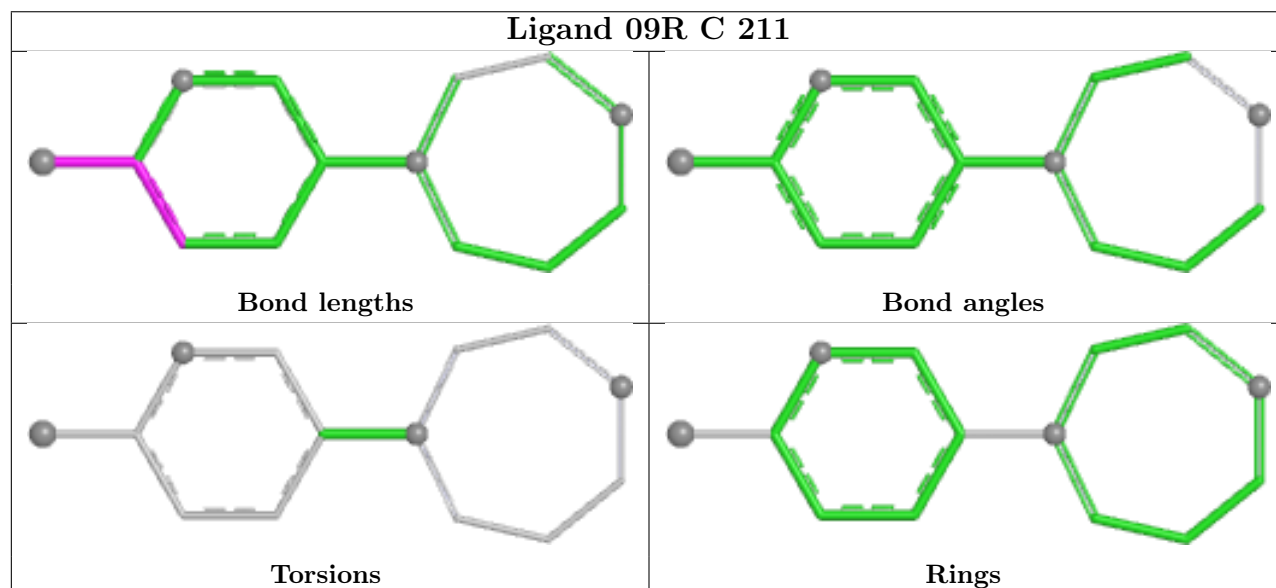
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



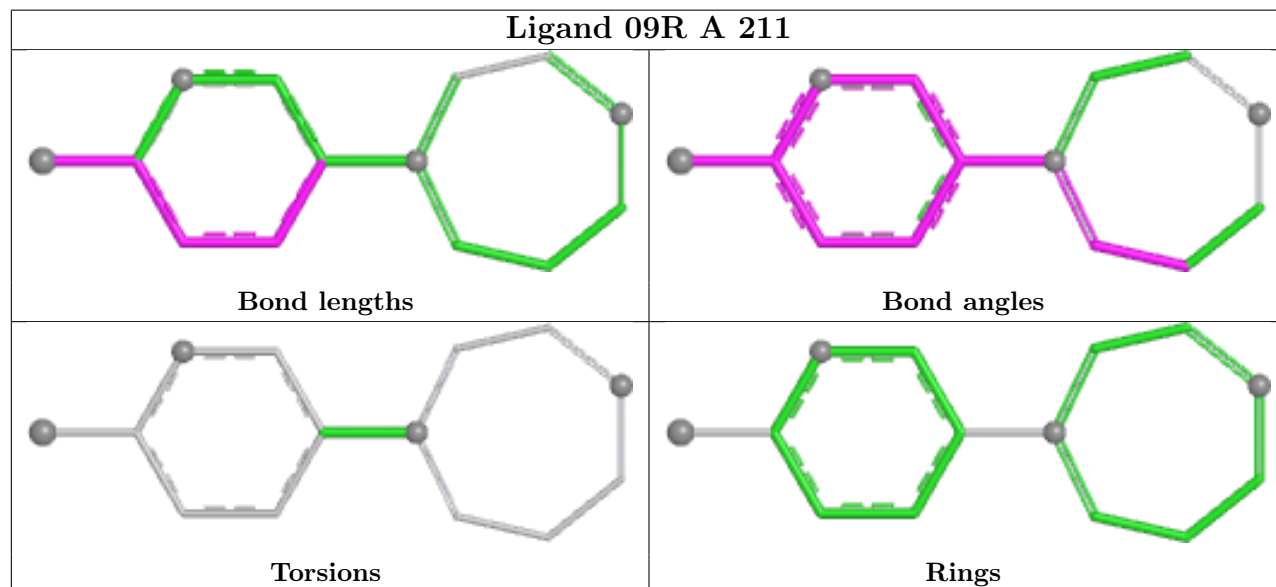
## Ligand 09R K 211



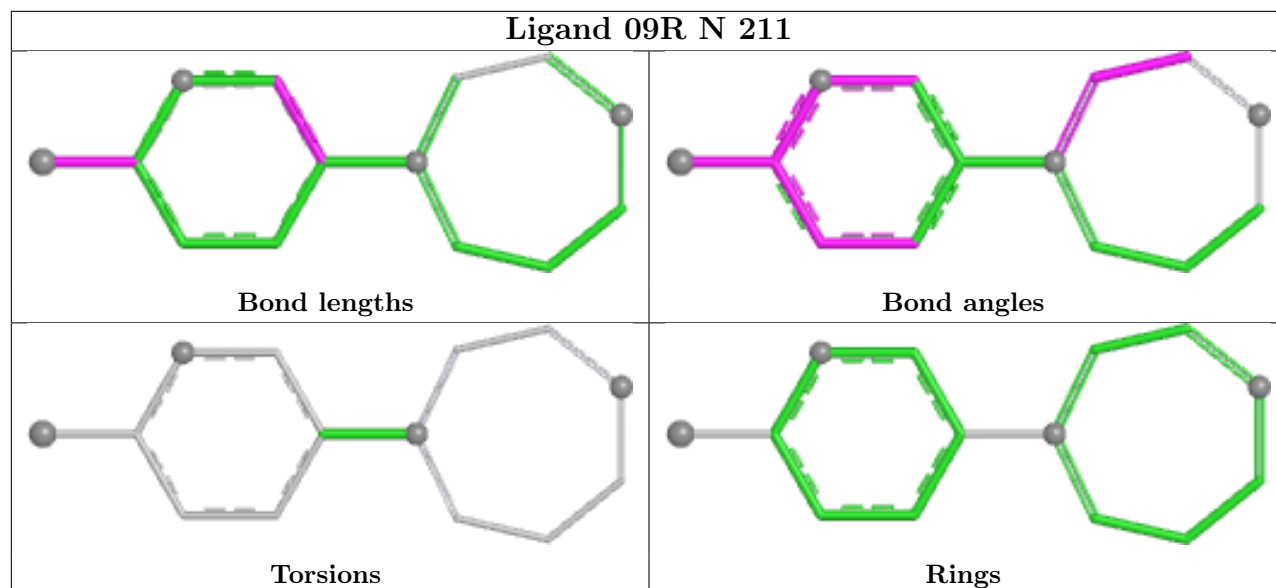
## Ligand 09R C 211



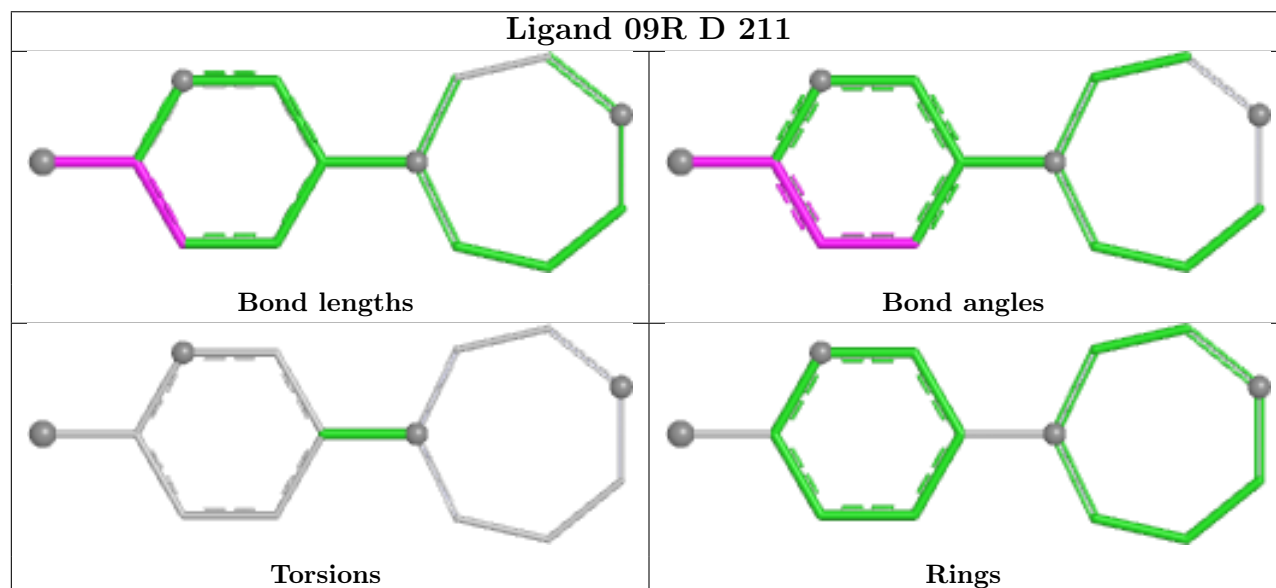
## Ligand 09R A 211



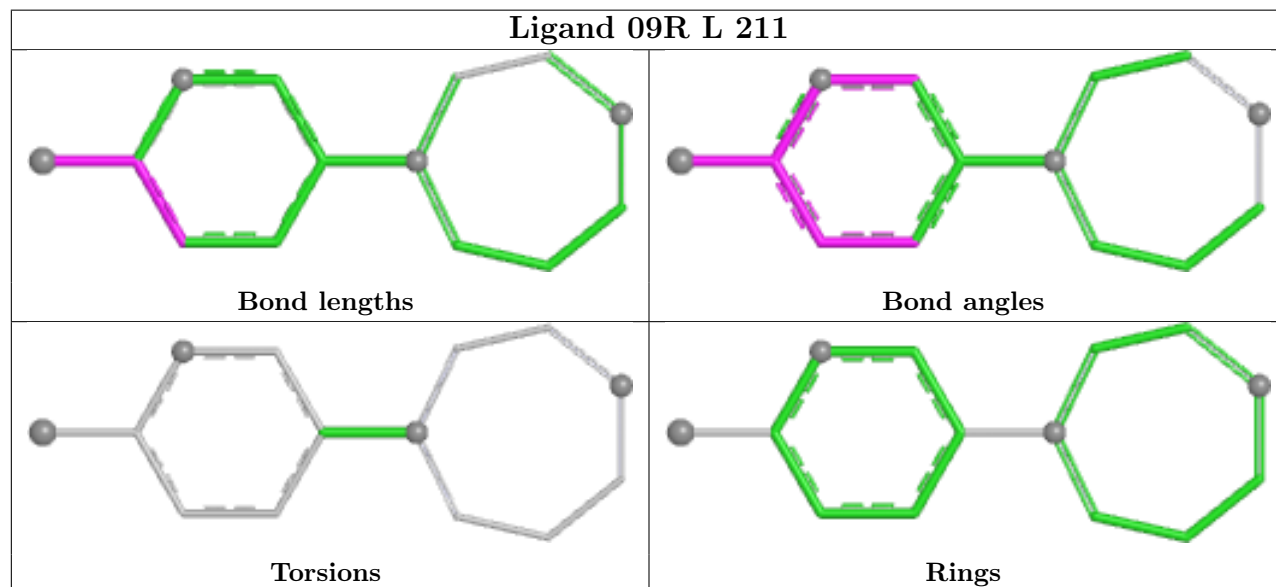
## Ligand 09R N 211



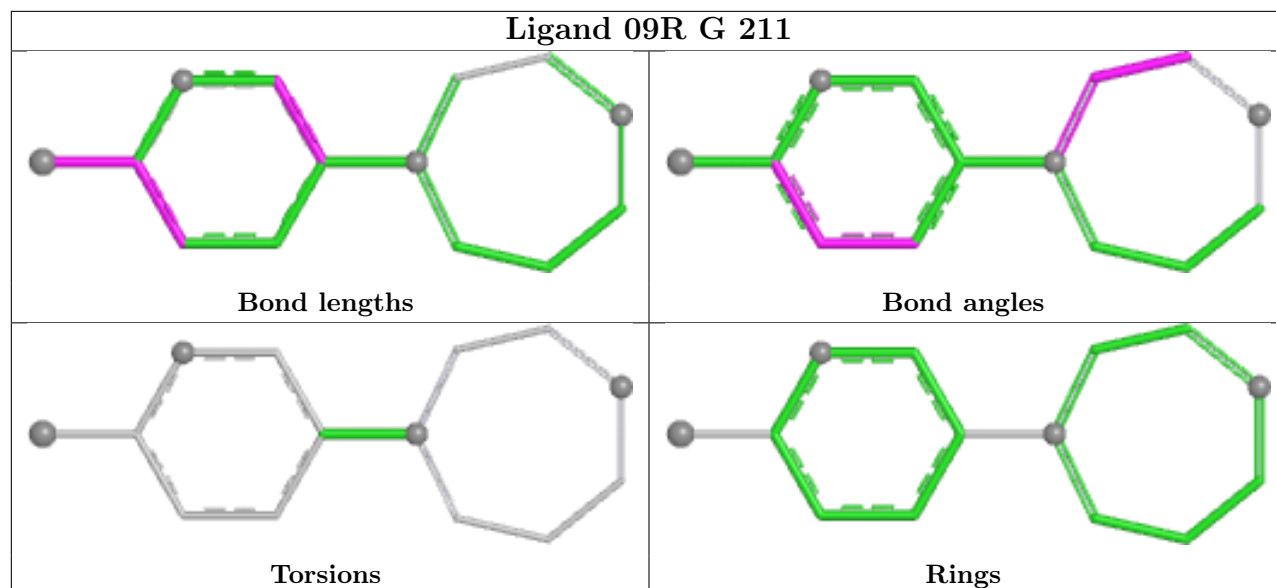
## Ligand 09R D 211



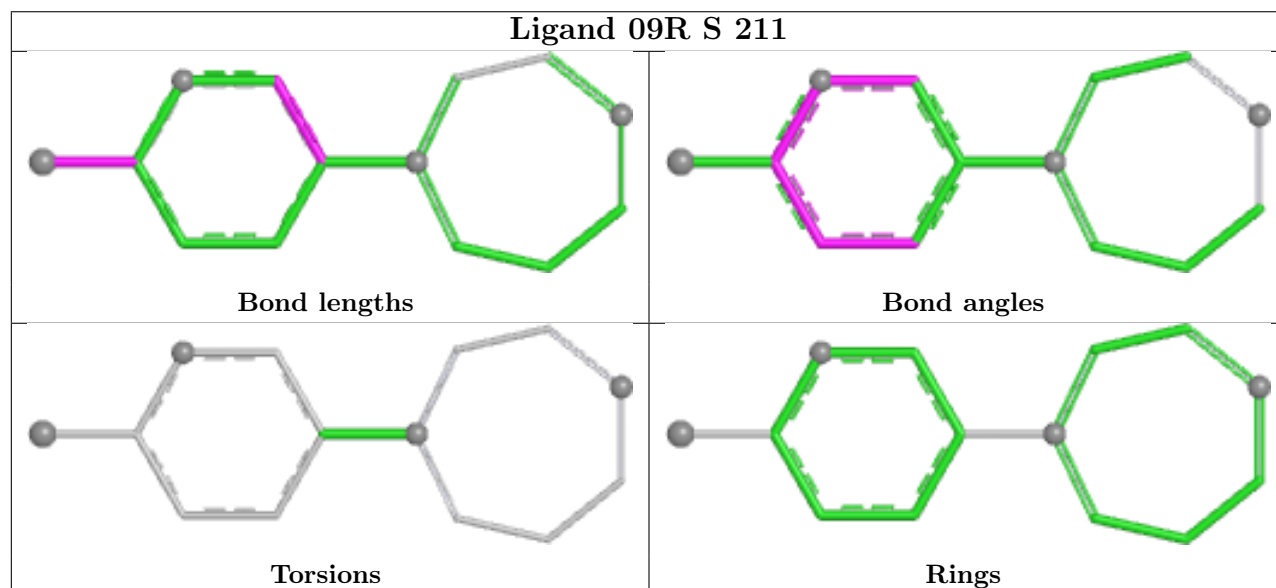
## Ligand 09R L 211



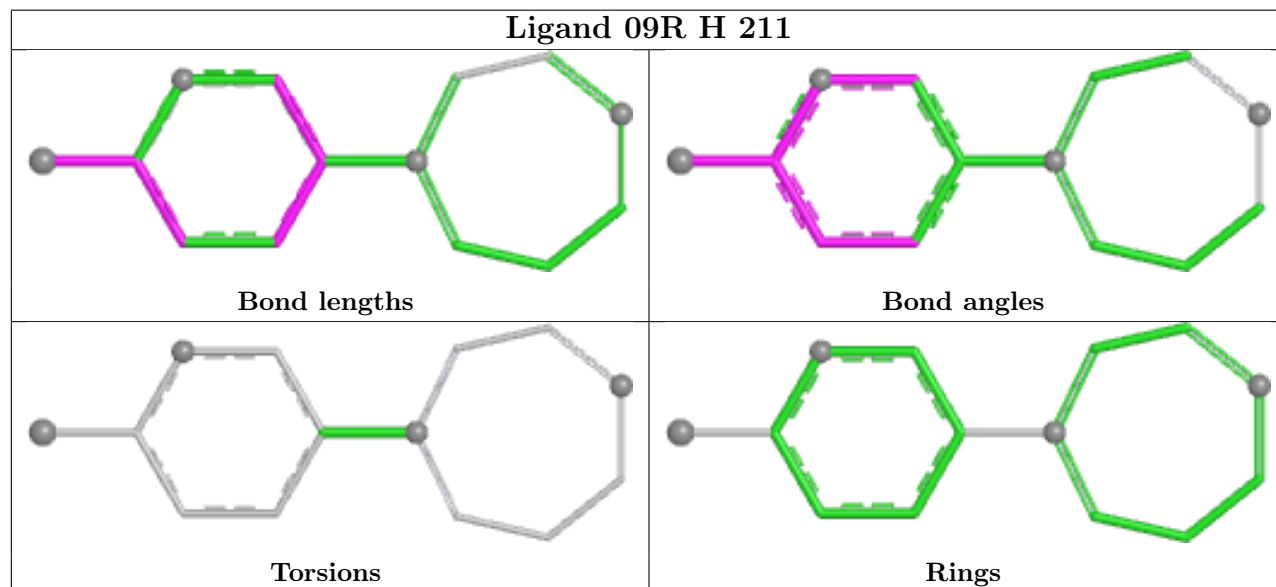
## Ligand 09R G 211



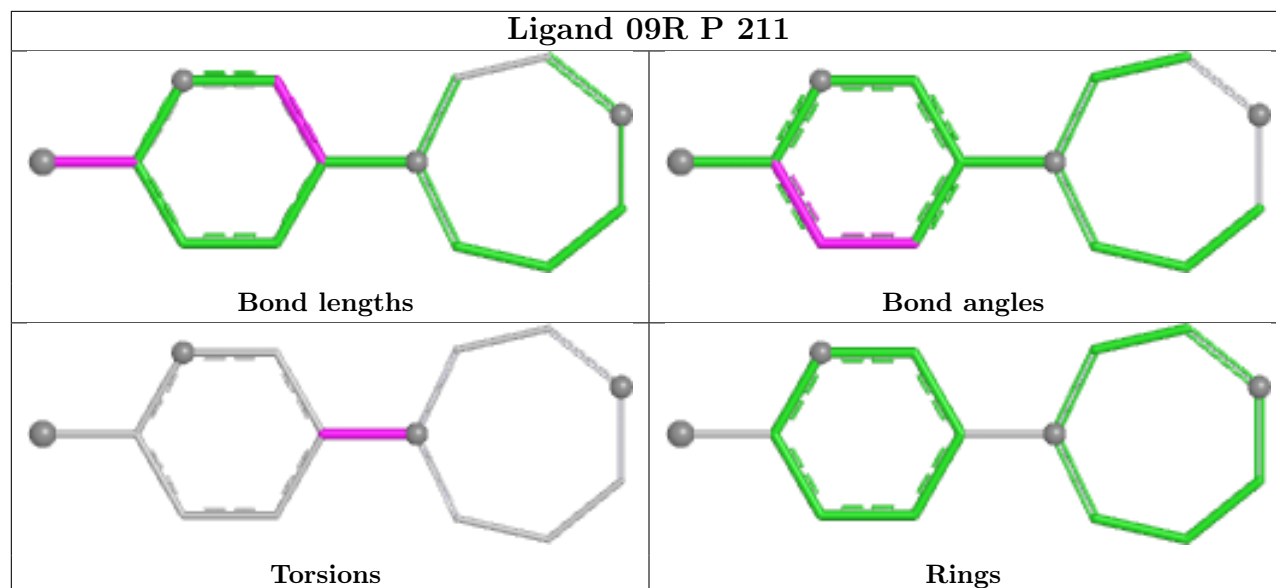
## Ligand 09R S 211



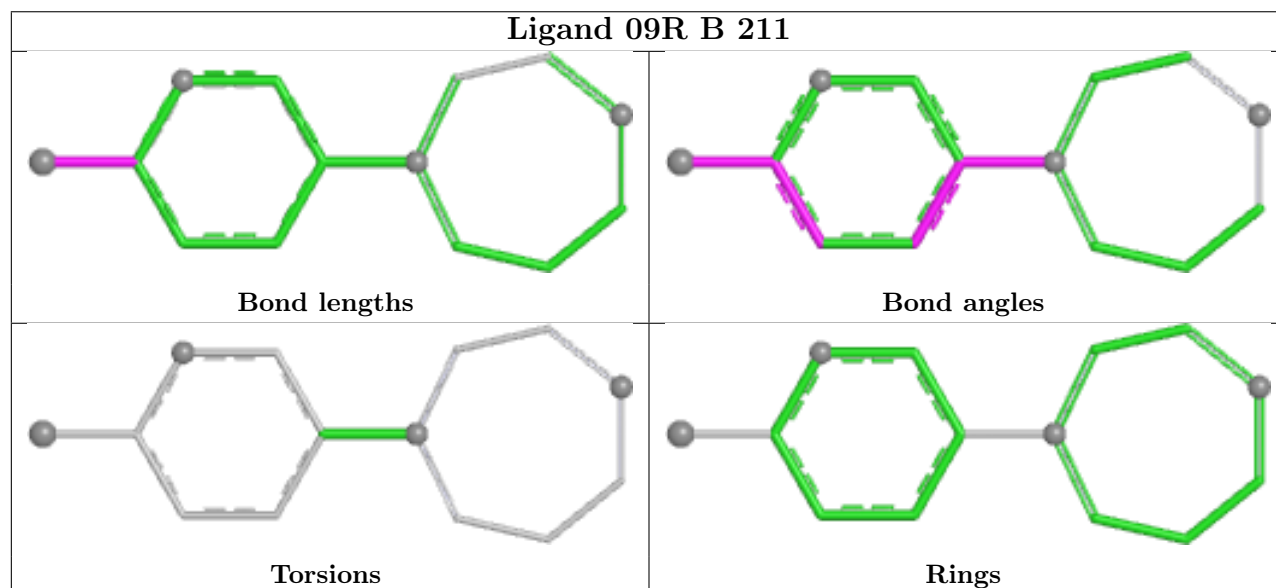
## Ligand 09R H 211



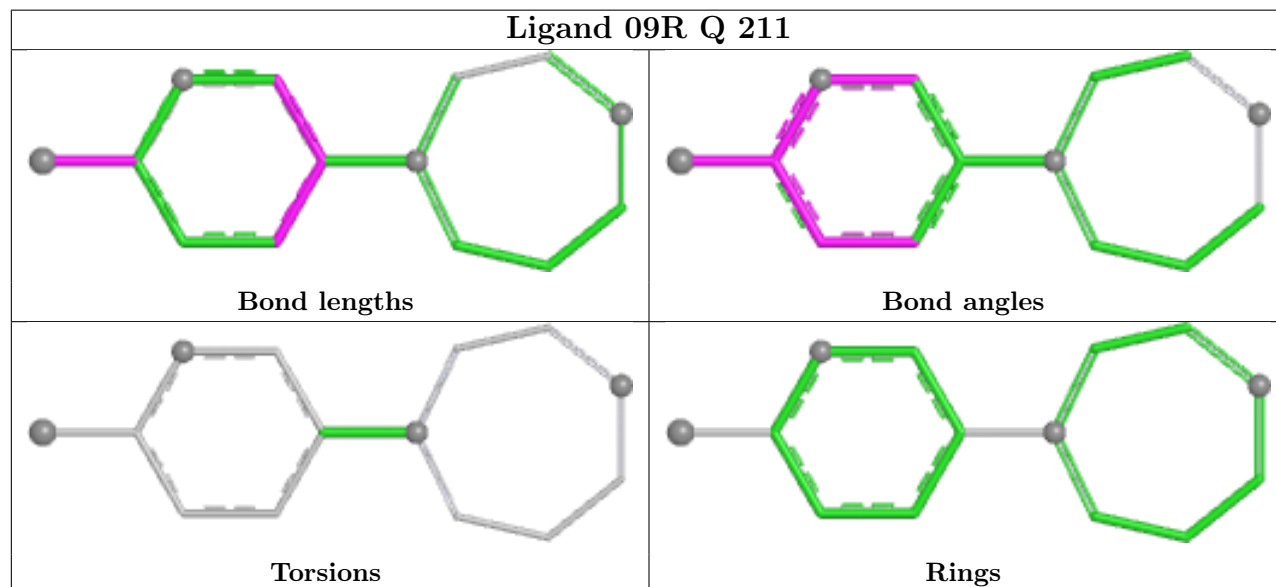
## Ligand 09R P 211



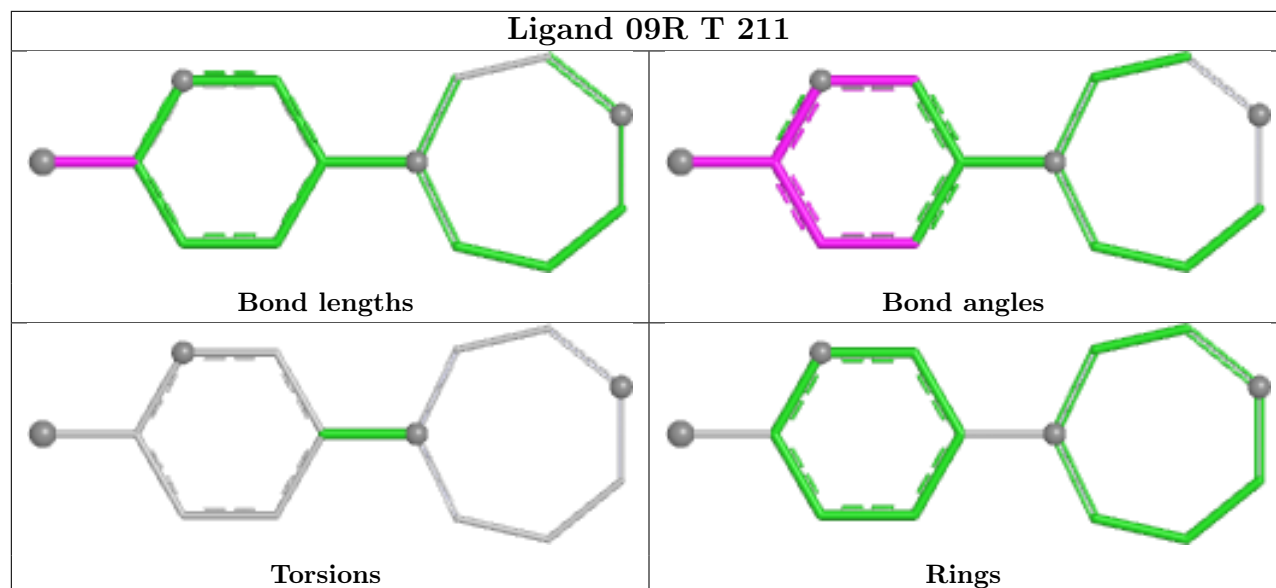
## Ligand 09R B 211



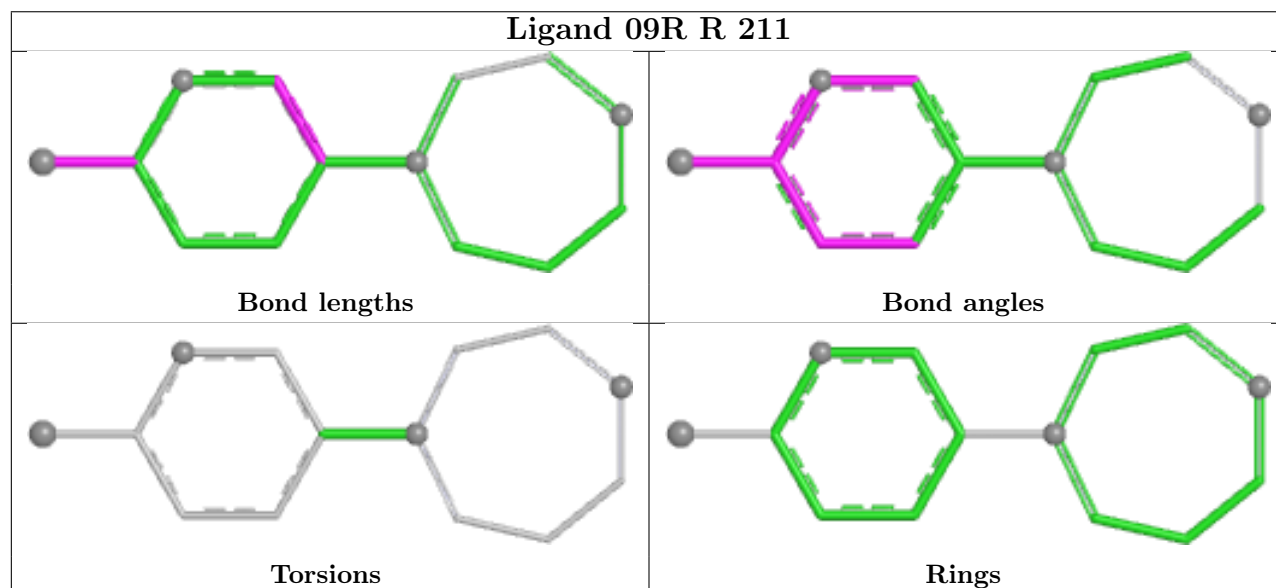
## Ligand 09R Q 211



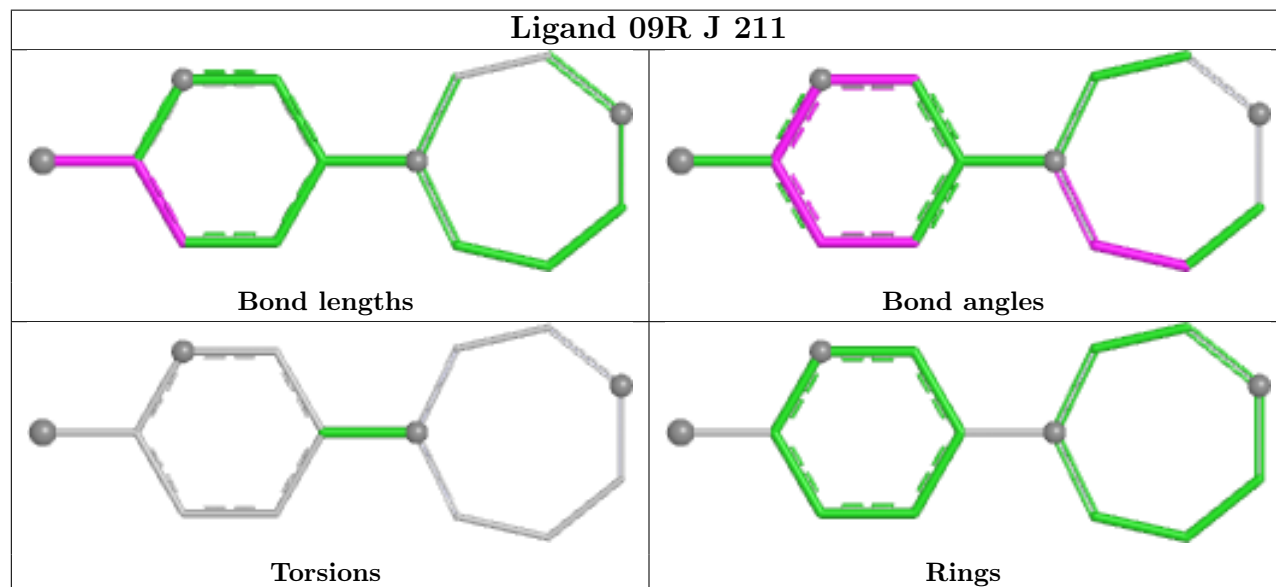
## Ligand 09R T 211



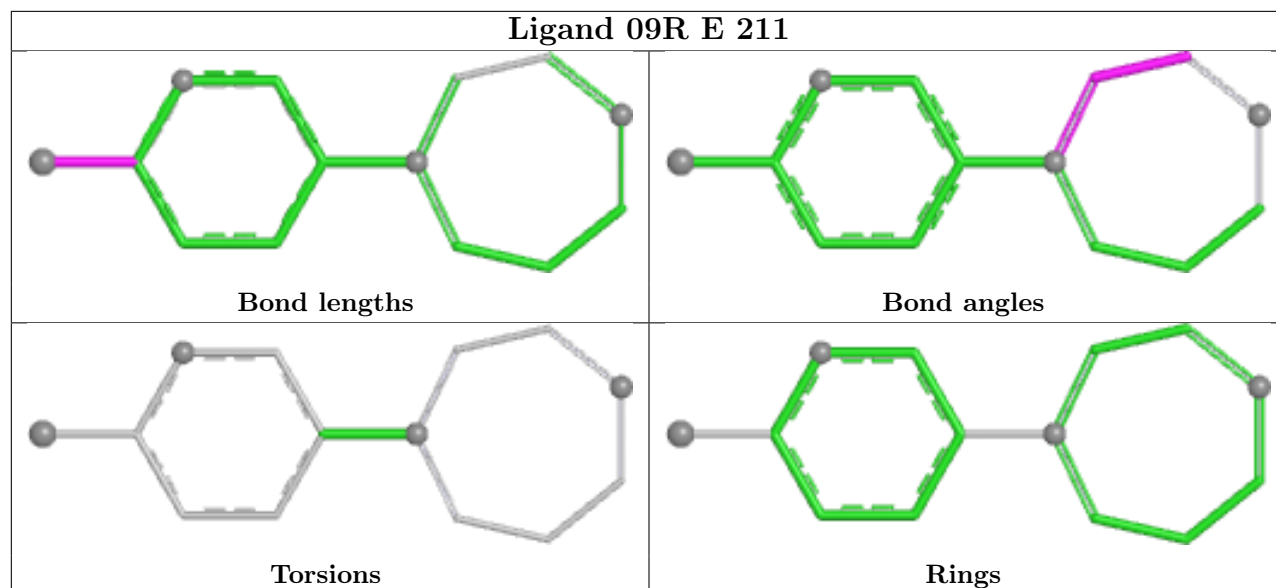
## Ligand 09R R 211



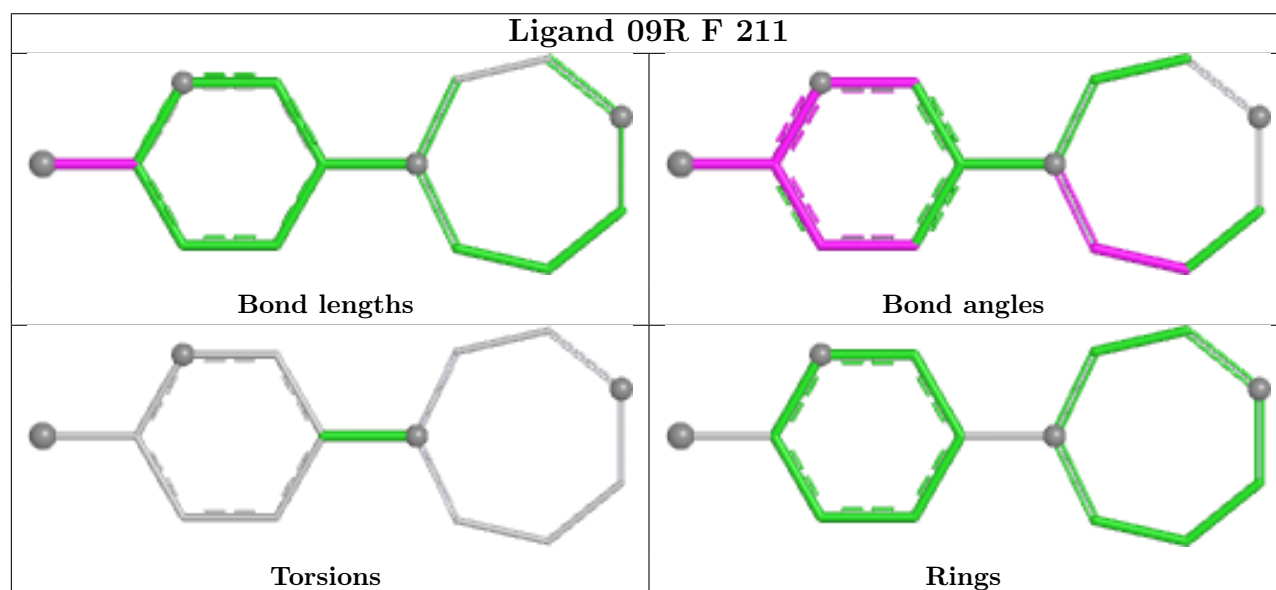
## Ligand 09R J 211



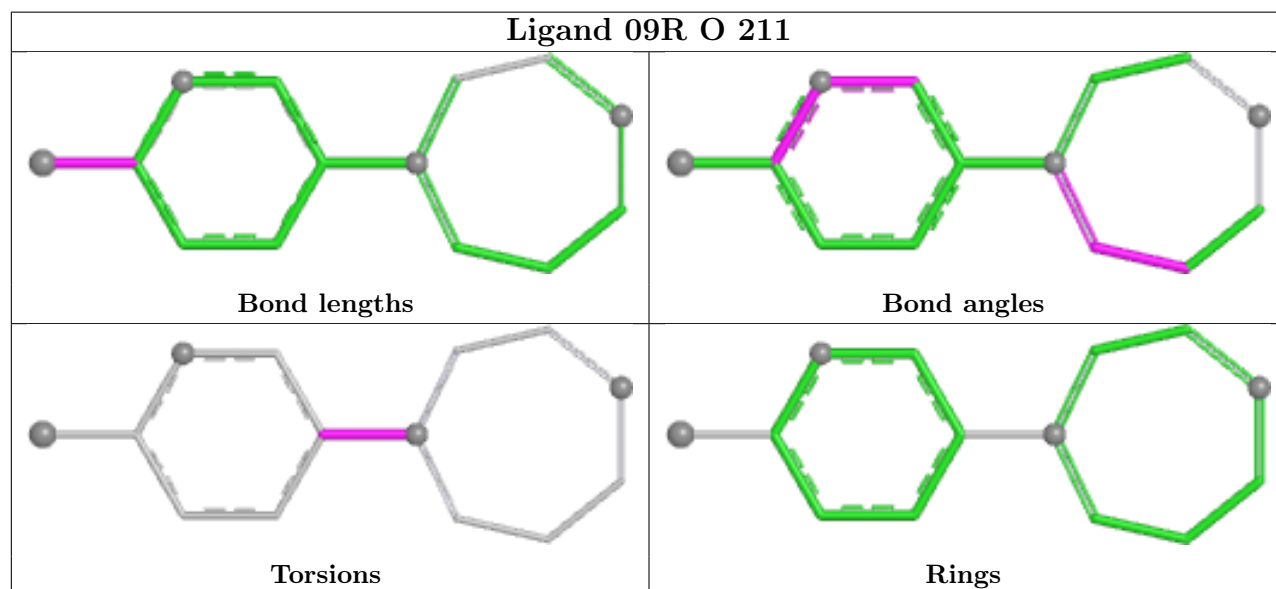
## Ligand 09R E 211

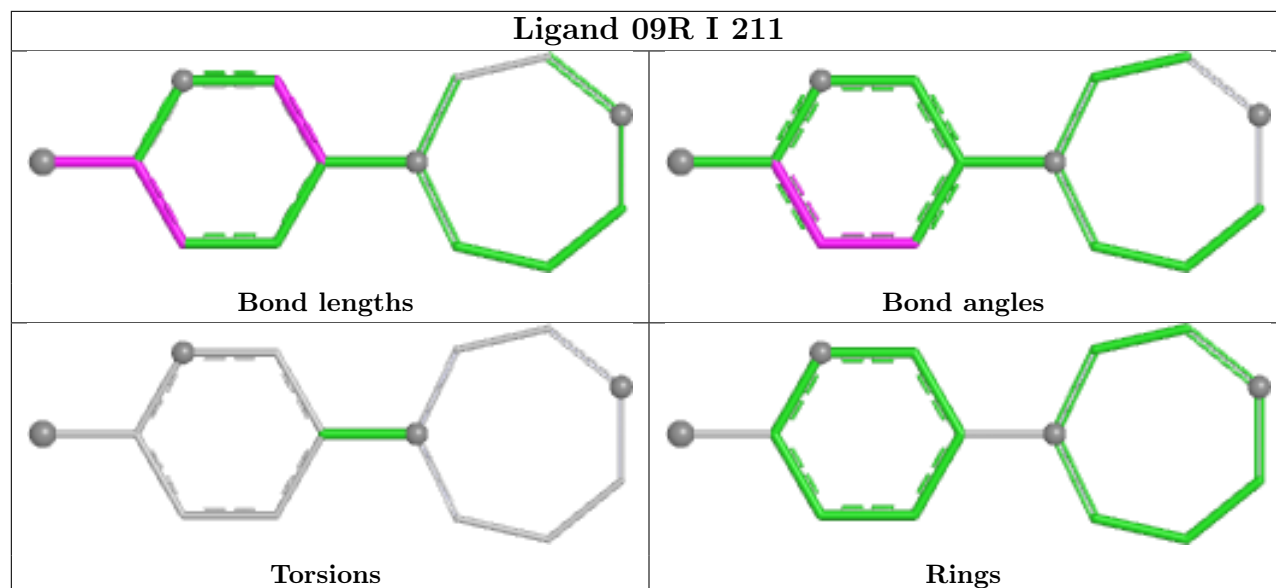


## Ligand 09R F 211



## Ligand 09R O 211





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 202/210 (96%)   | 0.08   | 7 (3%) 47 43  | 13, 27, 59, 76        | 1 (0%) |
| 1   | B     | 199/210 (94%)   | 0.08   | 5 (2%) 58 55  | 11, 27, 58, 88        | 0      |
| 1   | C     | 201/210 (95%)   | 0.09   | 5 (2%) 58 55  | 12, 27, 55, 77        | 0      |
| 1   | D     | 202/210 (96%)   | 0.07   | 7 (3%) 47 43  | 10, 27, 59, 78        | 1 (0%) |
| 1   | E     | 196/210 (93%)   | 0.05   | 3 (1%) 72 70  | 11, 26, 59, 79        | 1 (0%) |
| 1   | F     | 205/210 (97%)   | 0.13   | 8 (3%) 43 39  | 12, 28, 57, 78        | 0      |
| 1   | G     | 199/210 (94%)   | 0.12   | 4 (2%) 65 62  | 15, 28, 60, 88        | 0      |
| 1   | H     | 198/210 (94%)   | 0.14   | 2 (1%) 79 78  | 14, 28, 55, 90        | 0      |
| 1   | I     | 204/210 (97%)   | 0.07   | 3 (1%) 72 70  | 13, 29, 61, 85        | 0      |
| 1   | J     | 201/210 (95%)   | -0.05  | 3 (1%) 72 70  | 9, 29, 57, 84         | 0      |
| 1   | K     | 204/210 (97%)   | 0.13   | 3 (1%) 72 70  | 13, 28, 57, 77        | 0      |
| 1   | L     | 203/210 (96%)   | 0.08   | 6 (2%) 52 49  | 12, 27, 58, 91        | 0      |
| 1   | M     | 200/210 (95%)   | 0.16   | 7 (3%) 47 43  | 15, 27, 58, 78        | 1 (0%) |
| 1   | N     | 201/210 (95%)   | 0.13   | 3 (1%) 72 70  | 12, 28, 60, 77        | 1 (0%) |
| 1   | O     | 197/210 (93%)   | 0.20   | 6 (3%) 52 49  | 14, 29, 59, 78        | 0      |
| 1   | P     | 200/210 (95%)   | 0.13   | 4 (2%) 65 62  | 15, 28, 55, 77        | 0      |
| 1   | Q     | 199/210 (94%)   | 0.02   | 6 (3%) 52 49  | 14, 27, 56, 78        | 0      |
| 1   | R     | 199/210 (94%)   | 0.21   | 5 (2%) 58 55  | 14, 32, 60, 77        | 1 (0%) |
| 1   | S     | 200/210 (95%)   | 0.08   | 2 (1%) 79 78  | 16, 31, 60, 84        | 0      |
| 1   | T     | 200/210 (95%)   | 0.13   | 4 (2%) 65 62  | 15, 30, 57, 80        | 0      |
| All | All   | 4010/4200 (95%) | 0.10   | 93 (2%) 61 58 | 9, 28, 59, 91         | 6 (0%) |

All (93) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 14  | SER  | 4.3  |
| 1   | P     | 162 | SER  | 4.0  |
| 1   | G     | 162 | SER  | 3.9  |
| 1   | M     | 162 | SER  | 3.8  |
| 1   | F     | 24  | ASP  | 3.7  |
| 1   | D     | 67  | SER  | 3.4  |
| 1   | S     | 24  | ASP  | 3.4  |
| 1   | A     | 68  | SER  | 3.3  |
| 1   | T     | 186 | SER  | 3.3  |
| 1   | D     | 159 | SER  | 3.3  |
| 1   | F     | 68  | SER  | 3.2  |
| 1   | N     | 69  | HIS  | 3.1  |
| 1   | M     | 67  | SER  | 3.1  |
| 1   | L     | 161 | ASP  | 3.1  |
| 1   | M     | 161 | ASP  | 3.1  |
| 1   | C     | 68  | SER  | 3.0  |
| 1   | E     | 22  | GLN  | 2.9  |
| 1   | D     | 68  | SER  | 2.9  |
| 1   | B     | 162 | SER  | 2.9  |
| 1   | O     | 132 | SER  | 2.9  |
| 1   | Q     | 67  | SER  | 2.7  |
| 1   | R     | 162 | SER  | 2.7  |
| 1   | E     | 205 | GLY  | 2.6  |
| 1   | B     | 68  | SER  | 2.6  |
| 1   | C     | 162 | SER  | 2.6  |
| 1   | P     | 205 | GLY  | 2.6  |
| 1   | F     | 44  | ILE  | 2.5  |
| 1   | K     | 190 | GLU  | 2.5  |
| 1   | T     | 205 | GLY  | 2.5  |
| 1   | R     | 187 | CYS  | 2.5  |
| 1   | D     | 66  | ASN  | 2.5  |
| 1   | I     | 68  | SER  | 2.5  |
| 1   | O     | 68  | SER  | 2.5  |
| 1   | J     | 161 | ASP  | 2.5  |
| 1   | O     | 70  | SER  | 2.5  |
| 1   | P     | 155 | THR  | 2.5  |
| 1   | F     | 14  | SER  | 2.5  |
| 1   | T     | 162 | SER  | 2.5  |
| 1   | M     | 69  | HIS  | 2.5  |
| 1   | I     | 162 | SER  | 2.4  |
| 1   | N     | 24  | ASP  | 2.4  |
| 1   | J     | 23  | ARG  | 2.4  |
| 1   | R     | 178 | GLN  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 69  | HIS  | 2.4  |
| 1   | D     | 161 | ASP  | 2.3  |
| 1   | M     | 68  | SER  | 2.3  |
| 1   | F     | 187 | CYS  | 2.3  |
| 1   | D     | 69  | HIS  | 2.3  |
| 1   | L     | 162 | SER  | 2.3  |
| 1   | O     | 23  | ARG  | 2.3  |
| 1   | I     | 161 | ASP  | 2.3  |
| 1   | L     | 68  | SER  | 2.3  |
| 1   | A     | 69  | HIS  | 2.3  |
| 1   | A     | 24  | ASP  | 2.3  |
| 1   | B     | 67  | SER  | 2.3  |
| 1   | Q     | 162 | SER  | 2.2  |
| 1   | M     | 164 | TYR  | 2.2  |
| 1   | O     | 61  | ARG  | 2.2  |
| 1   | R     | 68  | SER  | 2.2  |
| 1   | Q     | 61  | ARG  | 2.2  |
| 1   | A     | 164 | TYR  | 2.2  |
| 1   | B     | 205 | GLY  | 2.2  |
| 1   | K     | 112 | LEU  | 2.2  |
| 1   | N     | 18  | VAL  | 2.2  |
| 1   | G     | 70  | SER  | 2.2  |
| 1   | K     | 69  | HIS  | 2.2  |
| 1   | Q     | 69  | HIS  | 2.2  |
| 1   | C     | 163 | GLU  | 2.1  |
| 1   | B     | 24  | ASP  | 2.1  |
| 1   | F     | 161 | ASP  | 2.1  |
| 1   | E     | 69  | HIS  | 2.1  |
| 1   | G     | 72  | ASP  | 2.1  |
| 1   | A     | 70  | SER  | 2.1  |
| 1   | Q     | 186 | SER  | 2.1  |
| 1   | S     | 59  | SER  | 2.1  |
| 1   | J     | 24  | ASP  | 2.1  |
| 1   | A     | 23  | ARG  | 2.1  |
| 1   | F     | 23  | ARG  | 2.1  |
| 1   | P     | 178 | GLN  | 2.1  |
| 1   | C     | 17  | ASP  | 2.0  |
| 1   | G     | 24  | ASP  | 2.0  |
| 1   | C     | 4   | ALA  | 2.0  |
| 1   | Q     | 205 | GLY  | 2.0  |
| 1   | M     | 25  | ARG  | 2.0  |
| 1   | L     | 24  | ASP  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 186 | SER  | 2.0  |
| 1   | H     | 70  | SER  | 2.0  |
| 1   | O     | 32  | SER  | 2.0  |
| 1   | T     | 155 | THR  | 2.0  |
| 1   | A     | 178 | GLN  | 2.0  |
| 1   | R     | 69  | HIS  | 2.0  |
| 1   | D     | 25  | ARG  | 2.0  |
| 1   | L     | 23  | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | SO4  | F     | 212 | 5/5   | 0.66 | 0.18 | 92,102,113,117             | 0     |
| 3   | SO4  | I     | 212 | 5/5   | 0.68 | 0.16 | 82,83,103,104              | 0     |
| 3   | SO4  | T     | 212 | 5/5   | 0.68 | 0.15 | 76,88,101,104              | 0     |
| 3   | SO4  | F     | 213 | 5/5   | 0.70 | 0.16 | 88,89,95,98                | 0     |
| 3   | SO4  | B     | 212 | 5/5   | 0.73 | 0.15 | 74,93,106,113              | 0     |
| 3   | SO4  | K     | 212 | 5/5   | 0.75 | 0.15 | 65,74,91,94                | 0     |
| 3   | SO4  | N     | 212 | 5/5   | 0.78 | 0.14 | 78,79,84,86                | 0     |
| 3   | SO4  | J     | 212 | 5/5   | 0.78 | 0.18 | 73,92,103,106              | 0     |
| 3   | SO4  | L     | 213 | 5/5   | 0.79 | 0.18 | 28,88,91,101               | 0     |
| 3   | SO4  | D     | 213 | 5/5   | 0.80 | 0.13 | 79,80,87,96                | 0     |
| 3   | SO4  | B     | 213 | 5/5   | 0.81 | 0.17 | 116,120,128,135            | 0     |
| 3   | SO4  | D     | 212 | 5/5   | 0.82 | 0.19 | 40,57,93,102               | 0     |
| 3   | SO4  | A     | 212 | 5/5   | 0.82 | 0.14 | 50,82,89,92                | 0     |
| 3   | SO4  | L     | 212 | 5/5   | 0.90 | 0.12 | 55,69,83,85                | 0     |
| 3   | SO4  | H     | 212 | 5/5   | 0.90 | 0.09 | 37,63,73,91                | 0     |

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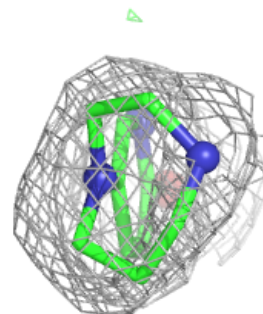
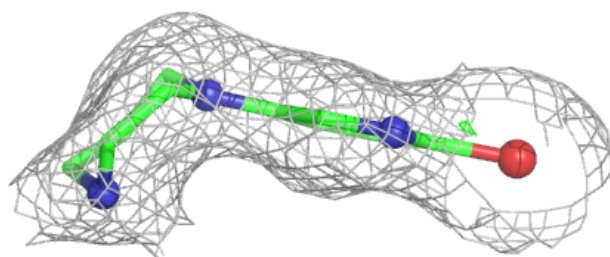
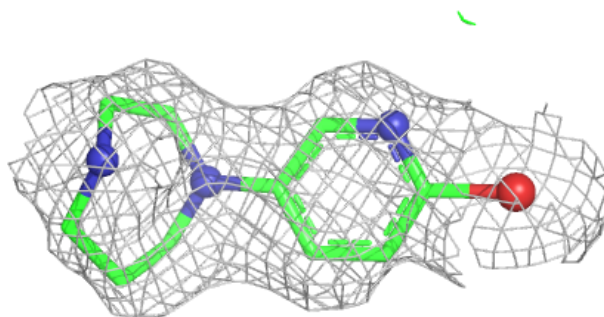
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | SO4  | D     | 214 | 5/5   | 0.91 | 0.12 | 52,55,63,64                 | 0     |
| 3   | SO4  | R     | 212 | 5/5   | 0.93 | 0.10 | 33,43,46,46                 | 0     |
| 2   | 09R  | S     | 211 | 14/14 | 0.98 | 0.07 | 4,35,49,49                  | 0     |
| 2   | 09R  | F     | 211 | 14/14 | 0.98 | 0.07 | 5,24,32,39                  | 0     |
| 2   | 09R  | T     | 211 | 14/14 | 0.99 | 0.05 | 7,25,41,45                  | 0     |
| 2   | 09R  | C     | 211 | 14/14 | 0.99 | 0.05 | 0,14,34,42                  | 0     |
| 2   | 09R  | D     | 211 | 14/14 | 0.99 | 0.05 | 0,19,30,31                  | 0     |
| 2   | 09R  | E     | 211 | 14/14 | 0.99 | 0.07 | 4,22,45,58                  | 0     |
| 2   | 09R  | A     | 211 | 14/14 | 0.99 | 0.07 | 0,11,50,51                  | 0     |
| 2   | 09R  | G     | 211 | 14/14 | 0.99 | 0.07 | 0,18,37,39                  | 0     |
| 2   | 09R  | H     | 211 | 14/14 | 0.99 | 0.06 | 3,13,39,45                  | 0     |
| 2   | 09R  | I     | 211 | 14/14 | 0.99 | 0.05 | 9,22,36,39                  | 0     |
| 2   | 09R  | J     | 211 | 14/14 | 0.99 | 0.06 | 0,20,46,63                  | 0     |
| 2   | 09R  | K     | 211 | 14/14 | 0.99 | 0.07 | 4,17,31,36                  | 0     |
| 2   | 09R  | L     | 211 | 14/14 | 0.99 | 0.07 | 0,23,42,49                  | 0     |
| 2   | 09R  | M     | 211 | 14/14 | 0.99 | 0.06 | 1,16,35,35                  | 0     |
| 2   | 09R  | N     | 211 | 14/14 | 0.99 | 0.07 | 9,19,51,52                  | 0     |
| 2   | 09R  | O     | 211 | 14/14 | 0.99 | 0.07 | 6,25,35,47                  | 0     |
| 2   | 09R  | P     | 211 | 14/14 | 0.99 | 0.07 | 0,23,57,74                  | 0     |
| 2   | 09R  | Q     | 211 | 14/14 | 0.99 | 0.07 | 2,18,35,40                  | 0     |
| 2   | 09R  | R     | 211 | 14/14 | 0.99 | 0.06 | 7,23,45,53                  | 0     |
| 2   | 09R  | B     | 211 | 14/14 | 0.99 | 0.05 | 0,11,34,40                  | 0     |

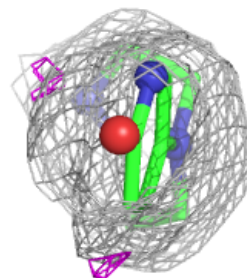
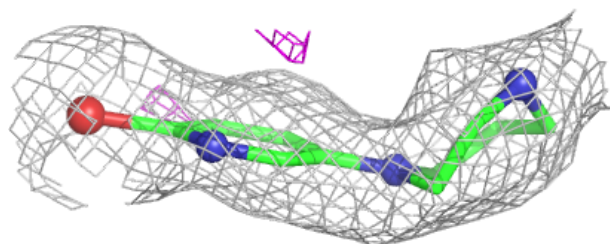
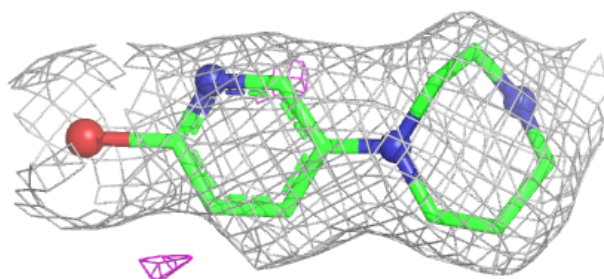
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 09R S 211:**

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

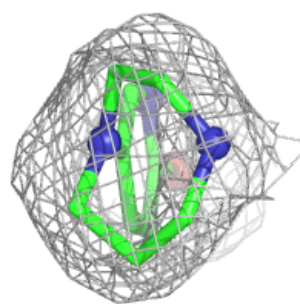
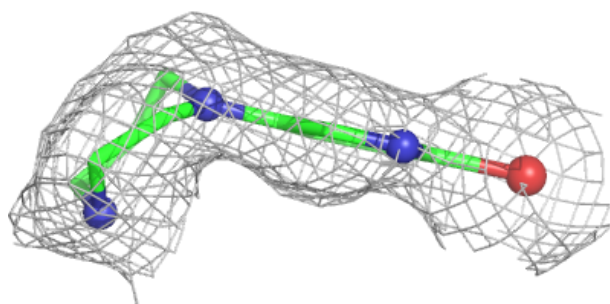
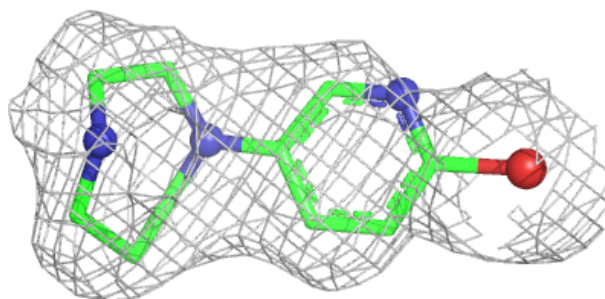
**Electron density around 09R F 211:**

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

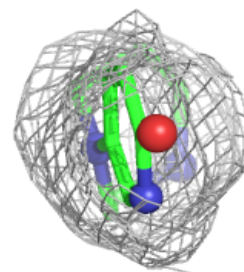
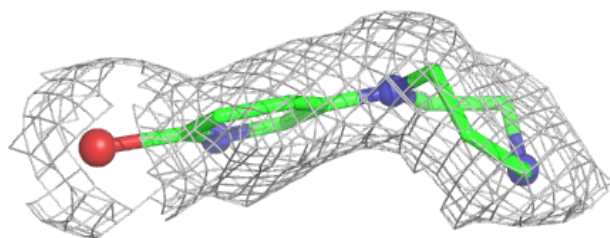
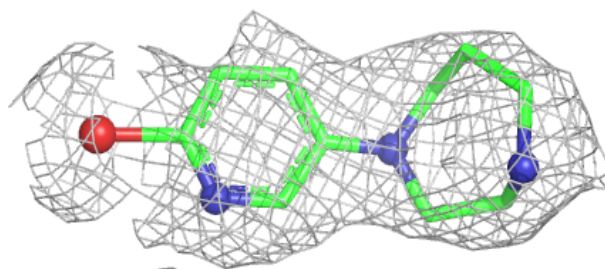


**Electron density around 09R T 211:**

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

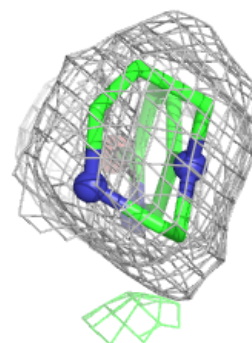
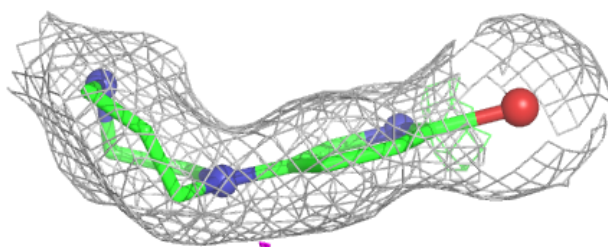
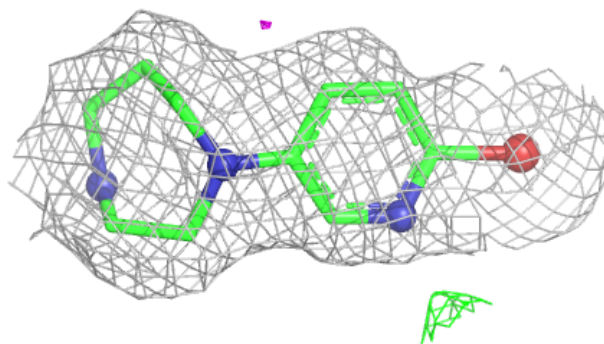
**Electron density around 09R C 211:**

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

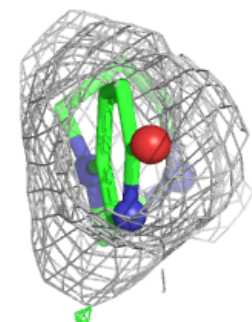
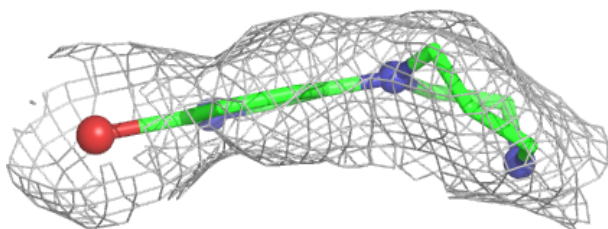
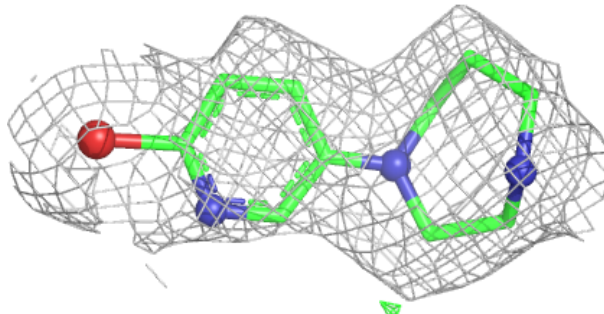


**Electron density around 09R D 211:**

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

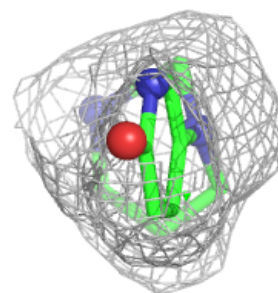
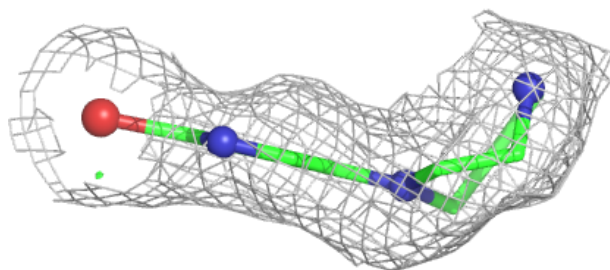
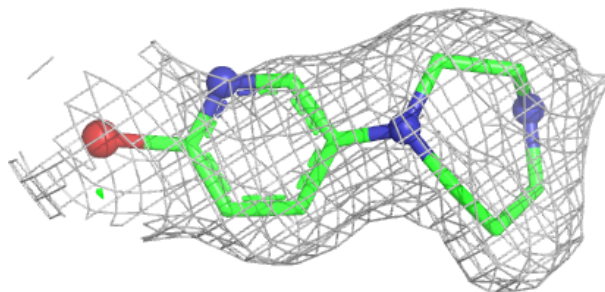
**Electron density around 09R E 211:**

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

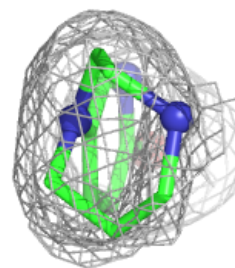
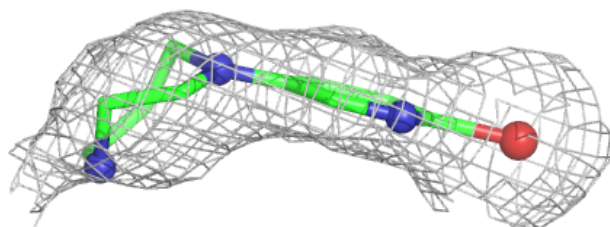
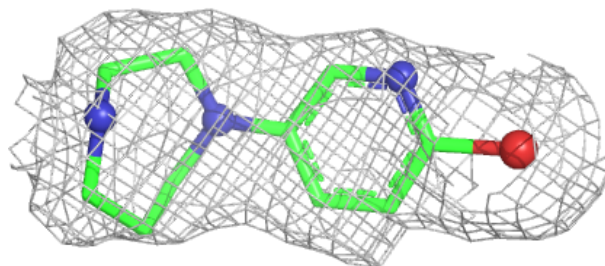


**Electron density around 09R A 211:**

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

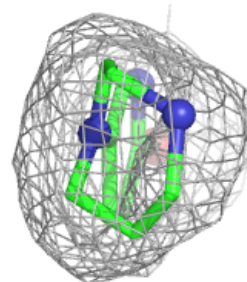
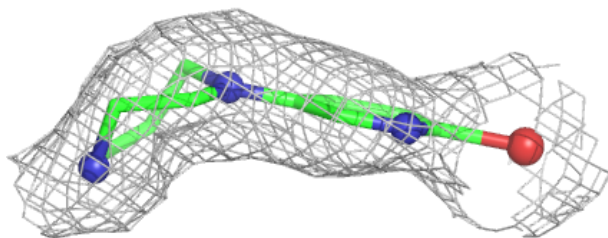
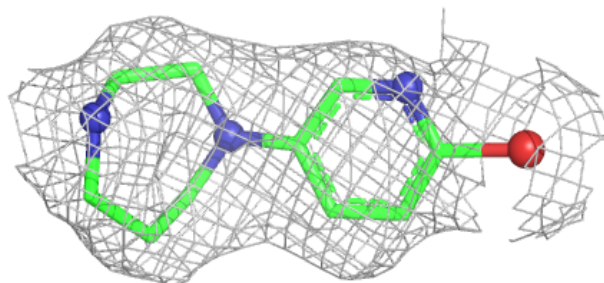
**Electron density around 09R G 211:**

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

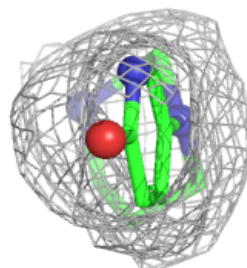
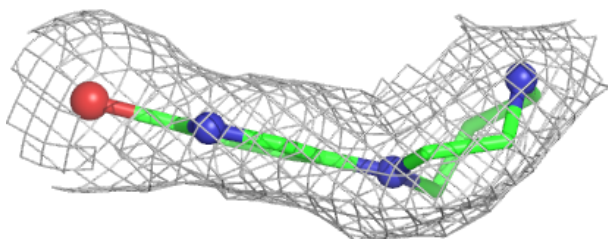
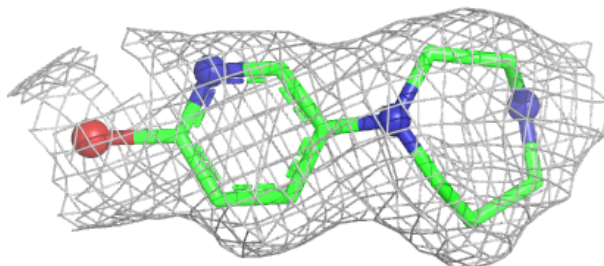


**Electron density around 09R H 211:**

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

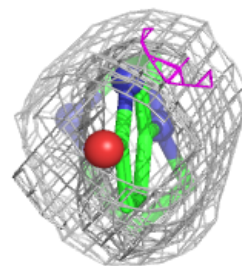
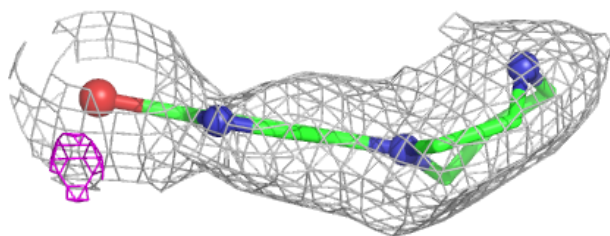
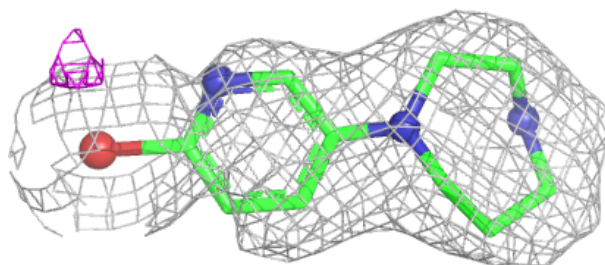
**Electron density around 09R I 211:**

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

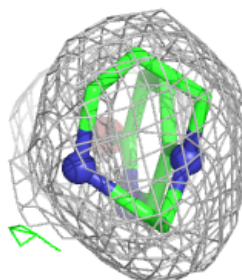
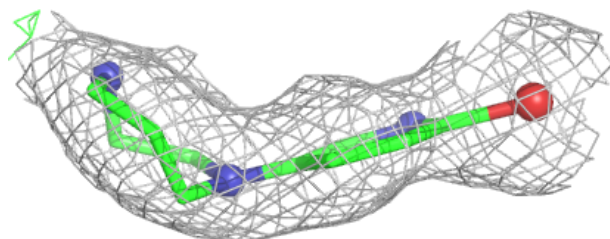
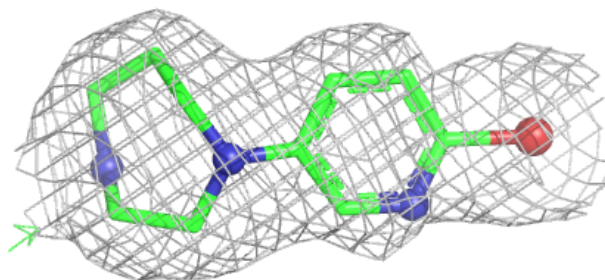


**Electron density around 09R J 211:**

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

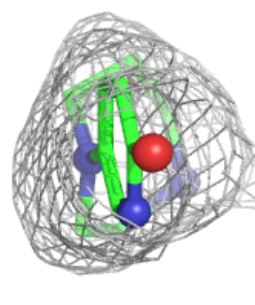
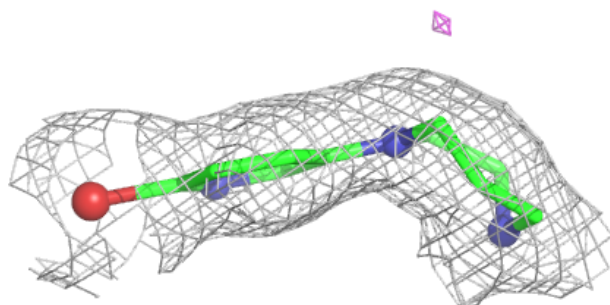
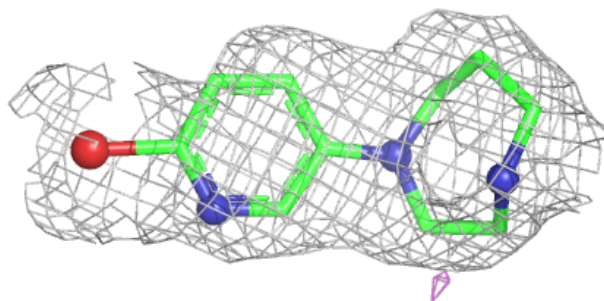
**Electron density around 09R K 211:**

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

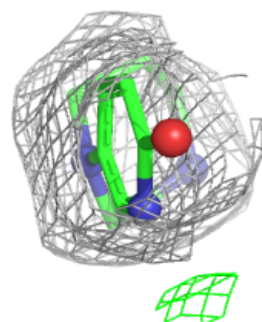
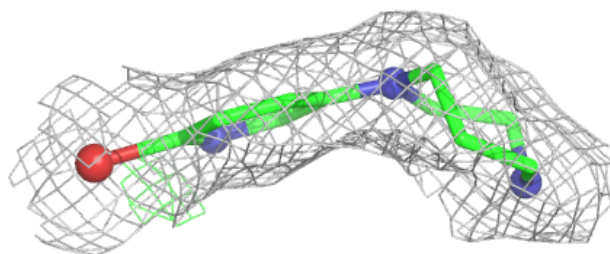
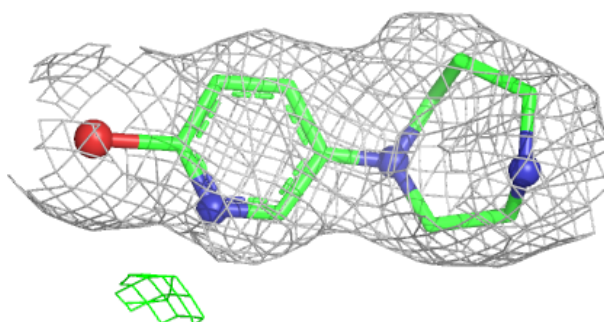


**Electron density around 09R L 211:**

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

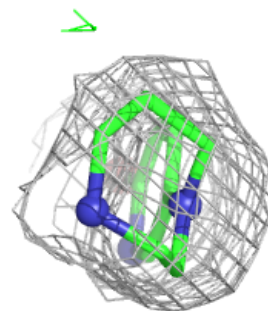
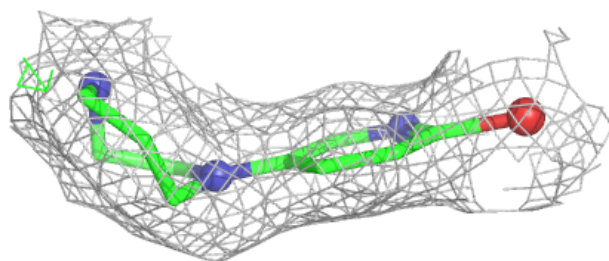
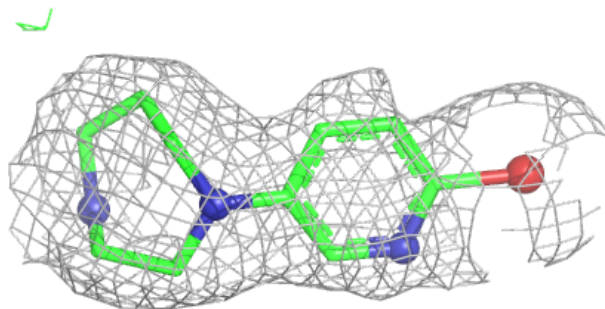
**Electron density around 09R M 211:**

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

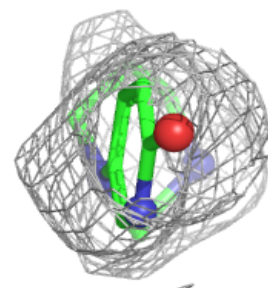
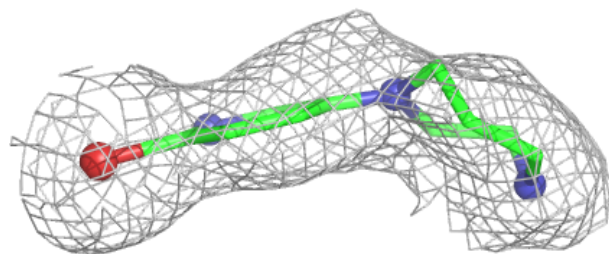
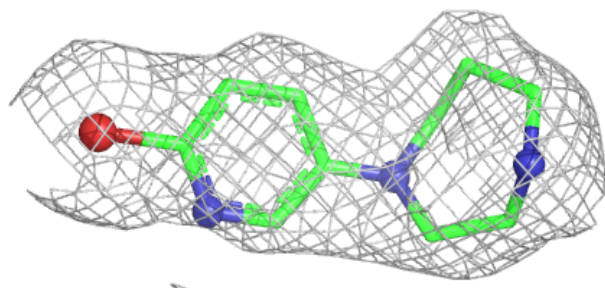


**Electron density around 09R N 211:**

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

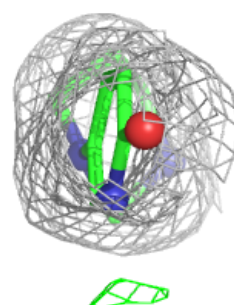
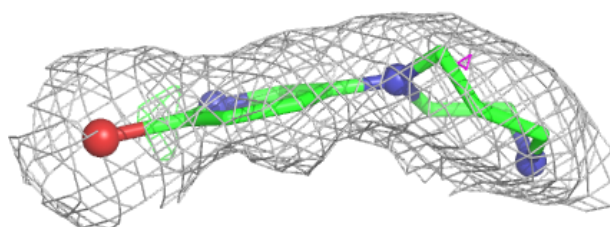
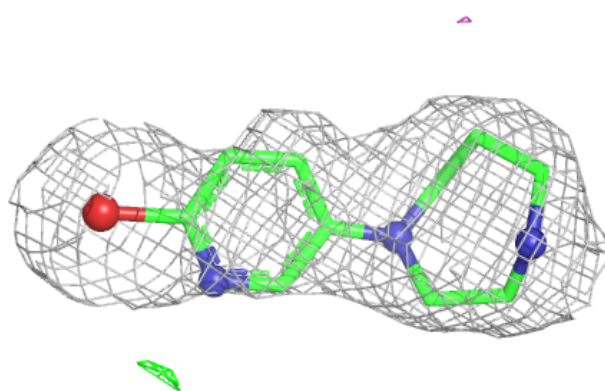
**Electron density around 09R O 211:**

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

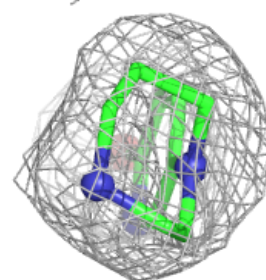
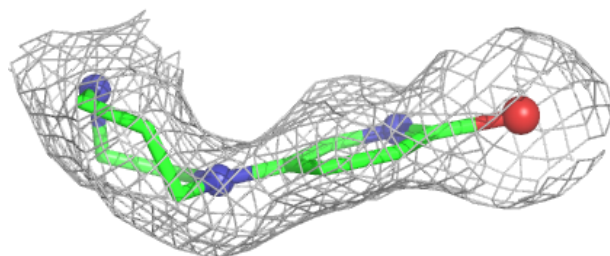
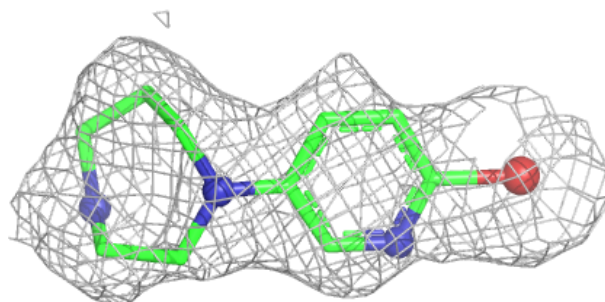


**Electron density around 09R P 211:**

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

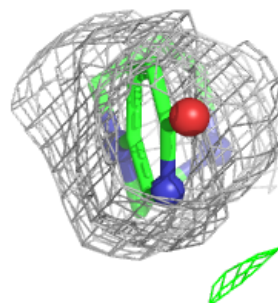
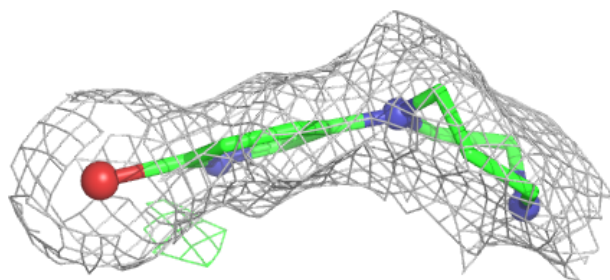
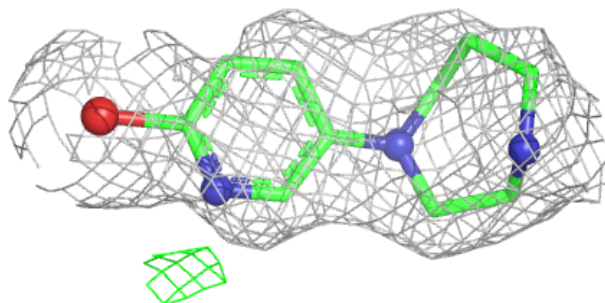
**Electron density around 09R Q 211:**

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

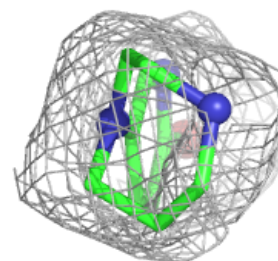
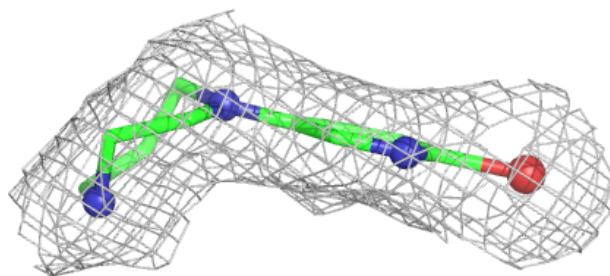
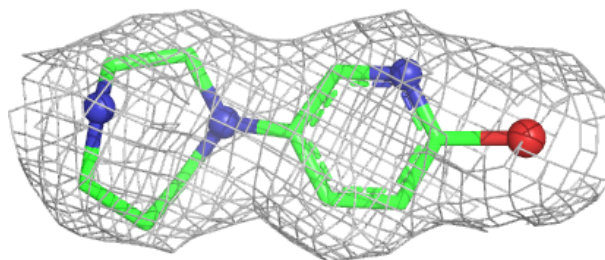


**Electron density around 09R R 211:**

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

**Electron density around 09R B 211:**

$2mF_o-DF_c$  (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.