



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:01 PM UTC

PDB ID : 3L70 / pdb\_00003L70  
Title : Cytochrome BC1 complex from chicken with trifloxystrobin bound  
Authors : Huang, L.; Berry, E.A.  
Deposited on : 2009-12-27  
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

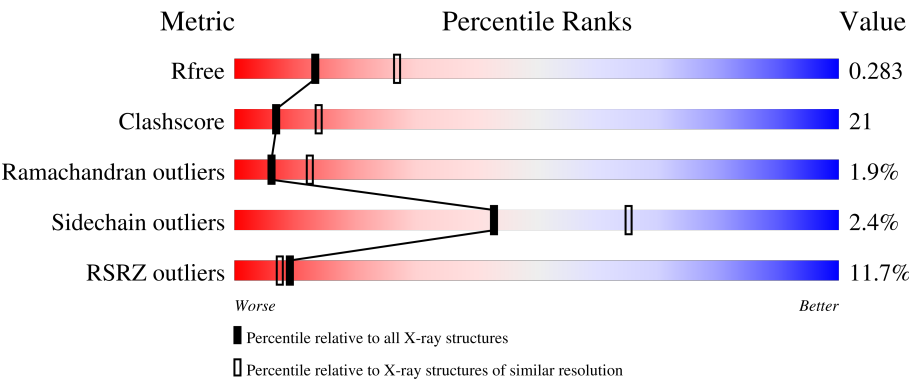
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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                      | 1009 (2.76-2.76)                                      |
| Clashscore            | 190562                      | 1044 (2.76-2.76)                                      |
| Ramachandran outliers | 187476                      | 1024 (2.76-2.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (2.76-2.76)                                      |
| RSRZ outliers         | 180081                      | 1009 (2.76-2.76)                                      |

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     | 446    |                  |
| 1   | N     | 446    |                  |
| 2   | B     | 441    |                  |
| 2   | O     | 441    |                  |
| 3   | C     | 380    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | P     | 380    |                  |
| 4   | D     | 241    |                  |
| 4   | Q     | 241    |                  |
| 5   | E     | 196    |                  |
| 5   | R     | 196    |                  |
| 6   | F     | 110    |                  |
| 6   | S     | 110    |                  |
| 7   | G     | 81     |                  |
| 7   | T     | 81     |                  |
| 8   | H     | 77     |                  |
| 8   | U     | 77     |                  |
| 9   | I     | 47     |                  |
| 9   | V     | 47     |                  |
| 10  | J     | 61     |                  |
| 10  | W     | 61     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 11  | PEE  | N     | 3008 | -         | X        | -       | -                |
| 18  | BOG  | D     | 2091 | -         | -        | -       | X                |
| 19  | FES  | E     | 501  | -         | -        | X       | -                |
| 19  | FES  | R     | 501  | -         | -        | X       | -                |

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32653 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 444      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3447  | 2160 | 607 | 659 | 21 |         |         |       |
| 1   | N     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3437  | 2154 | 605 | 657 | 21 |         |         |       |

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3133  | 1968 | 544 | 612 | 9  |         |         |       |
| 2   | O     | 422      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3147  | 1977 | 546 | 614 | 10 |         |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 380      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 2022 | 478 | 505 | 12 |         |         |       |
| 3   | P     | 379      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3012  | 2019 | 477 | 504 | 12 |         |         |       |

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1898  | 1212 | 327 | 347 | 12 |         |         |       |
| 4   | Q     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1898  | 1212 | 327 | 347 | 12 |         |         |       |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1513  | 952 | 263 | 292 | 6 |         |         |       |
| 5   | R     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1509  | 950 | 263 | 290 | 6 |         |         |       |

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 570 | 159 | 159 | 3 |         |         |       |
| 6   | S     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 570 | 159 | 159 | 3 |         |         |       |

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 7   | G     | 80       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 672   | 437 | 119 | 116 |         |         |       |
| 7   | T     | 79       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 662   | 432 | 117 | 113 |         |         |       |

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 574   | 350 | 105 | 114 | 5 |         |         |       |
| 8   | U     | 67       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 553   | 338 | 103 | 107 | 5 |         |         |       |

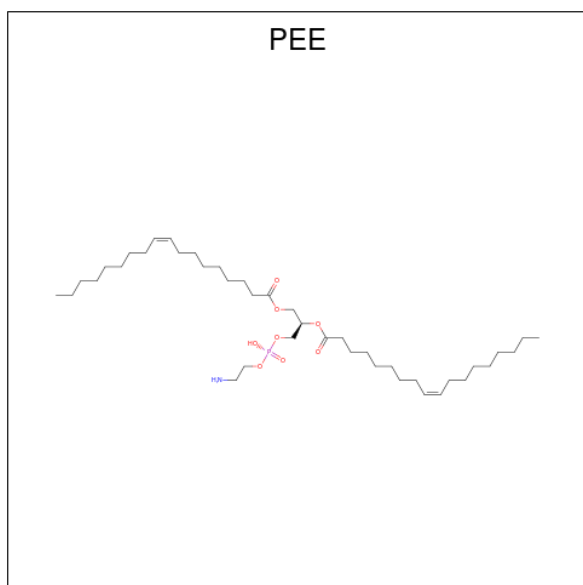
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | I     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 287   | 171 | 58 | 56 | 2 |         |         |       |
| 9   | V     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 277   | 167 | 55 | 53 | 2 |         |         |       |

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

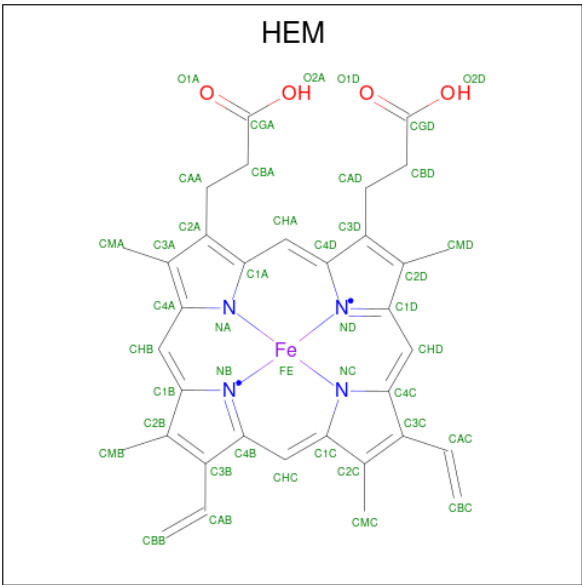
| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | J     | 61       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 497   | 321 | 87 | 89 |         |         |       |
| 10  | W     | 60       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 479   | 311 | 86 | 82 |         |         |       |

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



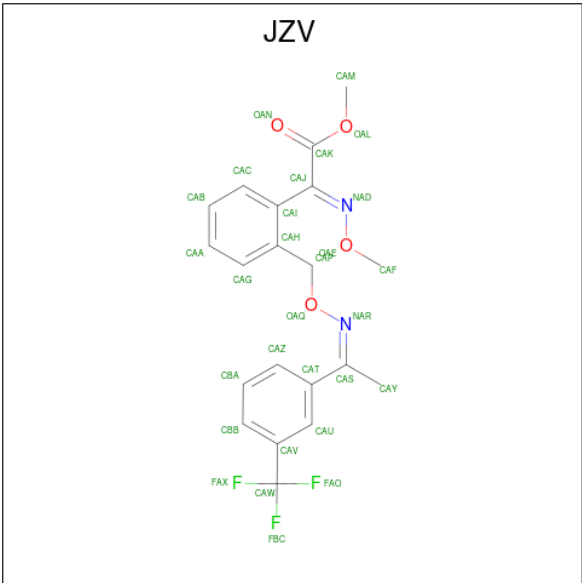
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 11  | A     | 1        | Total | C  | O | P |   | 0       | 0       |
|     |       |          | 21    | 12 | 8 | 1 |   |         |         |
| 11  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 11  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |         |
| 11  | N     | 1        | Total | O  | P |   |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |   |         |         |
| 11  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 11  | R     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |         |

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



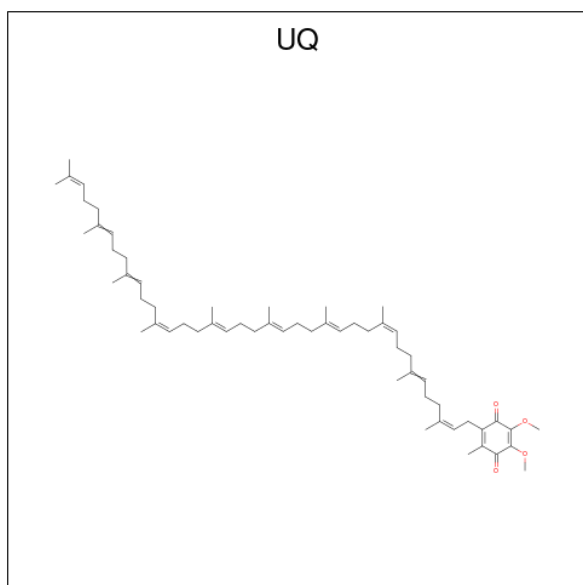
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 12  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 12  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 12  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 12  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 13 is methyl (2E)-(methoxyimino)(2-[[[(1Z)-1-[3-(trifluoromethyl)phenyl]ethylidene}amino)oxy]methyl]phenyl)ethanoate (CCD ID: JZV) (formula: C<sub>20</sub>H<sub>19</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>).



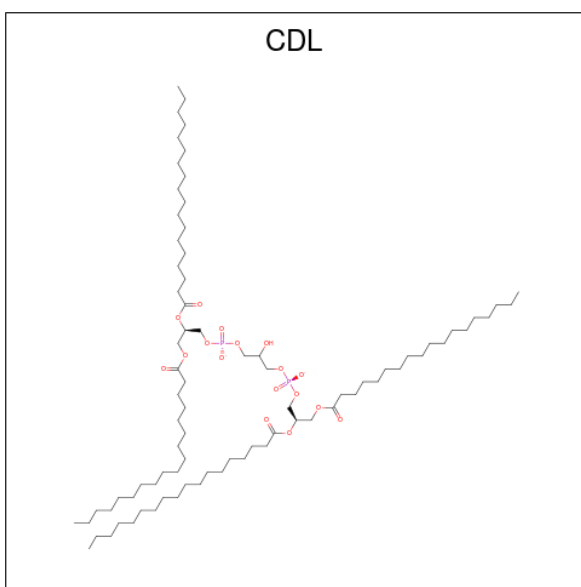
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 13  | C     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 29    | 20 | 3 | 2 | 4 |         |         |
| 13  | P     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 29    | 20 | 3 | 2 | 4 |         |         |

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



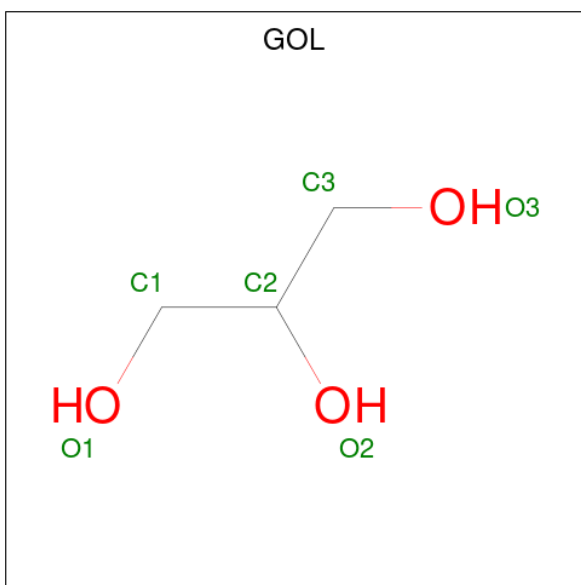
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 14  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 19    | 15 | 4 |         |         |
| 14  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 19    | 15 | 4 |         |         |

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



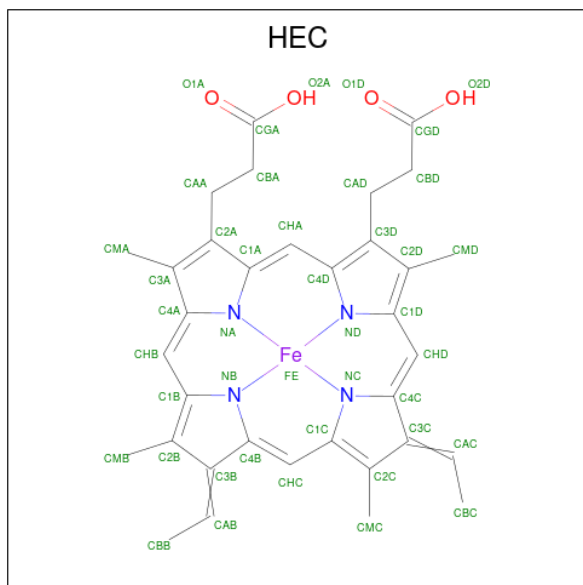
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 15  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 21 | 17 | 2 |         |         |
| 15  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 42    | 23 | 17 | 2 |         |         |
| 15  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 21 | 17 | 2 |         |         |
| 15  | Q     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 42    | 23 | 17 | 2 |         |         |

- Molecule 16 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



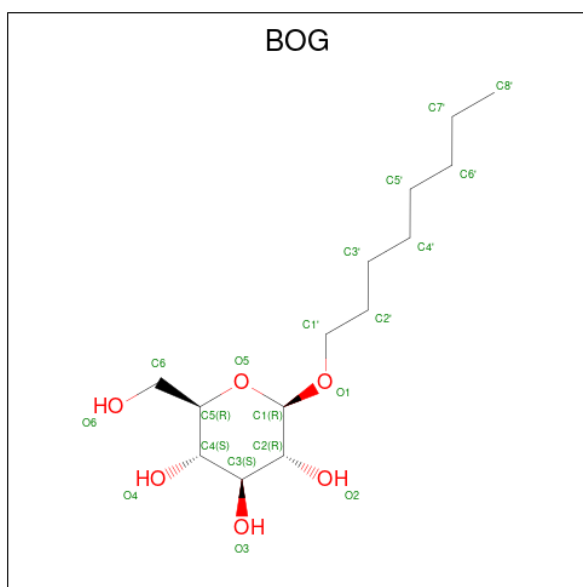
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 16  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 16  | P     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 17 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



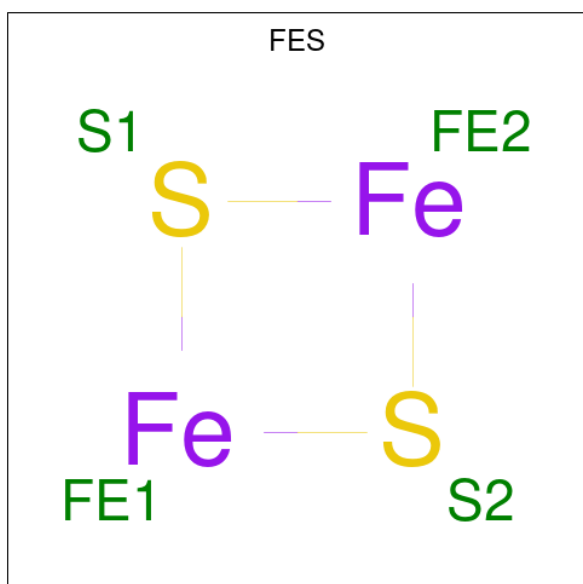
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 17  | D     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |
| 17  | Q     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |

- Molecule 18 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula:  $C_{14}H_{28}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 18  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 13    | 7  | 6 |         |         |
| 18  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 12    | 6  | 6 |         |         |
| 18  | Q     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 18  | Q     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 13    | 7  | 6 |         |         |

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 19  | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 19  | R     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 20 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 20  | C     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |
| 20  | E     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 20  | P     | 9        | Total | O | 0       | 0       |
|     |       |          | 9     | 9 |         |         |
| 20  | R     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

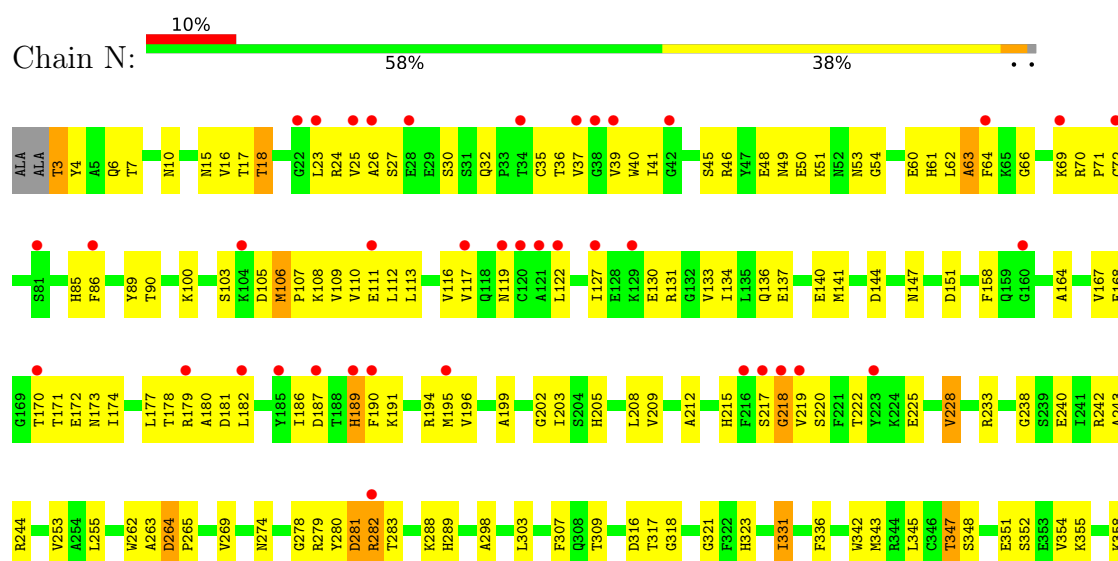
### 3 Residue-property plots

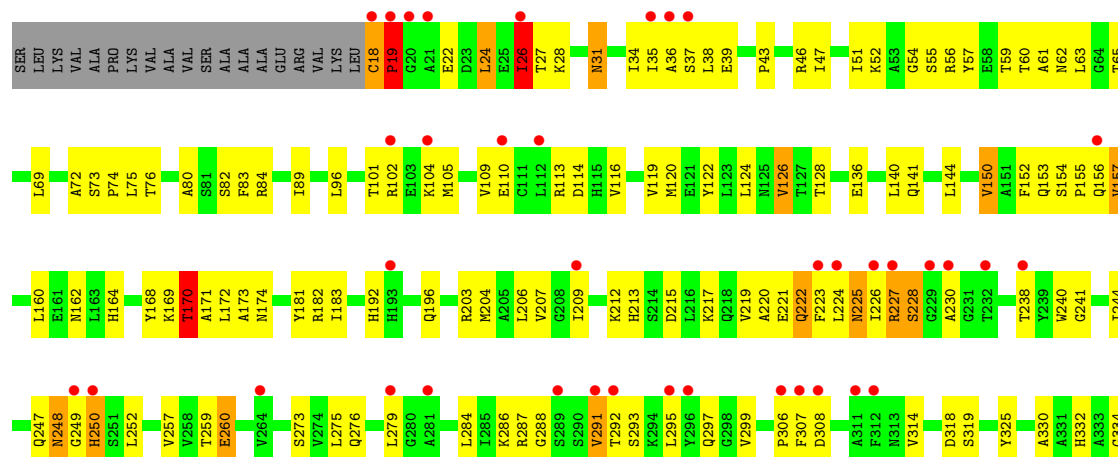
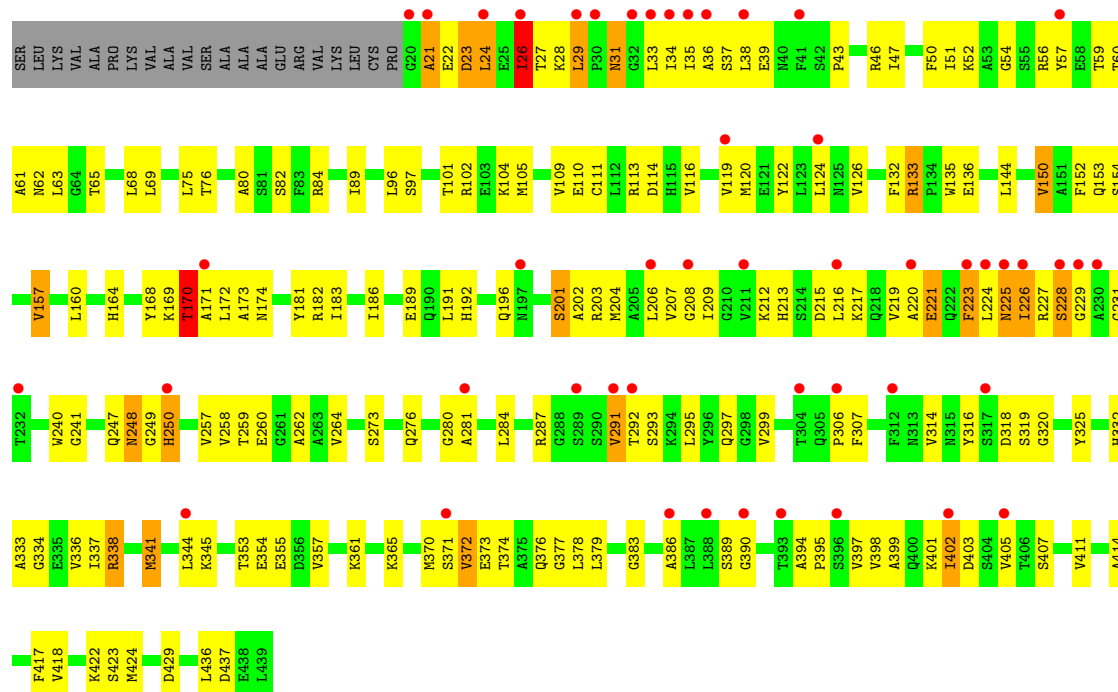
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

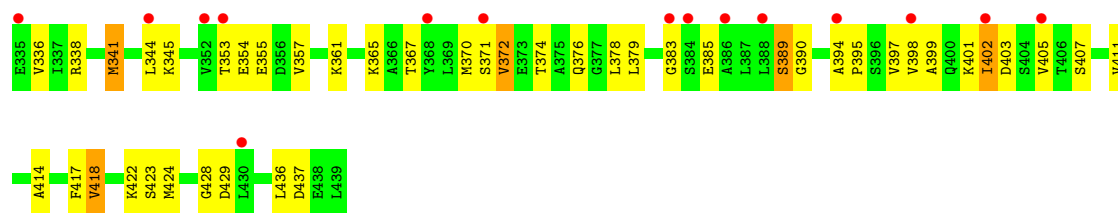
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



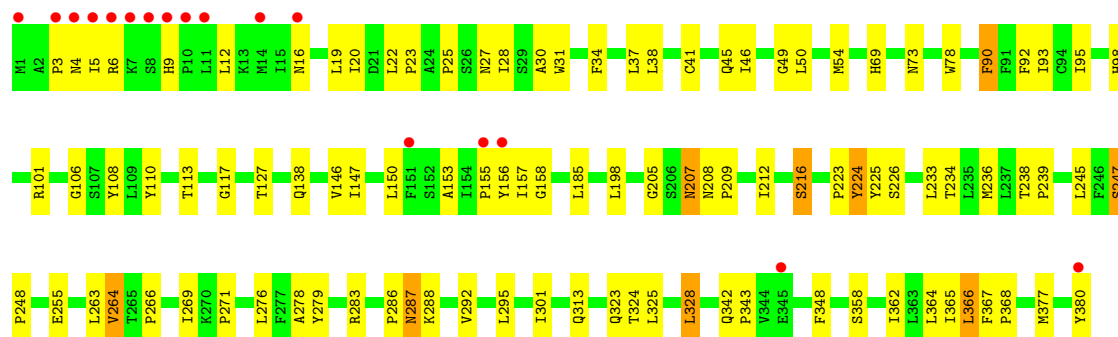
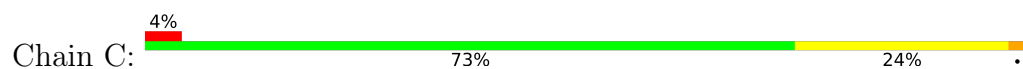
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



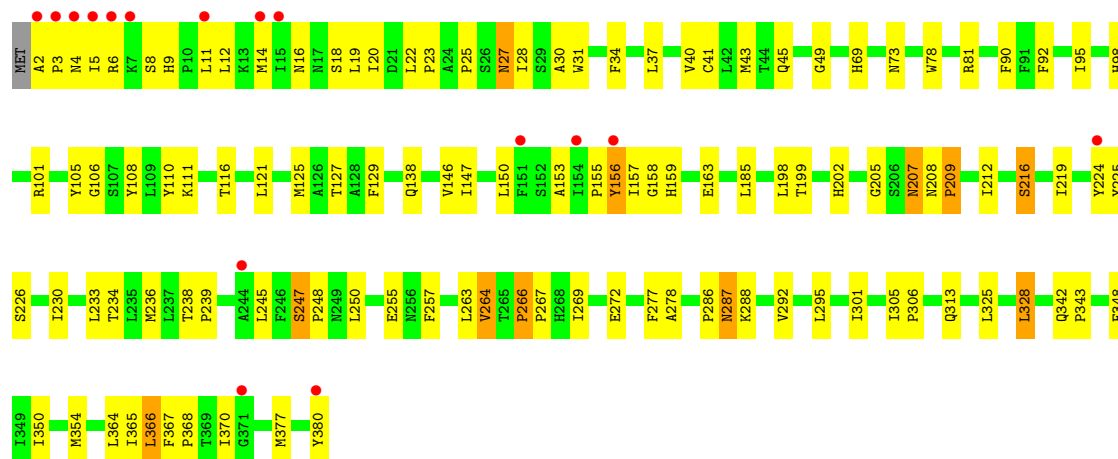




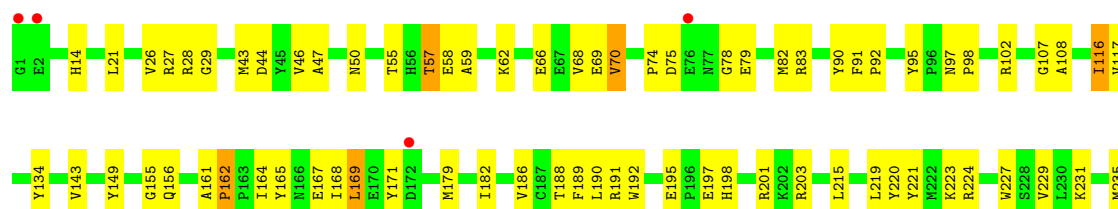
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b

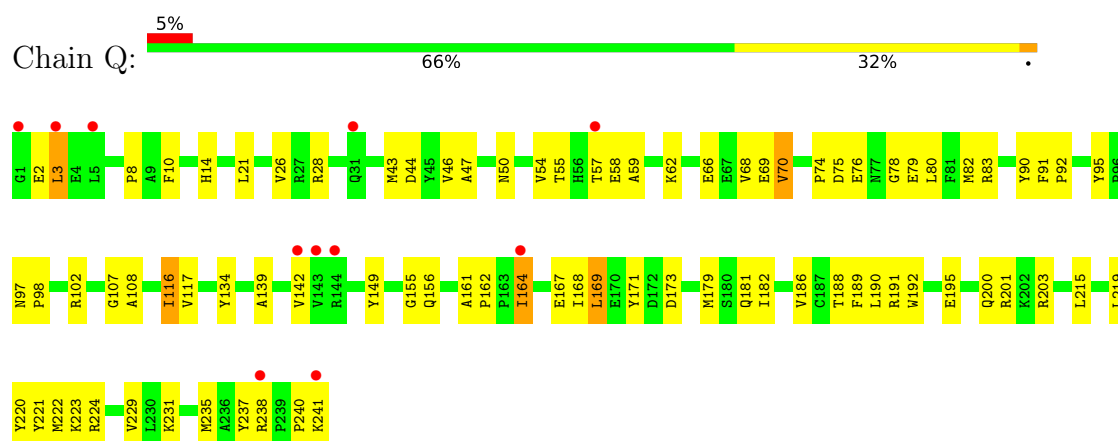


• Molecule 4: Mitochondrial cytochrome c1, heme protein

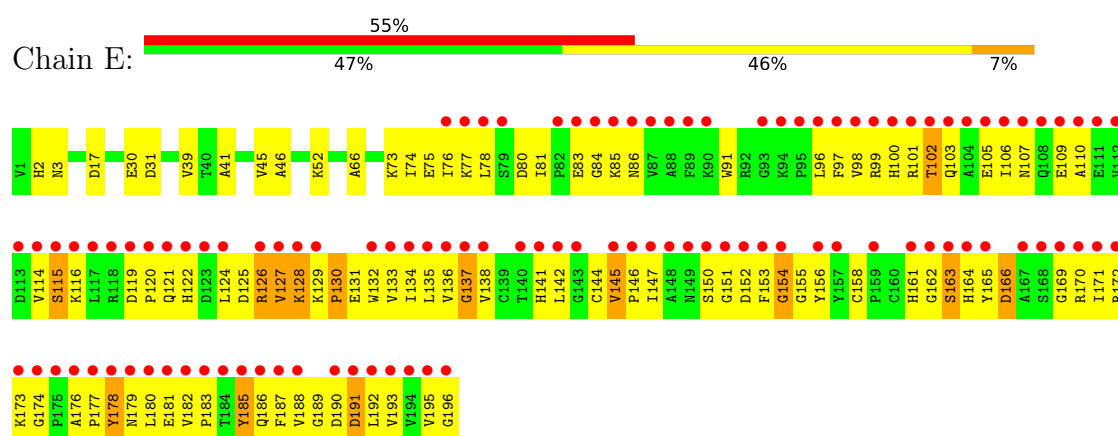




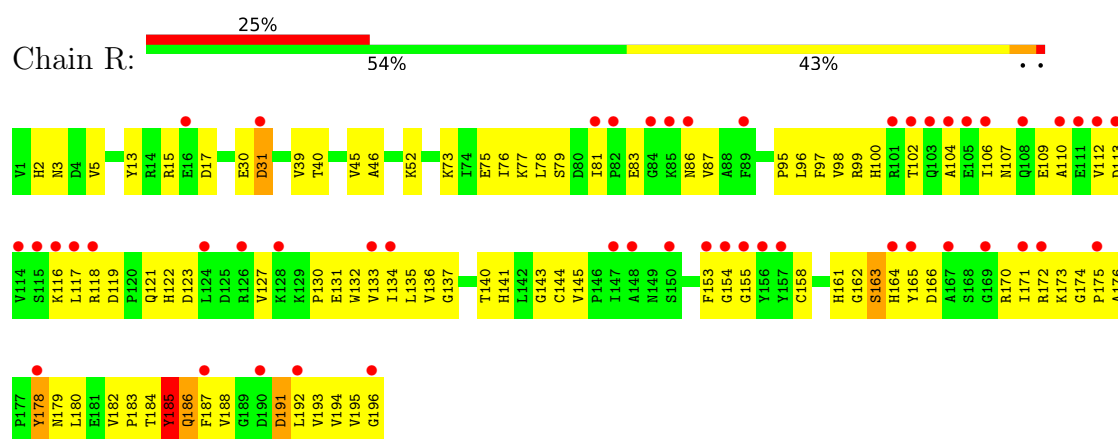
- Molecule 4: Mitochondrial cytochrome c1, heme protein



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

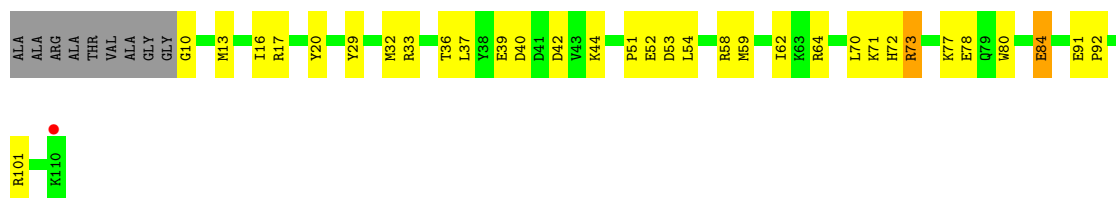


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

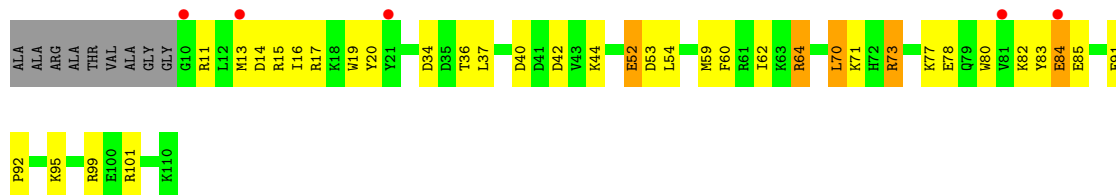


- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

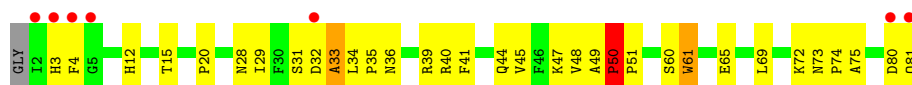




- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

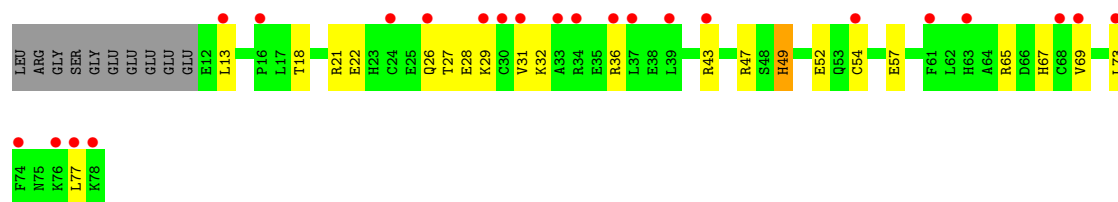


- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

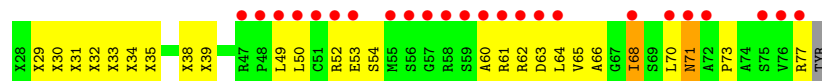
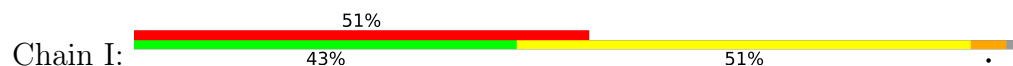


- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

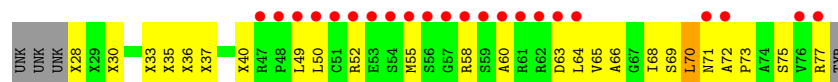




- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



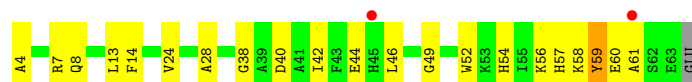
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 169.61Å 181.99Å 240.54Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 24.99 – 2.75<br>24.99 – 2.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (24.99-2.75)<br>99.2 (24.99-2.75)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.11                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.76 (at 2.69Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.267 , 0.297<br>0.256 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10214 reflections (4.99%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.603                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 50.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 32653                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: HEM, GOL, BOG, PEE, CDL, JZV, FES, HEC, UQ

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     | 0.53         | 0/3518         | 1.02        | 22/4767 (0.5%)   |
| 1   | N     | 0.49         | 0/3508         | 1.00        | 20/4753 (0.4%)   |
| 2   | B     | 0.46         | 0/3187         | 0.96        | 8/4321 (0.2%)    |
| 2   | O     | 0.49         | 0/3202         | 0.98        | 10/4343 (0.2%)   |
| 3   | C     | 0.63         | 1/3119 (0.0%)  | 1.02        | 16/4270 (0.4%)   |
| 3   | P     | 0.54         | 0/3114         | 1.01        | 19/4263 (0.4%)   |
| 4   | D     | 0.60         | 0/1956         | 1.03        | 7/2658 (0.3%)    |
| 4   | Q     | 0.47         | 0/1956         | 0.99        | 8/2658 (0.3%)    |
| 5   | E     | 0.47         | 0/1547         | 0.90        | 4/2103 (0.2%)    |
| 5   | R     | 0.45         | 0/1543         | 0.95        | 3/2098 (0.1%)    |
| 6   | F     | 0.62         | 1/911 (0.1%)   | 0.91        | 1/1219 (0.1%)    |
| 6   | S     | 0.47         | 0/911          | 0.91        | 1/1219 (0.1%)    |
| 7   | G     | 0.54         | 0/694          | 1.03        | 2/941 (0.2%)     |
| 7   | T     | 0.44         | 0/684          | 1.00        | 3/929 (0.3%)     |
| 8   | H     | 0.51         | 0/582          | 0.91        | 2/779 (0.3%)     |
| 8   | U     | 0.36         | 0/561          | 0.87        | 1/751 (0.1%)     |
| 9   | I     | 0.58         | 0/218          | 0.92        | 0/293            |
| 9   | V     | 0.55         | 0/218          | 1.02        | 1/293 (0.3%)     |
| 10  | J     | 0.53         | 0/508          | 0.88        | 2/682 (0.3%)     |
| 10  | W     | 0.48         | 0/490          | 0.88        | 2/660 (0.3%)     |
| All | All   | 0.52         | 2/32427 (0.0%) | 0.98        | 132/44000 (0.3%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | C     | 266 | PRO  | CA-C  | 5.73 | 1.55        | 1.51     |
| 6   | F     | 10  | GLY  | N-CA  | 5.15 | 1.53        | 1.45     |

All (132) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | O     | 227 | ARG  | N-CA-C  | 9.02  | 120.52      | 108.07   |
| 1   | N     | 32  | GLN  | CA-C-N  | 8.61  | 128.34      | 119.56   |
| 1   | N     | 32  | GLN  | C-N-CA  | 8.61  | 128.34      | 119.56   |
| 1   | A     | 32  | GLN  | CA-C-N  | 8.47  | 128.20      | 119.56   |
| 1   | A     | 32  | GLN  | C-N-CA  | 8.47  | 128.20      | 119.56   |
| 3   | C     | 185 | LEU  | N-CA-C  | 8.37  | 120.32      | 111.03   |
| 3   | P     | 185 | LEU  | N-CA-C  | 8.11  | 120.03      | 111.03   |
| 4   | D     | 44  | ASP  | N-CA-C  | 7.82  | 121.75      | 111.75   |
| 1   | A     | 432 | LEU  | N-CA-C  | 7.55  | 120.04      | 108.42   |
| 3   | P     | 365 | ILE  | N-CA-C  | 7.51  | 118.02      | 111.56   |
| 1   | N     | 432 | LEU  | N-CA-C  | 7.44  | 120.17      | 108.79   |
| 1   | N     | 32  | GLN  | N-CA-C  | 7.40  | 118.97      | 109.72   |
| 4   | Q     | 116 | ILE  | N-CA-C  | 7.39  | 118.12      | 110.36   |
| 1   | A     | 428 | ILE  | N-CA-C  | 7.38  | 119.23      | 112.29   |
| 1   | A     | 32  | GLN  | N-CA-C  | 7.33  | 118.88      | 109.72   |
| 5   | R     | 143 | GLY  | N-CA-C  | 6.88  | 125.50      | 114.90   |
| 1   | N     | 415 | ILE  | N-CA-C  | 6.82  | 117.43      | 111.56   |
| 4   | Q     | 44  | ASP  | N-CA-C  | 6.75  | 120.38      | 111.75   |
| 2   | O     | 157 | VAL  | N-CA-C  | 6.73  | 117.51      | 110.72   |
| 1   | A     | 119 | ASN  | N-CA-C  | 6.72  | 121.35      | 111.87   |
| 4   | D     | 116 | ILE  | N-CA-C  | 6.72  | 117.41      | 110.36   |
| 5   | E     | 17  | ASP  | N-CA-C  | 6.66  | 120.50      | 112.38   |
| 3   | C     | 365 | ILE  | N-CA-C  | 6.50  | 117.15      | 111.56   |
| 3   | C     | 207 | ASN  | N-CA-C  | -6.41 | 100.42      | 110.36   |
| 1   | A     | 248 | LEU  | CA-C-N  | 6.38  | 126.13      | 119.05   |
| 1   | A     | 248 | LEU  | C-N-CA  | 6.38  | 126.13      | 119.05   |
| 2   | B     | 174 | ASN  | CA-C-N  | 6.38  | 126.35      | 119.78   |
| 2   | B     | 174 | ASN  | C-N-CA  | 6.38  | 126.35      | 119.78   |
| 4   | D     | 155 | GLY  | N-CA-C  | -6.37 | 107.50      | 115.08   |
| 3   | P     | 247 | SER  | CA-C-N  | 6.37  | 127.80      | 119.84   |
| 3   | P     | 247 | SER  | C-N-CA  | 6.37  | 127.80      | 119.84   |
| 1   | A     | 331 | ILE  | CB-CA-C | -6.36 | 103.74      | 111.88   |
| 8   | U     | 73  | LEU  | N-CA-C  | 6.33  | 118.74      | 111.02   |
| 2   | O     | 226 | ILE  | N-CA-C  | -6.15 | 100.62      | 108.93   |
| 3   | P     | 207 | ASN  | N-CA-C  | -6.14 | 100.85      | 110.36   |
| 1   | N     | 331 | ILE  | CB-CA-C | -6.13 | 104.12      | 111.97   |
| 2   | O     | 126 | VAL  | N-CA-C  | 6.08  | 116.25      | 110.42   |
| 1   | N     | 263 | ALA  | N-CA-C  | 6.06  | 118.66      | 111.33   |
| 1   | N     | 119 | ASN  | N-CA-C  | 6.05  | 120.40      | 111.87   |
| 1   | A     | 66  | GLY  | N-CA-C  | 6.04  | 119.79      | 112.48   |
| 1   | A     | 263 | ALA  | N-CA-C  | 6.04  | 118.64      | 111.33   |
| 10  | W     | 13  | LEU  | N-CA-C  | 6.04  | 120.72      | 112.68   |
| 1   | N     | 348 | SER  | N-CA-C  | 6.01  | 118.13      | 110.61   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | P     | 110 | TYR  | N-CA-C | -5.99 | 100.63      | 109.62   |
| 7   | T     | 50  | PRO  | N-CA-C | 5.99  | 118.01      | 110.70   |
| 3   | C     | 209 | PRO  | N-CA-C | 5.97  | 121.61      | 113.84   |
| 1   | A     | 415 | ILE  | N-CA-C | 5.97  | 116.69      | 111.56   |
| 5   | R     | 17  | ASP  | N-CA-C | 5.95  | 119.64      | 112.38   |
| 4   | D     | 95  | TYR  | CA-C-N | 5.95  | 126.10      | 119.32   |
| 4   | D     | 95  | TYR  | C-N-CA | 5.95  | 126.10      | 119.32   |
| 3   | C     | 205 | GLY  | N-CA-C | -5.94 | 104.02      | 112.81   |
| 3   | C     | 247 | SER  | CA-C-N | 5.94  | 127.26      | 119.84   |
| 3   | C     | 247 | SER  | C-N-CA | 5.94  | 127.26      | 119.84   |
| 8   | H     | 73  | LEU  | N-CA-C | 5.91  | 118.23      | 111.02   |
| 3   | P     | 328 | LEU  | N-CA-C | -5.91 | 104.75      | 111.07   |
| 3   | C     | 328 | LEU  | N-CA-C | -5.90 | 104.75      | 111.07   |
| 2   | O     | 170 | THR  | N-CA-C | 5.90  | 115.88      | 108.45   |
| 3   | P     | 111 | LYS  | N-CA-C | 5.90  | 121.10      | 111.37   |
| 2   | B     | 157 | VAL  | N-CA-C | 5.89  | 116.67      | 110.72   |
| 1   | N     | 189 | HIS  | N-CA-C | 5.88  | 120.96      | 113.55   |
| 9   | V     | 70  | LEU  | N-CA-C | -5.87 | 106.28      | 113.50   |
| 1   | N     | 264 | ASP  | N-CA-C | 5.86  | 117.92      | 109.48   |
| 3   | P     | 257 | PHE  | N-CA-C | -5.86 | 106.04      | 112.72   |
| 7   | G     | 50  | PRO  | N-CA-C | 5.85  | 117.83      | 110.70   |
| 1   | A     | 189 | HIS  | N-CA-C | 5.84  | 120.92      | 113.55   |
| 1   | A     | 348 | SER  | N-CA-C | 5.84  | 117.30      | 110.41   |
| 5   | E     | 145 | VAL  | N-CA-C | 5.81  | 113.30      | 107.55   |
| 1   | N     | 347 | THR  | N-CA-C | 5.80  | 121.02      | 113.88   |
| 4   | Q     | 95  | TYR  | CA-C-N | 5.77  | 125.46      | 119.05   |
| 4   | Q     | 95  | TYR  | C-N-CA | 5.77  | 125.46      | 119.05   |
| 3   | C     | 366 | LEU  | N-CA-C | 5.77  | 117.37      | 111.14   |
| 3   | P     | 116 | THR  | N-CA-C | -5.76 | 105.00      | 111.28   |
| 3   | P     | 366 | LEU  | N-CA-C | 5.74  | 117.34      | 111.14   |
| 4   | Q     | 155 | GLY  | N-CA-C | -5.73 | 108.26      | 115.08   |
| 1   | A     | 431 | LEU  | N-CA-C | -5.64 | 100.49      | 109.96   |
| 10  | J     | 13  | LEU  | N-CA-C | 5.63  | 120.42      | 112.93   |
| 3   | C     | 226 | SER  | N-CA-C | -5.62 | 105.16      | 111.28   |
| 2   | O     | 174 | ASN  | CA-C-N | 5.60  | 125.55      | 119.78   |
| 2   | O     | 174 | ASN  | C-N-CA | 5.60  | 125.55      | 119.78   |
| 3   | C     | 113 | THR  | N-CA-C | -5.57 | 105.21      | 111.28   |
| 1   | A     | 228 | VAL  | CA-C-N | 5.57  | 125.84      | 119.83   |
| 1   | A     | 228 | VAL  | C-N-CA | 5.57  | 125.84      | 119.83   |
| 1   | A     | 264 | ASP  | CA-C-N | 5.55  | 125.39      | 119.28   |
| 1   | A     | 264 | ASP  | C-N-CA | 5.55  | 125.39      | 119.28   |
| 3   | C     | 90  | PHE  | N-CA-C | -5.55 | 105.23      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | T     | 12  | HIS  | N-CA-C | 5.54  | 119.33      | 112.24   |
| 3   | C     | 110 | TYR  | N-CA-C | -5.49 | 101.39      | 109.62   |
| 2   | B     | 133 | ARG  | CA-C-N | 5.47  | 124.93      | 119.24   |
| 2   | B     | 133 | ARG  | C-N-CA | 5.47  | 124.93      | 119.24   |
| 3   | P     | 266 | PRO  | CA-C-N | 5.47  | 124.66      | 118.97   |
| 3   | P     | 266 | PRO  | C-N-CA | 5.47  | 124.66      | 118.97   |
| 2   | O     | 225 | ASN  | N-CA-C | 5.46  | 120.31      | 113.43   |
| 2   | B     | 170 | THR  | N-CA-C | 5.42  | 115.39      | 108.24   |
| 7   | G     | 12  | HIS  | N-CA-C | 5.38  | 119.15      | 112.58   |
| 1   | A     | 347 | THR  | N-CA-C | 5.35  | 120.82      | 113.97   |
| 4   | D     | 162 | PRO  | CA-C-N | 5.35  | 124.86      | 119.19   |
| 4   | D     | 162 | PRO  | C-N-CA | 5.35  | 124.86      | 119.19   |
| 3   | C     | 27  | ASN  | N-CA-C | 5.34  | 119.10      | 112.59   |
| 1   | N     | 264 | ASP  | CA-C-N | 5.33  | 125.15      | 119.28   |
| 1   | N     | 264 | ASP  | C-N-CA | 5.33  | 125.15      | 119.28   |
| 1   | A     | 238 | GLY  | N-CA-C | -5.29 | 102.72      | 110.97   |
| 10  | W     | 14  | PHE  | N-CA-C | 5.28  | 119.72      | 113.28   |
| 1   | N     | 66  | GLY  | N-CA-C | 5.25  | 119.22      | 112.18   |
| 10  | J     | 14  | PHE  | N-CA-C | 5.25  | 119.68      | 113.28   |
| 3   | P     | 272 | GLU  | N-CA-C | -5.24 | 103.57      | 110.43   |
| 3   | C     | 93  | ILE  | N-CA-C | -5.21 | 105.41      | 110.42   |
| 1   | N     | 238 | GLY  | N-CA-C | -5.19 | 102.88      | 110.97   |
| 8   | H     | 50  | THR  | N-CA-C | 5.18  | 117.18      | 108.73   |
| 7   | T     | 23  | GLN  | N-CA-C | 5.18  | 117.15      | 109.69   |
| 2   | B     | 258 | VAL  | N-CA-C | 5.18  | 115.14      | 108.82   |
| 6   | F     | 39  | GLU  | N-CA-C | 5.17  | 117.62      | 109.39   |
| 1   | N     | 228 | VAL  | CA-C-N | 5.17  | 125.42      | 119.83   |
| 1   | N     | 228 | VAL  | C-N-CA | 5.17  | 125.42      | 119.83   |
| 1   | A     | 264 | ASP  | N-CA-C | 5.17  | 116.93      | 109.48   |
| 4   | Q     | 164 | ILE  | N-CA-C | 5.15  | 117.25      | 108.86   |
| 2   | B     | 223 | PHE  | N-CA-C | 5.14  | 119.91      | 113.43   |
| 1   | N     | 278 | GLY  | N-CA-C | 5.13  | 120.43      | 111.50   |
| 3   | C     | 224 | TYR  | N-CA-C | 5.12  | 117.27      | 111.02   |
| 5   | E     | 66  | ALA  | N-CA-C | 5.12  | 117.53      | 111.33   |
| 3   | P     | 27  | ASN  | N-CA-C | 5.10  | 118.81      | 112.59   |
| 3   | P     | 90  | PHE  | N-CA-C | -5.09 | 105.73      | 111.28   |
| 3   | P     | 209 | PRO  | N-CA-C | 5.08  | 120.51      | 113.65   |
| 3   | P     | 205 | GLY  | N-CA-C | -5.07 | 104.20      | 112.83   |
| 3   | P     | 226 | SER  | N-CA-C | -5.07 | 105.75      | 111.28   |
| 4   | Q     | 173 | ASP  | N-CA-C | -5.07 | 106.51      | 113.30   |
| 2   | O     | 141 | GLN  | CA-C-N | -5.05 | 114.87      | 119.82   |
| 2   | O     | 141 | GLN  | C-N-CA | -5.05 | 114.87      | 119.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | Q     | 80  | LEU  | N-CA-C | -5.04 | 103.74      | 110.55   |
| 5   | R     | 15  | ARG  | N-CA-C | -5.04 | 103.75      | 110.55   |
| 5   | E     | 126 | ARG  | N-CA-C | 5.03  | 115.62      | 107.32   |
| 1   | N     | 244 | ARG  | N-CA-C | 5.03  | 117.43      | 109.24   |
| 6   | S     | 15  | ARG  | N-CA-C | -5.01 | 106.02      | 112.68   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3447  | 0        | 3362     | 136     | 0            |
| 1   | N     | 3437  | 0        | 3349     | 153     | 0            |
| 2   | B     | 3133  | 0        | 3130     | 190     | 0            |
| 2   | O     | 3147  | 0        | 3146     | 196     | 0            |
| 3   | C     | 3017  | 0        | 3063     | 82      | 0            |
| 3   | P     | 3012  | 0        | 3058     | 104     | 0            |
| 4   | D     | 1898  | 0        | 1846     | 63      | 0            |
| 4   | Q     | 1898  | 0        | 1846     | 75      | 0            |
| 5   | E     | 1513  | 0        | 1478     | 126     | 0            |
| 5   | R     | 1509  | 0        | 1474     | 98      | 0            |
| 6   | F     | 891   | 0        | 893      | 24      | 0            |
| 6   | S     | 891   | 0        | 893      | 40      | 0            |
| 7   | G     | 672   | 0        | 653      | 34      | 0            |
| 7   | T     | 662   | 0        | 645      | 36      | 0            |
| 8   | H     | 574   | 0        | 548      | 16      | 0            |
| 8   | U     | 553   | 0        | 535      | 24      | 0            |
| 9   | I     | 287   | 0        | 250      | 37      | 0            |
| 9   | V     | 277   | 0        | 251      | 34      | 0            |
| 10  | J     | 497   | 0        | 490      | 16      | 0            |
| 10  | W     | 479   | 0        | 478      | 16      | 0            |
| 11  | A     | 21    | 0        | 13       | 0       | 0            |
| 11  | C     | 49    | 0        | 72       | 4       | 0            |
| 11  | E     | 50    | 0        | 77       | 1       | 0            |
| 11  | N     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | P     | 49    | 0        | 72       | 3       | 0            |
| 11  | R     | 50    | 0        | 77       | 2       | 0            |
| 12  | C     | 86    | 0        | 60       | 10      | 0            |
| 12  | P     | 86    | 0        | 60       | 8       | 0            |
| 13  | C     | 29    | 0        | 19       | 4       | 0            |
| 13  | P     | 29    | 0        | 19       | 4       | 0            |
| 14  | C     | 19    | 0        | 17       | 2       | 0            |
| 14  | P     | 19    | 0        | 17       | 3       | 0            |
| 15  | C     | 40    | 0        | 24       | 4       | 0            |
| 15  | D     | 42    | 0        | 28       | 4       | 0            |
| 15  | P     | 40    | 0        | 24       | 4       | 0            |
| 15  | Q     | 42    | 0        | 28       | 3       | 0            |
| 16  | C     | 6     | 0        | 8        | 0       | 0            |
| 16  | P     | 6     | 0        | 8        | 0       | 0            |
| 17  | D     | 43    | 0        | 30       | 0       | 0            |
| 17  | Q     | 43    | 0        | 30       | 0       | 0            |
| 18  | D     | 33    | 0        | 39       | 0       | 0            |
| 18  | P     | 12    | 0        | 11       | 2       | 0            |
| 18  | Q     | 33    | 0        | 39       | 1       | 0            |
| 19  | E     | 4     | 0        | 0        | 2       | 0            |
| 19  | R     | 4     | 0        | 0        | 2       | 0            |
| 20  | C     | 8     | 0        | 0        | 1       | 0            |
| 20  | E     | 1     | 0        | 0        | 0       | 0            |
| 20  | P     | 9     | 0        | 0        | 1       | 0            |
| 20  | R     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 32653 | 0        | 32160    | 1376    | 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 21.

All (1376) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 9:V:35:UNK:HG3   | 9:V:36:UNK:H    | 1.05                     | 1.14              |
| 5:E:121:GLN:HG2  | 5:E:170:ARG:HD3 | 1.15                     | 1.13              |
| 9:I:33:UNK:HG2   | 9:I:73:PRO:HB3  | 1.34                     | 1.07              |
| 2:B:76:THR:HG22  | 2:B:82:SER:H    | 1.18                     | 1.07              |
| 2:O:76:THR:HG22  | 2:O:82:SER:H    | 1.16                     | 1.07              |
| 2:O:353:THR:HG22 | 2:O:355:GLU:H   | 1.18                     | 1.05              |
| 2:B:353:THR:HG22 | 2:B:355:GLU:H   | 1.19                     | 1.03              |
| 2:O:338:ARG:HH11 | 2:O:338:ARG:HG3 | 1.27                     | 0.99              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:147:ILE:HG13 | 13:C:2001:JZV:HAP | 1.44                     | 0.99              |
| 2:B:338:ARG:HG3  | 2:B:338:ARG:HH11  | 1.28                     | 0.99              |
| 2:O:37:SER:HB3   | 2:O:213:HIS:ND1   | 1.78                     | 0.99              |
| 1:N:106:MET:HG3  | 1:N:203:ILE:HD13  | 1.42                     | 0.98              |
| 1:N:178:THR:HG22 | 1:N:180:ALA:H     | 1.25                     | 0.98              |
| 4:Q:47:ALA:H     | 4:Q:50:ASN:HD22   | 1.07                     | 0.97              |
| 1:A:178:THR:HG22 | 1:A:180:ALA:H     | 1.25                     | 0.96              |
| 3:P:9:HIS:HD2    | 3:P:12:LEU:H      | 1.09                     | 0.95              |
| 3:C:9:HIS:HD2    | 3:C:12:LEU:H      | 1.11                     | 0.93              |
| 4:D:47:ALA:H     | 4:D:50:ASN:HD22   | 1.12                     | 0.91              |
| 1:A:106:MET:HG3  | 1:A:203:ILE:HD13  | 1.50                     | 0.91              |
| 2:O:341:MET:HE1  | 2:O:417:PHE:HE2   | 1.36                     | 0.91              |
| 2:O:314:VAL:HG13 | 9:V:63:ASP:HB3    | 1.52                     | 0.91              |
| 2:O:51:ILE:HG12  | 2:O:204:MET:HG2   | 1.51                     | 0.90              |
| 9:V:49:LEU:HD13  | 9:V:55:MET:HG2    | 1.54                     | 0.90              |
| 1:A:69:LYS:HD2   | 1:A:70:ARG:HH21   | 1.36                     | 0.89              |
| 3:P:147:ILE:HG13 | 13:P:3001:JZV:HAP | 1.50                     | 0.88              |
| 2:O:157:VAL:HG23 | 9:V:64:LEU:HD21   | 1.54                     | 0.88              |
| 9:I:32:UNK:N     | 9:I:73:PRO:HG2    | 1.89                     | 0.88              |
| 2:B:341:MET:HE1  | 2:B:417:PHE:HE2   | 1.37                     | 0.88              |
| 7:T:41:PHE:O     | 7:T:45:VAL:HG23   | 1.75                     | 0.87              |
| 3:P:238:THR:HB   | 3:P:239:PRO:HD3   | 1.56                     | 0.86              |
| 3:P:301:ILE:HD11 | 3:P:364:LEU:HD21  | 1.56                     | 0.86              |
| 2:O:27:THR:HG22  | 2:O:28:LYS:H      | 1.40                     | 0.86              |
| 7:G:41:PHE:O     | 7:G:45:VAL:HG23   | 1.76                     | 0.85              |
| 2:O:248:ASN:HD22 | 2:O:248:ASN:C     | 1.83                     | 0.85              |
| 1:A:178:THR:HB   | 1:A:181:ASP:OD1   | 1.75                     | 0.85              |
| 2:B:124:LEU:HD11 | 2:B:223:PHE:HB3   | 1.57                     | 0.85              |
| 9:V:35:UNK:HG3   | 9:V:36:UNK:N      | 1.89                     | 0.85              |
| 5:E:136:VAL:HG23 | 5:E:183:PRO:HD3   | 1.58                     | 0.85              |
| 2:O:18:CYS:HB2   | 2:O:19:PRO:HD3    | 1.58                     | 0.84              |
| 3:C:301:ILE:HD11 | 3:C:364:LEU:HD21  | 1.60                     | 0.84              |
| 5:R:30:GLU:HB2   | 10:W:7:ARG:HG2    | 1.60                     | 0.84              |
| 9:V:64:LEU:HD12  | 9:V:77:ARG:O      | 1.78                     | 0.84              |
| 5:E:83:GLU:HB3   | 5:E:102:THR:HG22  | 1.59                     | 0.83              |
| 5:E:30:GLU:HB2   | 10:J:7:ARG:HG2    | 1.61                     | 0.83              |
| 5:E:121:GLN:HG2  | 5:E:170:ARG:CD    | 2.04                     | 0.83              |
| 2:B:248:ASN:C    | 2:B:248:ASN:HD22  | 1.87                     | 0.82              |
| 11:P:3007:PEE:H7 | 7:T:44:GLN:HE21   | 1.45                     | 0.82              |
| 5:E:127:VAL:HG12 | 5:E:128:LYS:H     | 1.43                     | 0.82              |
| 1:N:10:ASN:ND2   | 2:O:19:PRO:HD2    | 1.95                     | 0.81              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:314:VAL:HG13 | 9:I:63:ASP:HB3    | 1.62                     | 0.81              |
| 1:N:69:LYS:HD2   | 1:N:70:ARG:HH21   | 1.45                     | 0.81              |
| 2:B:157:VAL:HG23 | 9:I:64:LEU:HD21   | 1.62                     | 0.81              |
| 2:O:192:HIS:O    | 2:O:196:GLN:HG3   | 1.81                     | 0.81              |
| 9:I:34:UNK:HG3   | 9:I:35:UNK:N      | 1.96                     | 0.80              |
| 3:P:342:GLN:HE21 | 3:P:343:PRO:HD2   | 1.45                     | 0.80              |
| 2:B:80:ALA:HA    | 2:B:84:ARG:HH12   | 1.44                     | 0.80              |
| 2:B:51:ILE:HG12  | 2:B:204:MET:HG2   | 1.64                     | 0.80              |
| 3:C:238:THR:HB   | 3:C:239:PRO:HD3   | 1.64                     | 0.79              |
| 4:Q:47:ALA:H     | 4:Q:50:ASN:ND2    | 1.80                     | 0.79              |
| 1:A:443:TRP:HA   | 1:A:443:TRP:CE3   | 2.17                     | 0.79              |
| 3:C:22:LEU:HD21  | 14:C:2002:UQ:HM32 | 1.65                     | 0.79              |
| 2:B:209:ILE:HD13 | 2:B:378:LEU:HD23  | 1.65                     | 0.79              |
| 3:P:69:HIS:CD2   | 3:P:73:ASN:HD22   | 2.01                     | 0.78              |
| 2:B:47:ILE:HD13  | 2:B:120:MET:CE    | 2.14                     | 0.78              |
| 1:A:343:MET:HB3  | 1:A:444:ILE:HA    | 1.64                     | 0.78              |
| 1:N:178:THR:HB   | 1:N:181:ASP:OD1   | 1.82                     | 0.78              |
| 2:O:221:GLU:HG3  | 2:O:222:GLN:H     | 1.49                     | 0.77              |
| 2:O:154:SER:O    | 2:O:157:VAL:HG12  | 1.85                     | 0.77              |
| 1:A:7:THR:HG21   | 2:B:113:ARG:HD2   | 1.66                     | 0.77              |
| 2:O:80:ALA:HA    | 2:O:84:ARG:HH12   | 1.49                     | 0.77              |
| 2:O:206:LEU:HD23 | 2:O:220:ALA:HB2   | 1.66                     | 0.77              |
| 1:N:443:TRP:HA   | 1:N:443:TRP:CE3   | 2.19                     | 0.76              |
| 3:P:101:ARG:C    | 3:P:101:ARG:HD2   | 2.09                     | 0.76              |
| 5:E:122:HIS:HB3  | 5:E:125:ASP:CG    | 2.11                     | 0.76              |
| 7:T:72:LYS:HE2   | 8:U:57:GLU:OE1    | 1.86                     | 0.76              |
| 4:D:57:THR:HG22  | 4:D:59:ALA:H      | 1.49                     | 0.76              |
| 3:C:328:LEU:HD12 | 7:G:51:PRO:HB3    | 1.66                     | 0.76              |
| 2:O:181:TYR:CE1  | 2:O:182:ARG:HG3   | 2.21                     | 0.76              |
| 3:P:69:HIS:HD2   | 3:P:73:ASN:HD22   | 1.34                     | 0.75              |
| 2:B:192:HIS:O    | 2:B:196:GLN:HG3   | 1.87                     | 0.75              |
| 5:E:141:HIS:HB2  | 5:E:176:ALA:HB2   | 1.68                     | 0.75              |
| 1:N:111:GLU:HG3  | 1:N:215:HIS:CD2   | 2.22                     | 0.75              |
| 2:B:33:LEU:HD21  | 2:B:224:LEU:HD12  | 1.66                     | 0.75              |
| 5:E:81:ILE:HB    | 5:E:132:TRP:HH2   | 1.51                     | 0.75              |
| 11:C:2007:PEE:H7 | 7:G:44:GLN:HE21   | 1.49                     | 0.75              |
| 1:N:106:MET:HG3  | 1:N:203:ILE:CD1   | 2.17                     | 0.75              |
| 3:P:328:LEU:HD12 | 7:T:51:PRO:HB3    | 1.68                     | 0.75              |
| 5:E:119:ASP:HB3  | 5:E:179:ASN:HD21  | 1.51                     | 0.74              |
| 5:E:121:GLN:CG   | 5:E:170:ARG:HD3   | 2.06                     | 0.74              |
| 1:A:336:PHE:CZ   | 3:C:4:ASN:HB3     | 2.23                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:331:ILE:HG21 | 1:A:431:LEU:HB2  | 1.69                     | 0.74              |
| 2:B:399:ALA:O    | 2:B:402:ILE:HG22 | 1.87                     | 0.74              |
| 5:R:79:SER:OG    | 5:R:191:ASP:HB2  | 1.88                     | 0.74              |
| 5:E:129:LYS:HB3  | 5:E:132:TRP:HB2  | 1.68                     | 0.74              |
| 2:O:209:ILE:HD13 | 2:O:378:LEU:HD23 | 1.70                     | 0.74              |
| 2:O:338:ARG:HG3  | 2:O:338:ARG:NH1  | 2.00                     | 0.74              |
| 2:B:154:SER:O    | 2:B:157:VAL:HG12 | 1.88                     | 0.73              |
| 1:N:331:ILE:HG21 | 1:N:431:LEU:HB2  | 1.70                     | 0.73              |
| 2:O:27:THR:HG22  | 2:O:28:LYS:N     | 2.03                     | 0.73              |
| 1:A:443:TRP:HA   | 1:A:443:TRP:HE3  | 1.52                     | 0.73              |
| 3:C:69:HIS:HD2   | 3:C:73:ASN:HD22  | 1.35                     | 0.73              |
| 7:T:73:ASN:HD21  | 7:T:75:ALA:HB3   | 1.52                     | 0.73              |
| 1:A:336:PHE:CE2  | 3:C:4:ASN:HB3    | 2.24                     | 0.73              |
| 2:B:31:ASN:HD22  | 2:B:31:ASN:N     | 1.86                     | 0.73              |
| 1:N:443:TRP:HA   | 1:N:443:TRP:HE3  | 1.52                     | 0.72              |
| 3:P:23:PRO:HG2   | 7:T:3:HIS:HB3    | 1.71                     | 0.72              |
| 2:B:27:THR:HG22  | 2:B:28:LYS:H     | 1.53                     | 0.72              |
| 3:C:342:GLN:HE21 | 3:C:343:PRO:HD2  | 1.54                     | 0.72              |
| 1:N:170:THR:HG22 | 1:N:171:THR:N    | 2.03                     | 0.72              |
| 1:N:10:ASN:HD21  | 2:O:18:CYS:N     | 1.88                     | 0.72              |
| 4:Q:43:MET:HE2   | 4:Q:91:PHE:CE2   | 2.24                     | 0.72              |
| 5:R:78:LEU:HB3   | 5:R:132:TRP:CZ2  | 2.23                     | 0.72              |
| 2:B:37:SER:HB3   | 2:B:213:HIS:ND1  | 2.05                     | 0.72              |
| 1:N:7:THR:HG21   | 2:O:113:ARG:HD2  | 1.70                     | 0.72              |
| 1:A:111:GLU:HG3  | 1:A:215:HIS:CD2  | 2.25                     | 0.72              |
| 5:E:52:LYS:C     | 5:E:52:LYS:HD3   | 2.14                     | 0.72              |
| 5:E:166:ASP:OD2  | 5:E:170:ARG:HB2  | 1.88                     | 0.72              |
| 5:E:84:GLY:N     | 5:E:102:THR:HG23 | 2.05                     | 0.72              |
| 1:N:343:MET:HB3  | 1:N:444:ILE:HA   | 1.71                     | 0.72              |
| 7:T:73:ASN:ND2   | 7:T:75:ALA:HB3   | 2.03                     | 0.72              |
| 2:O:62:ASN:O     | 2:O:65:THR:HG22  | 1.90                     | 0.72              |
| 3:C:9:HIS:CD2    | 3:C:12:LEU:H     | 2.03                     | 0.72              |
| 2:B:181:TYR:CE1  | 2:B:182:ARG:HG3  | 2.26                     | 0.71              |
| 3:C:69:HIS:CD2   | 3:C:73:ASN:HD22  | 2.07                     | 0.71              |
| 1:N:369:LEU:HD12 | 1:N:392:LEU:HD11 | 1.72                     | 0.71              |
| 5:R:83:GLU:HB3   | 5:R:102:THR:HG22 | 1.71                     | 0.71              |
| 3:P:216:SER:HB3  | 6:S:59:MET:HE2   | 1.71                     | 0.71              |
| 2:B:338:ARG:HG3  | 2:B:338:ARG:NH1  | 2.01                     | 0.71              |
| 1:N:402:VAL:HG22 | 1:N:406:MET:HE2  | 1.71                     | 0.71              |
| 2:O:47:ILE:HD13  | 2:O:120:MET:CE   | 2.20                     | 0.71              |
| 3:C:245:LEU:O    | 4:D:201:ARG:HD2  | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:9:HIS:CD2    | 3:P:12:LEU:H     | 2.01                     | 0.71              |
| 2:O:399:ALA:O    | 2:O:402:ILE:HG22 | 1.90                     | 0.70              |
| 5:R:119:ASP:HB3  | 5:R:179:ASN:ND2  | 2.06                     | 0.70              |
| 5:R:170:ARG:HA   | 5:R:179:ASN:HB3  | 1.72                     | 0.70              |
| 3:C:23:PRO:HG2   | 7:G:3:HIS:HB3    | 1.71                     | 0.70              |
| 2:O:225:ASN:O    | 2:O:227:ARG:HG3  | 1.90                     | 0.70              |
| 1:A:281:ASP:CG   | 9:I:33:UNK:HB2   | 2.15                     | 0.70              |
| 2:B:202:ALA:HB3  | 2:B:229:GLY:O    | 1.91                     | 0.70              |
| 4:Q:26:VAL:HG12  | 4:Q:55:THR:HG21  | 1.71                     | 0.70              |
| 4:Q:164:ILE:O    | 4:Q:179:MET:HE2  | 1.91                     | 0.70              |
| 5:R:52:LYS:HD3   | 5:R:52:LYS:C     | 2.17                     | 0.70              |
| 2:O:314:VAL:CG1  | 9:V:63:ASP:HB3   | 2.22                     | 0.70              |
| 4:Q:57:THR:HG22  | 4:Q:59:ALA:H     | 1.55                     | 0.70              |
| 2:O:76:THR:HG23  | 2:O:136:GLU:OE1  | 1.92                     | 0.70              |
| 1:A:242:ARG:HH12 | 1:A:432:LEU:HA   | 1.56                     | 0.70              |
| 4:D:43:MET:HE2   | 4:D:91:PHE:CE2   | 2.26                     | 0.70              |
| 5:R:78:LEU:HD13  | 5:R:132:TRP:NE1  | 2.06                     | 0.70              |
| 3:P:245:LEU:O    | 4:Q:201:ARG:HD2  | 1.91                     | 0.69              |
| 1:A:106:MET:HE2  | 1:A:107:PRO:HA   | 1.75                     | 0.69              |
| 3:C:101:ARG:HD2  | 3:C:101:ARG:C    | 2.17                     | 0.69              |
| 4:D:43:MET:HE1   | 4:D:189:PHE:CZ   | 2.28                     | 0.69              |
| 5:E:76:ILE:HD13  | 5:E:98:VAL:HG21  | 1.74                     | 0.69              |
| 5:E:190:ASP:C    | 5:E:192:LEU:H    | 1.98                     | 0.69              |
| 4:D:47:ALA:H     | 4:D:50:ASN:ND2   | 1.89                     | 0.68              |
| 5:E:31:ASP:OD2   | 10:J:7:ARG:HG3   | 1.93                     | 0.68              |
| 1:N:85:HIS:CD2   | 2:O:284:LEU:HD22 | 2.27                     | 0.68              |
| 1:N:15:ASN:O     | 1:N:26:ALA:HA    | 1.93                     | 0.68              |
| 2:B:76:THR:HG22  | 2:B:82:SER:N     | 2.02                     | 0.68              |
| 7:G:36:ASN:OD1   | 7:G:39:ARG:NH1   | 2.26                     | 0.68              |
| 2:O:407:SER:O    | 2:O:411:VAL:HG23 | 1.94                     | 0.68              |
| 2:B:27:THR:HG22  | 2:B:28:LYS:N     | 2.07                     | 0.68              |
| 2:B:31:ASN:H     | 2:B:31:ASN:ND2   | 1.90                     | 0.68              |
| 4:Q:231:LYS:O    | 6:S:71:LYS:HE3   | 1.94                     | 0.68              |
| 1:N:105:ASP:O    | 1:N:109:VAL:HG23 | 1.92                     | 0.68              |
| 2:O:46:ARG:HG2   | 2:O:379:LEU:HD22 | 1.76                     | 0.68              |
| 2:O:101:THR:HG23 | 2:O:104:LYS:HE3  | 1.76                     | 0.68              |
| 4:D:26:VAL:HG12  | 4:D:55:THR:HG21  | 1.76                     | 0.68              |
| 4:Q:43:MET:HE1   | 4:Q:189:PHE:CZ   | 2.28                     | 0.68              |
| 1:N:242:ARG:HH12 | 1:N:432:LEU:HA   | 1.59                     | 0.67              |
| 2:O:128:THR:HG21 | 2:O:224:LEU:HD22 | 1.75                     | 0.67              |
| 5:R:166:ASP:OD2  | 5:R:170:ARG:HB2  | 1.95                     | 0.67              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 9:V:35:UNK:CG      | 9:V:36:UNK:H     | 1.89                     | 0.67              |
| 1:A:369:LEU:HD12   | 1:A:392:LEU:HD11 | 1.75                     | 0.67              |
| 1:A:170:THR:HG22   | 1:A:171:THR:N    | 2.08                     | 0.67              |
| 4:D:57:THR:HG22    | 4:D:59:ALA:N     | 2.08                     | 0.67              |
| 2:O:361:LYS:O      | 2:O:365:LYS:HG3  | 1.95                     | 0.67              |
| 9:I:31:UNK:C       | 9:I:73:PRO:HG2   | 2.25                     | 0.67              |
| 1:A:15:ASN:O       | 1:A:26:ALA:HA    | 1.95                     | 0.67              |
| 2:B:47:ILE:HD13    | 2:B:120:MET:HE1  | 1.75                     | 0.67              |
| 2:B:225:ASN:O      | 2:B:227:ARG:N    | 2.28                     | 0.67              |
| 2:O:47:ILE:HG21    | 2:O:120:MET:HE1  | 1.77                     | 0.67              |
| 1:N:336:PHE:CZ     | 3:P:4:ASN:HB3    | 2.30                     | 0.67              |
| 10:W:7:ARG:HB3     | 10:W:7:ARG:NH1   | 2.10                     | 0.67              |
| 2:B:241:GLY:HA2    | 2:B:423:SER:HB3  | 1.75                     | 0.66              |
| 3:C:377:MET:HE2    | 6:F:20:TYR:CD1   | 2.29                     | 0.66              |
| 2:B:80:ALA:HA      | 2:B:84:ARG:NH1   | 2.11                     | 0.66              |
| 4:D:62:LYS:O       | 4:D:66:GLU:HG3   | 1.95                     | 0.66              |
| 9:I:70:LEU:HD23    | 9:I:71:ASN:N     | 2.10                     | 0.66              |
| 5:R:186:GLN:HE21   | 5:R:188:VAL:HG13 | 1.59                     | 0.66              |
| 1:A:85:HIS:CD2     | 2:B:284:LEU:HD22 | 2.31                     | 0.66              |
| 3:P:153:ALA:HB2    | 3:P:288:LYS:HG2  | 1.78                     | 0.66              |
| 5:R:31:ASP:OD2     | 10:W:7:ARG:HG3   | 1.96                     | 0.66              |
| 5:E:129:LYS:CB     | 5:E:132:TRP:HB2  | 2.26                     | 0.66              |
| 10:J:7:ARG:HB3     | 10:J:7:ARG:NH1   | 2.10                     | 0.66              |
| 3:P:40:VAL:HA      | 3:P:43:MET:HE3   | 1.76                     | 0.66              |
| 15:P:3004:CDL:HA32 | 7:T:40:ARG:HB3   | 1.77                     | 0.66              |
| 2:B:46:ARG:HG2     | 2:B:379:LEU:HD22 | 1.77                     | 0.66              |
| 9:I:64:LEU:HD12    | 9:I:77:ARG:O     | 1.95                     | 0.66              |
| 4:D:164:ILE:O      | 4:D:179:MET:HE2  | 1.94                     | 0.66              |
| 2:B:62:ASN:O       | 2:B:65:THR:HG22  | 1.96                     | 0.66              |
| 1:N:402:VAL:HG22   | 1:N:406:MET:CE   | 2.25                     | 0.65              |
| 7:T:36:ASN:OD1     | 7:T:39:ARG:NH1   | 2.28                     | 0.65              |
| 9:I:70:LEU:HD23    | 9:I:71:ASN:H     | 1.61                     | 0.65              |
| 2:B:306:PRO:HA     | 9:I:52:ARG:CG    | 2.27                     | 0.65              |
| 1:N:282:ARG:HH21   | 9:V:36:UNK:HA    | 1.61                     | 0.65              |
| 4:Q:43:MET:HE3     | 4:Q:46:VAL:HG21  | 1.77                     | 0.65              |
| 5:E:127:VAL:HG12   | 5:E:128:LYS:N    | 2.11                     | 0.65              |
| 3:C:45:GLN:HB3     | 12:C:501:HEM:HAB | 1.78                     | 0.65              |
| 4:Q:62:LYS:O       | 4:Q:66:GLU:HG3   | 1.96                     | 0.65              |
| 2:B:160:LEU:HD12   | 9:I:64:LEU:HD13  | 1.78                     | 0.65              |
| 1:N:39:VAL:HG11    | 1:N:117:VAL:HG11 | 1.77                     | 0.65              |
| 2:O:22:GLU:HG2     | 2:O:39:GLU:HB3   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:81:ILE:HB     | 5:E:132:TRP:CH2   | 2.31                     | 0.64              |
| 2:O:219:VAL:O     | 2:O:223:PHE:HB2   | 1.97                     | 0.64              |
| 9:V:28:UNK:CB     | 9:V:72:ALA:HB2    | 2.26                     | 0.64              |
| 2:O:59:THR:HG22   | 2:O:61:ALA:H      | 1.62                     | 0.64              |
| 4:D:97:ASN:HB2    | 4:D:98:PRO:HD2    | 1.78                     | 0.64              |
| 12:P:502:HEM:HMC2 | 12:P:502:HEM:HBC2 | 1.79                     | 0.64              |
| 4:Q:57:THR:HG22   | 4:Q:59:ALA:N      | 2.12                     | 0.64              |
| 2:O:80:ALA:HA     | 2:O:84:ARG:NH1    | 2.12                     | 0.64              |
| 3:P:2:ALA:HB3     | 3:P:8:SER:HB3     | 1.80                     | 0.64              |
| 3:P:198:LEU:HD21  | 12:P:502:HEM:HMA3 | 1.78                     | 0.64              |
| 2:O:18:CYS:HB2    | 2:O:19:PRO:CD     | 2.27                     | 0.64              |
| 2:O:273:SER:O     | 2:O:276:GLN:HB3   | 1.97                     | 0.64              |
| 2:B:394:ALA:HB3   | 2:B:397:VAL:HG23  | 1.80                     | 0.64              |
| 1:N:37:VAL:HG12   | 1:N:199:ALA:HB1   | 1.79                     | 0.64              |
| 7:G:41:PHE:CE2    | 7:G:45:VAL:HG21   | 2.33                     | 0.64              |
| 5:E:119:ASP:HB3   | 5:E:179:ASN:ND2   | 2.13                     | 0.64              |
| 1:N:10:ASN:CG     | 2:O:19:PRO:HD2    | 2.21                     | 0.64              |
| 1:N:170:THR:HG22  | 1:N:172:GLU:H     | 1.62                     | 0.64              |
| 3:P:342:GLN:NE2   | 3:P:343:PRO:HD2   | 2.13                     | 0.64              |
| 9:V:70:LEU:HD23   | 9:V:71:ASN:N      | 2.14                     | 0.64              |
| 7:G:73:ASN:ND2    | 7:G:75:ALA:HB3    | 2.12                     | 0.63              |
| 1:N:336:PHE:CE2   | 3:P:4:ASN:HB3     | 2.32                     | 0.63              |
| 1:A:178:THR:HG22  | 1:A:180:ALA:N     | 2.07                     | 0.63              |
| 1:A:17:THR:HG23   | 1:A:205:HIS:NE2   | 2.14                     | 0.63              |
| 10:W:7:ARG:CB     | 10:W:7:ARG:HH11   | 2.11                     | 0.63              |
| 2:B:306:PRO:HA    | 9:I:52:ARG:HG3    | 1.79                     | 0.63              |
| 5:E:78:LEU:HD12   | 5:E:190:ASP:O     | 1.98                     | 0.63              |
| 2:O:160:LEU:HD12  | 9:V:64:LEU:HD13   | 1.79                     | 0.63              |
| 4:Q:74:PRO:HB2    | 4:Q:78:GLY:HA2    | 1.81                     | 0.63              |
| 10:J:7:ARG:CB     | 10:J:7:ARG:HH11   | 2.11                     | 0.63              |
| 2:B:38:LEU:HD12   | 2:B:39:GLU:N      | 2.14                     | 0.63              |
| 7:G:73:ASN:HD21   | 7:G:75:ALA:HB3    | 1.63                     | 0.63              |
| 1:A:4:TYR:HB3     | 2:B:114:ASP:OD2   | 1.99                     | 0.63              |
| 3:P:236:MET:O     | 3:P:239:PRO:HD2   | 1.99                     | 0.62              |
| 5:E:106:ILE:C     | 5:E:110:ALA:HB3   | 2.23                     | 0.62              |
| 3:P:37:LEU:HD21   | 3:P:233:LEU:HA    | 1.81                     | 0.62              |
| 1:N:106:MET:HE2   | 1:N:107:PRO:HA    | 1.81                     | 0.62              |
| 5:R:109:GLU:CG    | 5:R:123:ASP:HB2   | 2.28                     | 0.62              |
| 1:A:39:VAL:HG11   | 1:A:117:VAL:HG11  | 1.80                     | 0.62              |
| 1:A:60:GLU:OE2    | 1:A:90:THR:HG22   | 2.00                     | 0.62              |
| 5:E:187:PHE:C     | 5:E:189:GLY:H     | 2.06                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:248:ASN:HD21 | 2:O:250:HIS:HB2  | 1.64                     | 0.62              |
| 2:O:357:VAL:HG12 | 2:O:361:LYS:HE3  | 1.82                     | 0.62              |
| 4:Q:134:TYR:CG   | 4:Q:162:PRO:HG3  | 2.34                     | 0.62              |
| 1:A:106:MET:HG3  | 1:A:203:ILE:CD1  | 2.29                     | 0.62              |
| 2:B:69:LEU:HD23  | 2:B:105:MET:HE1  | 1.82                     | 0.62              |
| 2:O:217:LYS:O    | 2:O:221:GLU:HG2  | 1.99                     | 0.62              |
| 4:Q:43:MET:HE2   | 4:Q:91:PHE:CD2   | 2.34                     | 0.62              |
| 1:A:402:VAL:HG22 | 1:A:406:MET:HE2  | 1.81                     | 0.62              |
| 2:B:207:VAL:HG21 | 2:B:383:GLY:CA   | 2.29                     | 0.62              |
| 1:A:7:THR:HG21   | 2:B:113:ARG:CD   | 2.30                     | 0.62              |
| 5:E:130:PRO:HG2  | 5:E:131:GLU:CD   | 2.25                     | 0.62              |
| 5:E:171:ILE:HG22 | 5:E:179:ASN:OD1  | 2.00                     | 0.62              |
| 2:O:353:THR:HG22 | 2:O:355:GLU:N    | 2.02                     | 0.62              |
| 5:R:135:LEU:HD23 | 5:R:182:VAL:HG22 | 1.82                     | 0.62              |
| 5:E:83:GLU:HB3   | 5:E:102:THR:CG2  | 2.29                     | 0.62              |
| 3:P:25:PRO:HB2   | 3:P:28:ILE:HG23  | 1.82                     | 0.62              |
| 4:Q:97:ASN:HB2   | 4:Q:98:PRO:HD2   | 1.80                     | 0.62              |
| 8:U:28:GLU:O     | 8:U:32:LYS:HG3   | 1.99                     | 0.62              |
| 5:E:86:ASN:OD1   | 5:E:99:ARG:HB2   | 2.00                     | 0.61              |
| 7:T:79:ASN:O     | 7:T:80:ASP:HB2   | 2.00                     | 0.61              |
| 1:A:69:LYS:HD2   | 1:A:70:ARG:NH2   | 2.10                     | 0.61              |
| 2:B:357:VAL:HG12 | 2:B:361:LYS:HE3  | 1.81                     | 0.61              |
| 2:B:407:SER:O    | 2:B:411:VAL:HG23 | 2.00                     | 0.61              |
| 5:R:171:ILE:HD13 | 5:R:176:ALA:HB3  | 1.81                     | 0.61              |
| 1:A:37:VAL:HG12  | 1:A:199:ALA:HB1  | 1.80                     | 0.61              |
| 2:B:353:THR:HG22 | 2:B:355:GLU:N    | 2.04                     | 0.61              |
| 3:C:37:LEU:HD21  | 3:C:233:LEU:HA   | 1.82                     | 0.61              |
| 2:O:207:VAL:HG21 | 2:O:383:GLY:CA   | 2.30                     | 0.61              |
| 2:B:338:ARG:HH11 | 2:B:338:ARG:CG   | 2.10                     | 0.61              |
| 1:A:186:ILE:HG23 | 1:A:190:PHE:CD1  | 2.36                     | 0.61              |
| 1:N:182:LEU:O    | 1:N:186:ILE:HG13 | 2.01                     | 0.61              |
| 2:B:292:THR:HG22 | 2:B:292:THR:O    | 2.00                     | 0.61              |
| 3:C:236:MET:O    | 3:C:239:PRO:HD2  | 1.99                     | 0.61              |
| 2:B:248:ASN:C    | 2:B:248:ASN:ND2  | 2.59                     | 0.61              |
| 1:N:196:VAL:HG11 | 1:N:383:LEU:HD12 | 1.83                     | 0.61              |
| 8:H:18:THR:O     | 8:H:22:GLU:HG3   | 2.01                     | 0.61              |
| 8:H:28:GLU:O     | 8:H:32:LYS:HG3   | 2.01                     | 0.61              |
| 5:E:130:PRO:HG2  | 5:E:131:GLU:H    | 1.66                     | 0.61              |
| 6:F:59:MET:HE3   | 6:F:59:MET:HA    | 1.83                     | 0.60              |
| 9:V:64:LEU:HD12  | 9:V:77:ARG:C     | 2.26                     | 0.60              |
| 2:B:215:ASP:O    | 2:B:219:VAL:HG23 | 2.01                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:342:GLN:NE2  | 3:C:343:PRO:HD2   | 2.16                     | 0.60              |
| 5:R:83:GLU:HG3   | 5:R:100:HIS:CE1   | 2.37                     | 0.60              |
| 1:A:282:ARG:HH21 | 9:I:35:UNK:HA     | 1.67                     | 0.60              |
| 1:N:136:GLN:OE1  | 9:V:50:LEU:HB3    | 2.01                     | 0.60              |
| 2:O:394:ALA:HB3  | 2:O:397:VAL:HG23  | 1.83                     | 0.60              |
| 2:B:96:LEU:H     | 9:I:70:LEU:HD22   | 1.66                     | 0.60              |
| 1:N:371:GLY:O    | 1:N:375:VAL:HG23  | 2.01                     | 0.60              |
| 5:R:96:LEU:HD21  | 5:R:195:VAL:HG21  | 1.81                     | 0.60              |
| 1:A:23:LEU:HD23  | 1:A:24:ARG:N      | 2.17                     | 0.60              |
| 2:O:402:ILE:C    | 2:O:402:ILE:HD13  | 2.27                     | 0.60              |
| 5:R:81:ILE:HG22  | 5:R:100:HIS:HB2   | 1.83                     | 0.60              |
| 2:B:57:TYR:CE2   | 2:B:203:ARG:NH2   | 2.69                     | 0.60              |
| 2:O:27:THR:CG2   | 2:O:28:LYS:H      | 2.14                     | 0.60              |
| 5:R:83:GLU:HA    | 5:R:100:HIS:HB3   | 1.83                     | 0.60              |
| 6:F:42:ASP:OD1   | 6:F:101:ARG:NH1   | 2.34                     | 0.60              |
| 1:N:219:VAL:HG12 | 1:N:220:SER:N     | 2.16                     | 0.60              |
| 2:B:291:VAL:HA   | 2:B:297:GLN:HE21  | 1.65                     | 0.60              |
| 1:N:106:MET:HE3  | 1:N:110:VAL:HG21  | 1.84                     | 0.60              |
| 7:G:49:ALA:HB3   | 7:G:50:PRO:HD3    | 1.83                     | 0.60              |
| 1:N:395:TRP:HA   | 1:N:395:TRP:CE3   | 2.37                     | 0.60              |
| 5:R:78:LEU:HD11  | 5:R:187:PHE:CE1   | 2.37                     | 0.60              |
| 5:R:117:LEU:HD11 | 5:R:172:ARG:NH1   | 2.16                     | 0.59              |
| 4:D:43:MET:HE3   | 4:D:46:VAL:HG21   | 1.84                     | 0.59              |
| 1:N:178:THR:HG22 | 1:N:180:ALA:N     | 2.08                     | 0.59              |
| 3:P:22:LEU:HD21  | 14:P:3002:UQ:HM32 | 1.83                     | 0.59              |
| 5:R:134:ILE:HD12 | 5:R:185:TYR:CD1   | 2.37                     | 0.59              |
| 8:H:28:GLU:HG2   | 8:H:32:LYS:HE3    | 1.85                     | 0.59              |
| 6:S:17:ARG:HH11  | 6:S:17:ARG:HG2    | 1.68                     | 0.59              |
| 1:A:37:VAL:HG23  | 1:A:113:LEU:HD11  | 1.83                     | 0.59              |
| 2:B:59:THR:HG22  | 2:B:61:ALA:H      | 1.66                     | 0.59              |
| 1:N:269:VAL:HG22 | 1:N:406:MET:HE3   | 1.82                     | 0.59              |
| 5:R:109:GLU:OE1  | 5:R:123:ASP:HB2   | 2.02                     | 0.59              |
| 5:E:116:LYS:HD2  | 5:E:116:LYS:N     | 2.17                     | 0.59              |
| 5:E:122:HIS:HE1  | 5:E:124:LEU:HD12  | 1.68                     | 0.59              |
| 5:E:164:HIS:HD2  | 5:E:173:LYS:HB3   | 1.68                     | 0.59              |
| 8:H:27:THR:O     | 8:H:31:VAL:HG23   | 2.02                     | 0.59              |
| 5:R:81:ILE:HG12  | 5:R:87:VAL:HG21   | 1.84                     | 0.59              |
| 5:R:171:ILE:HG22 | 5:R:179:ASN:OD1   | 2.02                     | 0.59              |
| 4:D:74:PRO:HB2   | 4:D:78:GLY:HA2    | 1.84                     | 0.59              |
| 3:P:313:GLN:NE2  | 6:S:36:THR:OG1    | 2.36                     | 0.59              |
| 1:A:106:MET:HE2  | 1:A:107:PRO:CA    | 2.32                     | 0.59              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 15:C:2004:CDL:HA32 | 7:G:40:ARG:HB3   | 1.85                     | 0.59              |
| 1:N:69:LYS:HD2     | 1:N:70:ARG:NH2   | 2.15                     | 0.59              |
| 2:O:169:LYS:HG3    | 2:O:240:TRP:HB2  | 1.84                     | 0.59              |
| 3:P:212:ILE:HD12   | 6:S:62:ILE:HG23  | 1.85                     | 0.59              |
| 5:R:171:ILE:HG12   | 5:R:176:ALA:O    | 2.02                     | 0.59              |
| 8:U:27:THR:O       | 8:U:31:VAL:HG23  | 2.02                     | 0.59              |
| 2:B:361:LYS:O      | 2:B:365:LYS:HG3  | 2.02                     | 0.59              |
| 5:E:101:ARG:HA     | 5:E:105:GLU:OE1  | 2.03                     | 0.59              |
| 5:E:163:SER:HA     | 5:E:174:GLY:HA3  | 1.85                     | 0.59              |
| 5:R:76:ILE:O       | 5:R:193:VAL:HG12 | 2.03                     | 0.59              |
| 6:S:59:MET:HE3     | 6:S:59:MET:HA    | 1.85                     | 0.59              |
| 1:A:170:THR:HG22   | 1:A:172:GLU:H    | 1.68                     | 0.58              |
| 3:P:34:PHE:HB2     | 20:P:381:HOH:O   | 2.03                     | 0.58              |
| 1:A:106:MET:HE3    | 1:A:110:VAL:HG21 | 1.84                     | 0.58              |
| 2:B:207:VAL:HG21   | 2:B:383:GLY:HA3  | 1.86                     | 0.58              |
| 2:B:291:VAL:HA     | 2:B:297:GLN:NE2  | 2.17                     | 0.58              |
| 5:E:147:ILE:O      | 5:E:156:TYR:HA   | 2.04                     | 0.58              |
| 1:N:37:VAL:HG12    | 1:N:199:ALA:CB   | 2.33                     | 0.58              |
| 4:Q:76:GLU:CD      | 4:Q:76:GLU:H     | 2.10                     | 0.58              |
| 5:R:136:VAL:HG23   | 5:R:183:PRO:HD3  | 1.84                     | 0.58              |
| 1:A:430:GLN:HG3    | 7:G:4:PHE:O      | 2.03                     | 0.58              |
| 2:B:341:MET:CE     | 2:B:341:MET:HA   | 2.34                     | 0.58              |
| 1:N:63:ALA:O       | 1:N:116:VAL:HG13 | 2.03                     | 0.58              |
| 4:D:134:TYR:CG     | 4:D:162:PRO:HG3  | 2.39                     | 0.58              |
| 1:N:282:ARG:NH2    | 9:V:37:UNK:N     | 2.51                     | 0.58              |
| 2:O:341:MET:HE1    | 2:O:417:PHE:CE2  | 2.27                     | 0.58              |
| 1:A:103:SER:HB3    | 1:A:202:GLY:O    | 2.04                     | 0.58              |
| 5:E:86:ASN:HB2     | 5:E:99:ARG:HE    | 1.67                     | 0.58              |
| 2:O:422:LYS:O      | 2:O:436:LEU:HD21 | 2.02                     | 0.58              |
| 8:U:27:THR:HG22    | 8:U:29:LYS:H     | 1.67                     | 0.58              |
| 2:B:31:ASN:N       | 2:B:31:ASN:ND2   | 2.47                     | 0.58              |
| 1:N:112:LEU:O      | 1:N:116:VAL:HG23 | 2.03                     | 0.58              |
| 7:T:72:LYS:CE      | 8:U:57:GLU:OE1   | 2.51                     | 0.58              |
| 1:N:269:VAL:CG2    | 1:N:406:MET:HE3  | 2.33                     | 0.58              |
| 7:T:49:ALA:HB3     | 7:T:50:PRO:HD3   | 1.85                     | 0.58              |
| 1:A:371:GLY:O      | 1:A:375:VAL:HG23 | 2.04                     | 0.58              |
| 1:N:60:GLU:OE2     | 1:N:90:THR:HG22  | 2.03                     | 0.58              |
| 1:A:402:VAL:HG22   | 1:A:406:MET:CE   | 2.34                     | 0.58              |
| 2:B:101:THR:HG23   | 2:B:104:LYS:HE3  | 1.86                     | 0.58              |
| 1:N:298:ALA:HA     | 1:N:303:LEU:HB2  | 1.84                     | 0.58              |
| 2:O:414:ALA:O      | 2:O:418:VAL:HG23 | 2.04                     | 0.58              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:37:VAL:HG12  | 1:A:199:ALA:CB     | 2.34                     | 0.58              |
| 4:D:229:VAL:CG2  | 7:G:20:PRO:HG3     | 2.34                     | 0.58              |
| 5:E:76:ILE:O     | 5:E:193:VAL:HG12   | 2.04                     | 0.58              |
| 3:P:313:GLN:HE21 | 6:S:36:THR:CB      | 2.17                     | 0.58              |
| 5:E:76:ILE:CD1   | 5:E:98:VAL:HG21    | 2.34                     | 0.57              |
| 5:E:99:ARG:HD3   | 5:E:105:GLU:OE2    | 2.03                     | 0.57              |
| 2:O:241:GLY:HA2  | 2:O:423:SER:HB3    | 1.86                     | 0.57              |
| 2:O:332:HIS:O    | 2:O:336:VAL:HG23   | 2.03                     | 0.57              |
| 2:O:341:MET:CE   | 2:O:417:PHE:HE2    | 2.15                     | 0.57              |
| 2:O:215:ASP:O    | 2:O:219:VAL:HG23   | 2.04                     | 0.57              |
| 3:P:377:MET:HE2  | 6:S:20:TYR:CD1     | 2.39                     | 0.57              |
| 3:C:153:ALA:HB2  | 3:C:288:LYS:HG2    | 1.85                     | 0.57              |
| 4:D:195:GLU:OE1  | 4:D:201:ARG:NH2    | 2.38                     | 0.57              |
| 5:R:102:THR:O    | 5:R:106:ILE:HG13   | 2.04                     | 0.57              |
| 7:T:41:PHE:CE2   | 7:T:45:VAL:HG21    | 2.39                     | 0.57              |
| 1:A:274:ASN:ND2  | 1:A:309:THR:HB     | 2.20                     | 0.57              |
| 2:B:341:MET:HA   | 2:B:341:MET:HE2    | 1.86                     | 0.57              |
| 6:F:84:GLU:H     | 6:F:84:GLU:CD      | 2.12                     | 0.57              |
| 1:N:186:ILE:HG23 | 1:N:190:PHE:CD1    | 2.40                     | 0.57              |
| 4:Q:75:ASP:OD2   | 4:Q:79:GLU:HB2     | 2.04                     | 0.57              |
| 3:C:147:ILE:CG1  | 13:C:2001:JZV:HAP  | 2.29                     | 0.57              |
| 4:D:169:LEU:C    | 4:D:169:LEU:HD23   | 2.30                     | 0.57              |
| 5:E:84:GLY:N     | 5:E:100:HIS:O      | 2.33                     | 0.57              |
| 2:O:338:ARG:HH11 | 2:O:338:ARG:CG     | 2.09                     | 0.57              |
| 1:A:178:THR:CG2  | 1:A:179:ARG:N      | 2.68                     | 0.57              |
| 2:B:150:VAL:O    | 2:B:153:GLN:HG3    | 2.05                     | 0.57              |
| 3:C:30:ALA:HB1   | 15:D:2003:CDL:H111 | 1.86                     | 0.57              |
| 4:D:231:LYS:O    | 6:F:71:LYS:HE3     | 2.05                     | 0.57              |
| 6:S:91:GLU:HG2   | 6:S:95:LYS:HE3     | 1.86                     | 0.57              |
| 6:S:95:LYS:O     | 6:S:99:ARG:HG3     | 2.03                     | 0.57              |
| 5:E:136:VAL:CG2  | 5:E:183:PRO:HD3    | 2.33                     | 0.57              |
| 7:G:65:GLU:O     | 7:G:69:LEU:HG      | 2.04                     | 0.57              |
| 1:N:18:THR:HG23  | 1:N:24:ARG:HG3     | 1.87                     | 0.57              |
| 2:O:292:THR:HG22 | 2:O:292:THR:O      | 2.02                     | 0.57              |
| 5:R:86:ASN:OD1   | 5:R:99:ARG:HB2     | 2.05                     | 0.57              |
| 1:A:364:ALA:O    | 1:A:368:GLN:HG3    | 2.05                     | 0.57              |
| 1:N:85:HIS:NE2   | 2:O:284:LEU:HD22   | 2.20                     | 0.57              |
| 4:Q:2:GLU:O      | 4:Q:3:LEU:O        | 2.22                     | 0.57              |
| 2:B:75:LEU:HD22  | 2:B:136:GLU:HB3    | 1.86                     | 0.56              |
| 2:B:357:VAL:O    | 2:B:361:LYS:HG3    | 2.05                     | 0.56              |
| 1:N:364:ALA:O    | 1:N:368:GLN:HG3    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:63:LEU:HB2   | 2:O:182:ARG:HD3  | 1.87                     | 0.56              |
| 2:B:206:LEU:HD23 | 2:B:220:ALA:HB2  | 1.86                     | 0.56              |
| 4:D:43:MET:HE2   | 4:D:91:PHE:CD2   | 2.40                     | 0.56              |
| 5:R:186:GLN:O    | 5:R:193:VAL:HG23 | 2.04                     | 0.56              |
| 2:B:31:ASN:HD22  | 2:B:31:ASN:H     | 1.48                     | 0.56              |
| 2:B:341:MET:HE1  | 2:B:417:PHE:CE2  | 2.28                     | 0.56              |
| 5:E:144:CYS:HB2  | 5:E:158:CYS:SG   | 2.45                     | 0.56              |
| 1:N:36:THR:HG21  | 1:N:373:THR:HA   | 1.86                     | 0.56              |
| 1:N:321:GLY:HA2  | 1:N:342:TRP:HZ2  | 1.70                     | 0.56              |
| 1:N:430:GLN:HG3  | 7:T:4:PHE:O      | 2.05                     | 0.56              |
| 4:Q:169:LEU:HD22 | 4:Q:182:ILE:HD11 | 1.87                     | 0.56              |
| 7:G:28:ASN:HB3   | 7:G:31:SER:OG    | 2.06                     | 0.56              |
| 2:O:299:VAL:HG11 | 2:O:336:VAL:HG13 | 1.86                     | 0.56              |
| 5:R:45:VAL:HG13  | 10:W:28:ALA:HA   | 1.87                     | 0.56              |
| 2:B:264:VAL:HG23 | 2:B:316:TYR:C    | 2.30                     | 0.56              |
| 2:B:332:HIS:O    | 2:B:336:VAL:HG23 | 2.06                     | 0.56              |
| 2:B:402:ILE:HD13 | 2:B:402:ILE:C    | 2.31                     | 0.56              |
| 2:O:206:LEU:CD2  | 2:O:220:ALA:HB2  | 2.35                     | 0.56              |
| 4:Q:139:ALA:HB3  | 8:U:54:CYS:SG    | 2.45                     | 0.56              |
| 9:V:70:LEU:HD23  | 9:V:71:ASN:OD1   | 2.06                     | 0.56              |
| 1:N:178:THR:CG2  | 1:N:179:ARG:N    | 2.68                     | 0.56              |
| 5:R:106:ILE:O    | 5:R:109:GLU:HB3  | 2.05                     | 0.56              |
| 1:A:269:VAL:HG22 | 1:A:406:MET:HE3  | 1.87                     | 0.56              |
| 1:A:395:TRP:HA   | 1:A:395:TRP:CE3  | 2.41                     | 0.56              |
| 3:C:301:ILE:CD1  | 3:C:364:LEU:HD21 | 2.34                     | 0.56              |
| 1:N:170:THR:CG2  | 1:N:171:THR:N    | 2.68                     | 0.56              |
| 1:N:382:HIS:HB3  | 1:N:388:ARG:O    | 2.06                     | 0.56              |
| 2:B:414:ALA:O    | 2:B:418:VAL:HG23 | 2.06                     | 0.56              |
| 5:E:109:GLU:OE2  | 5:E:153:PHE:HB3  | 2.06                     | 0.56              |
| 2:O:69:LEU:HD23  | 2:O:105:MET:HE1  | 1.86                     | 0.56              |
| 1:N:279:ARG:HH22 | 9:V:30:UNK:C     | 2.19                     | 0.56              |
| 4:Q:43:MET:HE1   | 4:Q:189:PHE:HZ   | 1.68                     | 0.56              |
| 2:B:28:LYS:O     | 2:B:29:LEU:O     | 2.24                     | 0.56              |
| 1:N:37:VAL:HG23  | 1:N:113:LEU:HD11 | 1.88                     | 0.56              |
| 1:N:187:ASP:O    | 1:N:191:LYS:HE3  | 2.06                     | 0.56              |
| 5:R:86:ASN:HB2   | 5:R:99:ARG:HE    | 1.70                     | 0.56              |
| 6:S:53:ASP:OD1   | 6:S:54:LEU:N     | 2.39                     | 0.56              |
| 2:O:38:LEU:HD12  | 2:O:39:GLU:N     | 2.21                     | 0.55              |
| 2:B:47:ILE:HG21  | 2:B:120:MET:HE1  | 1.87                     | 0.55              |
| 2:B:395:PRO:HA   | 2:B:398:VAL:HG12 | 1.89                     | 0.55              |
| 3:P:106:GLY:HA2  | 3:P:108:TYR:CE2  | 2.41                     | 0.55              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 5:R:186:GLN:NE2    | 5:R:188:VAL:HG13 | 2.20                     | 0.55              |
| 2:B:23:ASP:OD1     | 2:B:24:LEU:N     | 2.38                     | 0.55              |
| 2:B:201:SER:OG     | 2:B:228:SER:HA   | 2.07                     | 0.55              |
| 1:N:4:TYR:HB3      | 2:O:114:ASP:OD2  | 2.07                     | 0.55              |
| 2:O:56:ARG:HH12    | 2:O:172:LEU:HG   | 1.71                     | 0.55              |
| 2:O:150:VAL:O      | 2:O:153:GLN:HG3  | 2.06                     | 0.55              |
| 15:P:3004:CDL:OA4  | 7:T:40:ARG:HD2   | 2.07                     | 0.55              |
| 4:Q:222:MET:HE3    | 5:R:40:THR:OG1   | 2.06                     | 0.55              |
| 4:Q:237:TYR:HB2    | 6:S:60:PHE:CG    | 2.40                     | 0.55              |
| 5:R:117:LEU:HD21   | 5:R:172:ARG:NH1  | 2.21                     | 0.55              |
| 1:A:85:HIS:NE2     | 2:B:284:LEU:HD22 | 2.22                     | 0.55              |
| 9:I:29:UNK:O       | 9:I:30:UNK:HB2   | 2.05                     | 0.55              |
| 1:N:170:THR:HG22   | 1:N:171:THR:H    | 1.71                     | 0.55              |
| 2:O:397:VAL:O      | 2:O:401:LYS:HG2  | 2.07                     | 0.55              |
| 5:R:118:ARG:NH1    | 5:R:174:GLY:O    | 2.40                     | 0.55              |
| 1:A:282:ARG:NH2    | 9:I:35:UNK:HA    | 2.22                     | 0.55              |
| 2:B:63:LEU:HB2     | 2:B:182:ARG:HD3  | 1.87                     | 0.55              |
| 7:G:72:LYS:HE2     | 8:H:57:GLU:OE1   | 2.06                     | 0.55              |
| 1:N:35:CYS:SG      | 1:N:203:ILE:HD11 | 2.46                     | 0.55              |
| 1:A:187:ASP:O      | 1:A:191:LYS:HE3  | 2.07                     | 0.55              |
| 2:B:248:ASN:HD21   | 2:B:250:HIS:HB2  | 1.71                     | 0.55              |
| 5:E:106:ILE:O      | 5:E:110:ALA:HB3  | 2.07                     | 0.55              |
| 5:R:134:ILE:HD12   | 5:R:185:TYR:CE1  | 2.41                     | 0.55              |
| 3:C:301:ILE:HD11   | 3:C:364:LEU:CD2  | 2.34                     | 0.55              |
| 5:E:45:VAL:HG13    | 10:J:28:ALA:HA   | 1.89                     | 0.55              |
| 5:R:164:HIS:HD2    | 5:R:173:LYS:HB3  | 1.72                     | 0.55              |
| 2:B:341:MET:CE     | 2:B:417:PHE:HE2  | 2.14                     | 0.55              |
| 2:B:422:LYS:O      | 2:B:436:LEU:HD21 | 2.06                     | 0.55              |
| 2:O:247:GLN:HE22   | 2:O:429:ASP:HA   | 1.71                     | 0.55              |
| 2:O:341:MET:CE     | 2:O:341:MET:HA   | 2.37                     | 0.55              |
| 6:S:42:ASP:OD1     | 6:S:101:ARG:NH1  | 2.39                     | 0.55              |
| 2:B:299:VAL:HG11   | 2:B:336:VAL:HG13 | 1.88                     | 0.55              |
| 2:B:338:ARG:NH1    | 2:B:338:ARG:CG   | 2.69                     | 0.55              |
| 2:O:47:ILE:HD13    | 2:O:120:MET:HE1  | 1.89                     | 0.55              |
| 3:P:78:TRP:CZ3     | 4:Q:201:ARG:HG3  | 2.42                     | 0.55              |
| 15:Q:3003:CDL:HB22 | 7:T:40:ARG:NH2   | 2.22                     | 0.55              |
| 8:U:28:GLU:HG2     | 8:U:32:LYS:HE3   | 1.89                     | 0.55              |
| 2:O:152:PHE:HA     | 2:O:157:VAL:HG11 | 1.88                     | 0.55              |
| 3:C:286:PRO:O      | 3:C:287:ASN:HB2  | 2.08                     | 0.54              |
| 1:N:3:THR:HG23     | 1:N:6:GLN:OE1    | 2.07                     | 0.54              |
| 1:N:10:ASN:ND2     | 2:O:19:PRO:CD    | 2.70                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:291:VAL:HA     | 2:O:297:GLN:NE2    | 2.22                     | 0.54              |
| 2:O:338:ARG:NH1    | 2:O:338:ARG:CG     | 2.68                     | 0.54              |
| 1:N:106:MET:HE2    | 1:N:107:PRO:CA     | 2.37                     | 0.54              |
| 2:O:152:PHE:HA     | 2:O:157:VAL:CG1    | 2.37                     | 0.54              |
| 2:O:31:ASN:N       | 2:O:31:ASN:HD22    | 2.05                     | 0.54              |
| 8:U:18:THR:O       | 8:U:22:GLU:HG3     | 2.07                     | 0.54              |
| 1:A:298:ALA:HA     | 1:A:303:LEU:HB2    | 1.88                     | 0.54              |
| 1:N:233:ARG:HH21   | 1:N:316:ASP:HB2    | 1.73                     | 0.54              |
| 2:O:56:ARG:NH1     | 2:O:172:LEU:HG     | 2.22                     | 0.54              |
| 2:O:57:TYR:CE2     | 2:O:203:ARG:NH2    | 2.71                     | 0.54              |
| 5:E:135:LEU:HD11   | 5:E:169:GLY:HA3    | 1.88                     | 0.54              |
| 5:E:146:PRO:HG2    | 5:E:180:LEU:HD21   | 1.89                     | 0.54              |
| 5:E:188:VAL:HG12   | 5:E:188:VAL:O      | 2.08                     | 0.54              |
| 2:O:207:VAL:HG21   | 2:O:383:GLY:HA2    | 1.88                     | 0.54              |
| 2:O:357:VAL:O      | 2:O:361:LYS:HG3    | 2.07                     | 0.54              |
| 2:B:56:ARG:NH1     | 2:B:172:LEU:HG     | 2.22                     | 0.54              |
| 2:B:76:THR:CG2     | 2:B:82:SER:H       | 2.06                     | 0.54              |
| 3:P:199:THR:HA     | 18:P:2010:BOG:O1   | 2.08                     | 0.54              |
| 5:R:184:THR:O      | 5:R:185:TYR:HB3    | 2.07                     | 0.54              |
| 1:A:307:PHE:CD1    | 1:A:307:PHE:C      | 2.85                     | 0.54              |
| 2:B:124:LEU:HD11   | 2:B:223:PHE:CB     | 2.33                     | 0.54              |
| 3:P:325:LEU:HD21   | 3:P:366:LEU:HB3    | 1.89                     | 0.54              |
| 4:Q:70:VAL:HG21    | 4:Q:83:ARG:CZ      | 2.38                     | 0.54              |
| 1:A:196:VAL:HG11   | 1:A:383:LEU:HD12   | 1.90                     | 0.54              |
| 3:C:328:LEU:CD1    | 7:G:51:PRO:HB3     | 2.37                     | 0.54              |
| 6:F:53:ASP:OD1     | 6:F:54:LEU:N       | 2.39                     | 0.54              |
| 2:O:168:TYR:CE2    | 2:O:172:LEU:HD12   | 2.42                     | 0.54              |
| 2:O:374:THR:HG22   | 2:O:376:GLN:H      | 1.72                     | 0.54              |
| 5:R:165:TYR:CD2    | 5:R:180:LEU:HG     | 2.43                     | 0.54              |
| 10:J:7:ARG:NH1     | 10:J:7:ARG:CB      | 2.70                     | 0.54              |
| 3:P:30:ALA:HB1     | 15:Q:3003:CDL:H111 | 1.90                     | 0.54              |
| 2:B:168:TYR:CE2    | 2:B:172:LEU:HD12   | 2.43                     | 0.53              |
| 5:E:84:GLY:CA      | 5:E:102:THR:HG23   | 2.38                     | 0.53              |
| 1:N:23:LEU:HD23    | 1:N:24:ARG:N       | 2.23                     | 0.53              |
| 1:N:209:VAL:O      | 1:N:212:ALA:HB3    | 2.07                     | 0.53              |
| 1:N:281:ASP:HB2    | 9:V:33:UNK:HB2     | 1.91                     | 0.53              |
| 15:P:3004:CDL:H712 | 11:P:3007:PEE:H50  | 1.90                     | 0.53              |
| 1:A:151:ASP:OD2    | 5:E:2:HIS:NE2      | 2.28                     | 0.53              |
| 2:B:24:LEU:HD12    | 2:B:37:SER:O       | 2.07                     | 0.53              |
| 3:C:216:SER:HB3    | 6:F:59:MET:HE2     | 1.88                     | 0.53              |
| 3:C:263:LEU:O      | 3:C:264:VAL:HG23   | 2.08                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:J:56:LYS:O      | 10:J:60:GLU:HB2   | 2.08                     | 0.53              |
| 2:O:47:ILE:HD11    | 2:O:116:VAL:HG13  | 1.90                     | 0.53              |
| 2:O:291:VAL:HA     | 2:O:297:GLN:HE21  | 1.74                     | 0.53              |
| 11:R:3005:PEE:H58  | 10:W:24:VAL:HG11  | 1.90                     | 0.53              |
| 1:A:36:THR:HG21    | 1:A:373:THR:HA    | 1.91                     | 0.53              |
| 2:B:247:GLN:HE22   | 2:B:429:ASP:HA    | 1.73                     | 0.53              |
| 5:E:81:ILE:HG22    | 5:E:100:HIS:HB2   | 1.88                     | 0.53              |
| 2:O:252:LEU:HD13   | 9:V:55:MET:HE3    | 1.91                     | 0.53              |
| 4:Q:221:TYR:CD2    | 5:R:39:VAL:HG11   | 2.43                     | 0.53              |
| 7:T:65:GLU:O       | 7:T:69:LEU:HG     | 2.08                     | 0.53              |
| 15:D:2003:CDL:HB22 | 7:G:40:ARG:NH2    | 2.23                     | 0.53              |
| 8:U:22:GLU:O       | 8:U:26:GLN:HG2    | 2.08                     | 0.53              |
| 1:A:105:ASP:O      | 1:A:109:VAL:HG23  | 2.08                     | 0.53              |
| 5:E:131:GLU:CD     | 5:E:131:GLU:H     | 2.17                     | 0.53              |
| 2:O:372:VAL:HG12   | 2:O:372:VAL:O     | 2.08                     | 0.53              |
| 5:R:119:ASP:HB3    | 5:R:179:ASN:HD21  | 1.74                     | 0.53              |
| 3:C:278:ALA:HB1    | 3:C:295:LEU:CD1   | 2.38                     | 0.53              |
| 3:C:325:LEU:HD21   | 3:C:366:LEU:HB3   | 1.90                     | 0.53              |
| 4:D:70:VAL:HG21    | 4:D:83:ARG:CZ     | 2.39                     | 0.53              |
| 5:E:165:TYR:HA     | 5:E:170:ARG:O     | 2.09                     | 0.53              |
| 6:S:84:GLU:CD      | 6:S:84:GLU:H      | 2.15                     | 0.53              |
| 3:C:45:GLN:CB      | 12:C:501:HEM:HAB  | 2.38                     | 0.53              |
| 3:C:127:THR:HG21   | 12:C:501:HEM:HBB2 | 1.91                     | 0.53              |
| 1:A:170:THR:CG2    | 1:A:171:THR:N     | 2.72                     | 0.53              |
| 2:B:36:ALA:HB3     | 2:B:207:VAL:HG13  | 1.91                     | 0.53              |
| 2:B:189:GLU:OE1    | 2:B:189:GLU:N     | 2.42                     | 0.53              |
| 9:I:65:VAL:HG12    | 9:I:66:ALA:N      | 2.24                     | 0.53              |
| 1:A:358:LYS:HE3    | 1:A:399:ILE:O     | 2.08                     | 0.53              |
| 2:B:152:PHE:HA     | 2:B:157:VAL:HG11  | 1.91                     | 0.53              |
| 2:B:206:LEU:HG     | 2:B:216:LEU:HD11  | 1.90                     | 0.53              |
| 2:B:374:THR:HG22   | 2:B:376:GLN:H     | 1.74                     | 0.53              |
| 4:D:215:LEU:HD13   | 5:E:46:ALA:HB3    | 1.90                     | 0.53              |
| 5:E:101:ARG:HB2    | 5:E:131:GLU:HA    | 1.90                     | 0.53              |
| 2:O:124:LEU:HD11   | 2:O:223:PHE:HB3   | 1.91                     | 0.53              |
| 5:R:131:GLU:OE1    | 5:R:131:GLU:N     | 2.40                     | 0.53              |
| 4:D:229:VAL:HG23   | 7:G:20:PRO:HG3    | 1.91                     | 0.52              |
| 1:N:7:THR:HG21     | 2:O:113:ARG:CD    | 2.38                     | 0.52              |
| 2:O:248:ASN:C      | 2:O:248:ASN:ND2   | 2.56                     | 0.52              |
| 2:O:299:VAL:CG1    | 2:O:336:VAL:HG13  | 2.39                     | 0.52              |
| 10:W:52:TRP:O      | 10:W:56:LYS:HB2   | 2.09                     | 0.52              |
| 2:B:56:ARG:HH12    | 2:B:172:LEU:HG    | 1.73                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:437:ASP:C    | 2:B:437:ASP:OD1   | 2.52                     | 0.52              |
| 8:H:27:THR:HG22  | 8:H:29:LYS:H      | 1.74                     | 0.52              |
| 1:N:395:TRP:HA   | 1:N:395:TRP:HE3   | 1.72                     | 0.52              |
| 2:B:152:PHE:HA   | 2:B:157:VAL:CG1   | 2.40                     | 0.52              |
| 3:C:25:PRO:HB2   | 3:C:28:ILE:HG23   | 1.90                     | 0.52              |
| 1:N:48:GLU:CD    | 1:N:54:GLY:H      | 2.18                     | 0.52              |
| 2:B:344:LEU:HD13 | 2:B:417:PHE:CE2   | 2.44                     | 0.52              |
| 1:N:331:ILE:CG2  | 1:N:431:LEU:HB2   | 2.38                     | 0.52              |
| 2:O:75:LEU:HD22  | 2:O:136:GLU:HB3   | 1.92                     | 0.52              |
| 7:T:50:PRO:HB2   | 7:T:51:PRO:CD     | 2.39                     | 0.52              |
| 5:R:164:HIS:CD2  | 5:R:173:LYS:HB3   | 2.45                     | 0.52              |
| 1:A:280:TYR:CG   | 1:A:281:ASP:N     | 2.78                     | 0.52              |
| 2:B:76:THR:HG23  | 2:B:136:GLU:OE1   | 2.09                     | 0.52              |
| 3:C:234:THR:HG21 | 4:D:219:LEU:HD12  | 1.92                     | 0.52              |
| 3:C:313:GLN:HE21 | 6:F:36:THR:CB     | 2.22                     | 0.52              |
| 4:D:47:ALA:HA    | 4:D:90:TYR:HA     | 1.91                     | 0.52              |
| 4:D:68:VAL:HG11  | 4:D:92:PRO:HG3    | 1.91                     | 0.52              |
| 4:Q:229:VAL:CG2  | 7:T:20:PRO:HG3    | 2.39                     | 0.52              |
| 2:B:372:VAL:HG12 | 2:B:372:VAL:O     | 2.09                     | 0.52              |
| 3:P:127:THR:HG21 | 12:P:501:HEM:HBB2 | 1.90                     | 0.52              |
| 3:P:286:PRO:O    | 3:P:287:ASN:HB2   | 2.09                     | 0.52              |
| 4:Q:167:GLU:CG   | 8:U:13:LEU:HD12   | 2.40                     | 0.52              |
| 5:R:113:ASP:HB2  | 5:R:116:LYS:HB2   | 1.92                     | 0.52              |
| 1:A:106:MET:HE2  | 1:A:106:MET:C     | 2.34                     | 0.52              |
| 1:A:217:SER:O    | 1:A:218:GLY:C     | 2.52                     | 0.52              |
| 2:B:59:THR:HG22  | 2:B:60:THR:N      | 2.25                     | 0.52              |
| 5:E:78:LEU:HD11  | 5:E:187:PHE:CD2   | 2.45                     | 0.52              |
| 5:E:102:THR:O    | 5:E:103:GLN:HG3   | 2.10                     | 0.52              |
| 5:E:164:HIS:CD2  | 5:E:173:LYS:HB3   | 2.44                     | 0.52              |
| 1:N:317:THR:HG23 | 1:N:318:GLY:N     | 2.25                     | 0.52              |
| 1:N:358:LYS:HE3  | 1:N:399:ILE:O     | 2.09                     | 0.52              |
| 2:O:47:ILE:HD13  | 2:O:120:MET:HE2   | 1.91                     | 0.52              |
| 3:P:234:THR:HG21 | 4:Q:219:LEU:HD12  | 1.90                     | 0.52              |
| 5:E:114:VAL:HG21 | 5:E:172:ARG:NH1   | 2.24                     | 0.52              |
| 4:Q:161:ALA:O    | 4:Q:162:PRO:C     | 2.53                     | 0.52              |
| 8:U:43:ARG:O     | 8:U:47:ARG:HG3    | 2.09                     | 0.52              |
| 9:V:65:VAL:HG12  | 9:V:66:ALA:N      | 2.25                     | 0.52              |
| 1:A:288:LYS:HE3  | 1:A:289:HIS:CE1   | 2.45                     | 0.52              |
| 4:D:43:MET:HE1   | 4:D:189:PHE:HZ    | 1.70                     | 0.52              |
| 4:D:75:ASP:OD2   | 4:D:79:GLU:HB2    | 2.10                     | 0.52              |
| 8:H:10:GLU:O     | 8:H:11:GLU:HG3    | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:173:ASN:O    | 1:N:177:LEU:HG   | 2.10                     | 0.52              |
| 1:N:217:SER:O    | 1:N:218:GLY:C    | 2.52                     | 0.52              |
| 1:N:307:PHE:CD1  | 1:N:307:PHE:C    | 2.86                     | 0.52              |
| 2:O:35:ILE:HD13  | 2:O:217:LYS:HA   | 1.92                     | 0.52              |
| 2:O:221:GLU:C    | 2:O:223:PHE:H    | 2.17                     | 0.52              |
| 2:O:222:GLN:O    | 2:O:222:GLN:HG2  | 2.10                     | 0.52              |
| 2:O:344:LEU:HD13 | 2:O:417:PHE:CE2  | 2.45                     | 0.52              |
| 7:T:48:VAL:O     | 7:T:51:PRO:HD2   | 2.10                     | 0.52              |
| 1:A:222:THR:OG1  | 1:A:225:GLU:HG3  | 2.09                     | 0.51              |
| 2:B:35:ILE:HD13  | 2:B:217:LYS:HA   | 1.92                     | 0.51              |
| 5:E:135:LEU:HD23 | 5:E:182:VAL:HG22 | 1.92                     | 0.51              |
| 2:O:56:ARG:HG3   | 2:O:56:ARG:HH11  | 1.75                     | 0.51              |
| 3:P:301:ILE:HD11 | 3:P:364:LEU:CD2  | 2.35                     | 0.51              |
| 3:C:31:TRP:NE1   | 11:C:2007:PEE:O4 | 2.43                     | 0.51              |
| 3:C:279:TYR:O    | 3:C:283:ARG:HG3  | 2.10                     | 0.51              |
| 1:N:131:ARG:NH2  | 1:N:177:LEU:O    | 2.44                     | 0.51              |
| 2:O:203:ARG:HD2  | 2:O:230:ALA:O    | 2.10                     | 0.51              |
| 2:O:395:PRO:HA   | 2:O:398:VAL:HG12 | 1.91                     | 0.51              |
| 5:R:163:SER:H    | 5:R:175:PRO:HD2  | 1.75                     | 0.51              |
| 6:S:91:GLU:O     | 6:S:95:LYS:HG3   | 2.09                     | 0.51              |
| 4:D:169:LEU:HD22 | 4:D:182:ILE:HD11 | 1.92                     | 0.51              |
| 1:N:45:SER:HA    | 1:N:48:GLU:HG3   | 1.92                     | 0.51              |
| 1:N:140:GLU:HG3  | 9:V:50:LEU:HD12  | 1.92                     | 0.51              |
| 4:Q:2:GLU:HB3    | 4:Q:3:LEU:HD12   | 1.91                     | 0.51              |
| 4:D:102:ARG:HB3  | 4:D:107:GLY:HA2  | 1.92                     | 0.51              |
| 10:W:40:ASP:O    | 10:W:44:GLU:HG3  | 2.09                     | 0.51              |
| 1:A:140:GLU:OE2  | 9:I:49:LEU:HA    | 2.10                     | 0.51              |
| 3:C:78:TRP:CZ3   | 4:D:201:ARG:HG3  | 2.45                     | 0.51              |
| 2:O:248:ASN:ND2  | 2:O:250:HIS:H    | 2.09                     | 0.51              |
| 4:Q:68:VAL:HG11  | 4:Q:92:PRO:HG3   | 1.93                     | 0.51              |
| 4:Q:237:TYR:HB2  | 6:S:60:PHE:CD1   | 2.46                     | 0.51              |
| 3:P:9:HIS:CD2    | 3:P:12:LEU:HG    | 2.46                     | 0.51              |
| 2:B:57:TYR:N     | 2:B:57:TYR:CD1   | 2.78                     | 0.51              |
| 5:E:190:ASP:O    | 5:E:192:LEU:N    | 2.43                     | 0.51              |
| 2:O:207:VAL:HG21 | 2:O:383:GLY:HA3  | 1.93                     | 0.51              |
| 5:R:77:LYS:HA    | 5:R:191:ASP:O    | 2.10                     | 0.51              |
| 5:R:78:LEU:HD11  | 5:R:187:PHE:CD1  | 2.46                     | 0.51              |
| 10:W:58:LYS:HB2  | 10:W:59:TYR:CE1  | 2.45                     | 0.51              |
| 5:E:187:PHE:C    | 5:E:189:GLY:N    | 2.66                     | 0.51              |
| 1:N:60:GLU:OE2   | 1:N:89:TYR:HA    | 2.11                     | 0.51              |
| 2:O:26:ILE:HG12  | 2:O:26:ILE:O     | 2.09                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:O:57:TYR:CD1   | 2:O:57:TYR:N      | 2.78                     | 0.51              |
| 2:O:437:ASP:OD1  | 2:O:437:ASP:C     | 2.54                     | 0.51              |
| 2:B:402:ILE:HG23 | 2:B:403:ASP:N     | 2.26                     | 0.51              |
| 6:S:11:ARG:HA    | 6:S:14:ASP:HB2    | 1.93                     | 0.51              |
| 2:B:299:VAL:CG1  | 2:B:336:VAL:HG13  | 2.40                     | 0.50              |
| 9:I:71:ASN:H     | 9:I:71:ASN:HD22   | 1.59                     | 0.50              |
| 1:N:41:ILE:HD13  | 1:N:190:PHE:CD2   | 2.46                     | 0.50              |
| 2:O:222:GLN:O    | 2:O:223:PHE:CD2   | 2.64                     | 0.50              |
| 10:W:7:ARG:NH1   | 10:W:7:ARG:CB     | 2.72                     | 0.50              |
| 1:A:48:GLU:CD    | 1:A:54:GLY:H      | 2.19                     | 0.50              |
| 9:I:49:LEU:HD22  | 9:I:54:SER:HB3    | 1.93                     | 0.50              |
| 2:O:43:PRO:O     | 2:O:113:ARG:HG3   | 2.11                     | 0.50              |
| 6:S:13:MET:HA    | 6:S:16:ILE:HD12   | 1.93                     | 0.50              |
| 1:A:269:VAL:CG2  | 1:A:406:MET:HE3   | 2.42                     | 0.50              |
| 1:A:331:ILE:CG2  | 1:A:431:LEU:HB2   | 2.40                     | 0.50              |
| 1:N:106:MET:HE2  | 1:N:106:MET:C     | 2.36                     | 0.50              |
| 1:N:368:GLN:O    | 1:N:369:LEU:HD23  | 2.12                     | 0.50              |
| 2:O:357:VAL:CG1  | 2:O:361:LYS:HE3   | 2.41                     | 0.50              |
| 2:O:361:LYS:HA   | 2:O:402:ILE:HD11  | 1.92                     | 0.50              |
| 1:N:10:ASN:HD21  | 2:O:19:PRO:HD2    | 1.75                     | 0.50              |
| 2:B:357:VAL:CG1  | 2:B:361:LYS:HE3   | 2.41                     | 0.50              |
| 3:C:207:ASN:ND2  | 3:C:208:ASN:H     | 2.10                     | 0.50              |
| 4:D:14:HIS:HB3   | 4:D:21:LEU:HA     | 1.94                     | 0.50              |
| 1:N:17:THR:HG23  | 1:N:205:HIS:NE2   | 2.27                     | 0.50              |
| 4:Q:240:PRO:O    | 4:Q:241:LYS:OXT   | 2.30                     | 0.50              |
| 5:R:162:GLY:O    | 5:R:163:SER:C     | 2.53                     | 0.50              |
| 5:R:165:TYR:HA   | 5:R:170:ARG:O     | 2.11                     | 0.50              |
| 2:B:402:ILE:HG23 | 2:B:403:ASP:H     | 1.77                     | 0.50              |
| 3:C:106:GLY:HA2  | 3:C:108:TYR:CE2   | 2.47                     | 0.50              |
| 5:E:165:TYR:CD2  | 5:E:180:LEU:HG    | 2.46                     | 0.50              |
| 1:N:64:PHE:HE2   | 1:N:86:PHE:CZ     | 2.30                     | 0.50              |
| 3:P:147:ILE:CG1  | 13:P:3001:JZV:HAP | 2.32                     | 0.50              |
| 1:A:62:LEU:HD11  | 1:A:127:ILE:HG12  | 1.94                     | 0.50              |
| 5:E:101:ARG:NH2  | 5:E:130:PRO:O     | 2.45                     | 0.50              |
| 5:E:190:ASP:C    | 5:E:192:LEU:N     | 2.67                     | 0.50              |
| 3:P:45:GLN:HB3   | 12:P:501:HEM:HAB  | 1.94                     | 0.50              |
| 8:U:36:ARG:HB3   | 8:U:36:ARG:CZ     | 2.41                     | 0.50              |
| 2:B:109:VAL:HG21 | 2:B:119:VAL:HG12  | 1.93                     | 0.50              |
| 2:B:225:ASN:O    | 2:B:226:ILE:C     | 2.54                     | 0.50              |
| 3:P:6:ARG:HG2    | 3:P:16:ASN:HB2    | 1.92                     | 0.50              |
| 3:P:101:ARG:C    | 3:P:101:ARG:CD    | 2.83                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:R:185:TYR:HB3  | 5:R:195:VAL:HA   | 1.94                     | 0.50              |
| 1:A:362:ARG:O    | 1:A:365:MET:HG2  | 2.11                     | 0.50              |
| 2:B:259:THR:HG22 | 2:B:260:GLU:N    | 2.26                     | 0.50              |
| 2:B:395:PRO:O    | 2:B:398:VAL:HG12 | 2.11                     | 0.50              |
| 4:D:29:GLY:HA3   | 4:D:189:PHE:HB2  | 1.94                     | 0.50              |
| 4:D:167:GLU:HG3  | 8:H:13:LEU:CD2   | 2.41                     | 0.50              |
| 1:N:151:ASP:OD2  | 5:R:2:HIS:NE2    | 2.30                     | 0.50              |
| 3:P:278:ALA:HB1  | 3:P:295:LEU:CD1  | 2.42                     | 0.50              |
| 7:T:50:PRO:HB2   | 7:T:51:PRO:HD3   | 1.94                     | 0.50              |
| 1:A:106:MET:HE2  | 1:A:107:PRO:N    | 2.27                     | 0.49              |
| 9:I:38:UNK:O     | 9:I:39:UNK:C     | 2.59                     | 0.49              |
| 9:V:33:UNK:HA    | 9:V:73:PRO:HB3   | 1.94                     | 0.49              |
| 2:B:207:VAL:HG21 | 2:B:383:GLY:HA2  | 1.94                     | 0.49              |
| 1:N:158:PHE:O    | 1:N:164:ALA:HB2  | 2.12                     | 0.49              |
| 5:R:178:TYR:N    | 5:R:178:TYR:CD1  | 2.80                     | 0.49              |
| 2:B:169:LYS:HG3  | 2:B:240:TRP:HB2  | 1.93                     | 0.49              |
| 3:C:377:MET:HE2  | 6:F:20:TYR:CG    | 2.47                     | 0.49              |
| 2:O:76:THR:HG22  | 2:O:82:SER:N     | 2.02                     | 0.49              |
| 2:O:109:VAL:HG21 | 2:O:119:VAL:HG12 | 1.94                     | 0.49              |
| 2:O:334:GLY:O    | 2:O:338:ARG:HG2  | 2.12                     | 0.49              |
| 2:B:33:LEU:CD2   | 2:B:224:LEU:HD12 | 2.37                     | 0.49              |
| 3:C:19:LEU:C     | 3:C:20:ILE:HG13  | 2.36                     | 0.49              |
| 2:O:47:ILE:CD1   | 2:O:116:VAL:HG13 | 2.41                     | 0.49              |
| 2:O:52:LYS:O     | 2:O:203:ARG:NH2  | 2.38                     | 0.49              |
| 4:Q:21:LEU:HD21  | 4:Q:191:ARG:HG3  | 1.93                     | 0.49              |
| 7:T:34:LEU:HB2   | 7:T:35:PRO:HD3   | 1.94                     | 0.49              |
| 2:B:26:ILE:HG12  | 2:B:26:ILE:O     | 2.12                     | 0.49              |
| 2:B:287:ARG:HB3  | 9:I:53:GLU:HG3   | 1.94                     | 0.49              |
| 7:G:80:ASP:O     | 7:G:81:GLN:C     | 2.55                     | 0.49              |
| 3:P:138:GLN:HB2  | 3:P:255:GLU:O    | 2.12                     | 0.49              |
| 3:P:238:THR:HB   | 3:P:239:PRO:CD   | 2.37                     | 0.49              |
| 4:Q:43:MET:HE2   | 4:Q:91:PHE:HE2   | 1.75                     | 0.49              |
| 5:R:144:CYS:HB2  | 5:R:158:CYS:SG   | 2.52                     | 0.49              |
| 2:B:402:ILE:O    | 2:B:405:VAL:HG23 | 2.13                     | 0.49              |
| 1:N:362:ARG:O    | 1:N:365:MET:HG2  | 2.12                     | 0.49              |
| 2:O:341:MET:HA   | 2:O:341:MET:HE2  | 1.93                     | 0.49              |
| 3:P:159:HIS:O    | 3:P:163:GLU:HG3  | 2.13                     | 0.49              |
| 3:P:301:ILE:CD1  | 3:P:364:LEU:HD21 | 2.36                     | 0.49              |
| 7:T:28:ASN:HB3   | 7:T:31:SER:OG    | 2.13                     | 0.49              |
| 1:A:131:ARG:NH2  | 1:A:177:LEU:O    | 2.45                     | 0.49              |
| 5:E:106:ILE:O    | 5:E:106:ILE:HG22 | 2.12                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:Q:200:GLN:NE2   | 18:Q:3091:BOG:H5 | 2.28                     | 0.49              |
| 6:S:40:ASP:O      | 6:S:44:LYS:HG3   | 2.13                     | 0.49              |
| 1:A:64:PHE:HE2    | 1:A:86:PHE:CZ    | 2.31                     | 0.49              |
| 2:B:397:VAL:O     | 2:B:401:LYS:HG2  | 2.13                     | 0.49              |
| 3:C:34:PHE:HB2    | 20:C:381:HOH:O   | 2.12                     | 0.49              |
| 3:C:263:LEU:O     | 3:C:264:VAL:CG2  | 2.61                     | 0.49              |
| 5:E:130:PRO:HG2   | 5:E:131:GLU:OE2  | 2.11                     | 0.49              |
| 1:N:321:GLY:HA2   | 1:N:342:TRP:CZ2  | 2.48                     | 0.49              |
| 5:R:95:PRO:HG2    | 5:R:145:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:321:GLY:HA2   | 1:A:342:TRP:HZ2  | 1.76                     | 0.49              |
| 3:C:138:GLN:HB2   | 3:C:255:GLU:O    | 2.13                     | 0.49              |
| 4:D:21:LEU:HD21   | 4:D:191:ARG:HG3  | 1.94                     | 0.49              |
| 4:D:43:MET:HE2    | 4:D:91:PHE:HE2   | 1.73                     | 0.49              |
| 5:E:122:HIS:HB3   | 5:E:125:ASP:OD1  | 2.13                     | 0.49              |
| 1:A:173:ASN:O     | 1:A:177:LEU:HG   | 2.13                     | 0.49              |
| 1:A:205:HIS:O     | 1:A:208:LEU:HB3  | 2.13                     | 0.49              |
| 2:B:47:ILE:HD11   | 2:B:116:VAL:HG13 | 1.95                     | 0.49              |
| 7:G:36:ASN:O      | 7:G:40:ARG:HG3   | 2.13                     | 0.49              |
| 2:B:306:PRO:HA    | 9:I:52:ARG:HG2   | 1.94                     | 0.48              |
| 2:B:334:GLY:O     | 2:B:338:ARG:HG2  | 2.13                     | 0.48              |
| 15:C:2004:CDL:OA4 | 7:G:40:ARG:HD2   | 2.13                     | 0.48              |
| 1:N:64:PHE:HE2    | 1:N:86:PHE:CE1   | 2.31                     | 0.48              |
| 2:O:325:TYR:CD1   | 9:V:60:ALA:HB3   | 2.48                     | 0.48              |
| 3:C:287:ASN:O     | 3:C:288:LYS:C    | 2.56                     | 0.48              |
| 5:E:127:VAL:O     | 5:E:128:LYS:HB2  | 2.13                     | 0.48              |
| 10:J:52:TRP:O     | 10:J:56:LYS:HB2  | 2.13                     | 0.48              |
| 1:N:106:MET:HE3   | 1:N:110:VAL:CG2  | 2.42                     | 0.48              |
| 1:A:23:LEU:HD23   | 1:A:23:LEU:C     | 2.38                     | 0.48              |
| 2:B:104:LYS:HD2   | 2:B:104:LYS:C    | 2.38                     | 0.48              |
| 4:D:149:TYR:CE1   | 4:D:156:GLN:HB3  | 2.47                     | 0.48              |
| 5:E:178:TYR:HD1   | 5:E:178:TYR:H    | 1.61                     | 0.48              |
| 10:J:49:GLY:N     | 10:J:54:HIS:ND1  | 2.61                     | 0.48              |
| 4:Q:229:VAL:HG23  | 7:T:20:PRO:HG3   | 1.94                     | 0.48              |
| 5:R:73:LYS:HB3    | 5:R:196:GLY:O    | 2.14                     | 0.48              |
| 1:A:35:CYS:SG     | 1:A:203:ILE:HD11 | 2.53                     | 0.48              |
| 1:A:422:LEU:HD22  | 1:A:437:ILE:CD1  | 2.42                     | 0.48              |
| 5:E:3:ASN:HD22    | 5:E:3:ASN:H      | 1.62                     | 0.48              |
| 1:N:46:ARG:NH1    | 1:N:316:ASP:OD1  | 2.36                     | 0.48              |
| 1:A:182:LEU:O     | 1:A:186:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:191:LYS:CA    | 1:A:195:MET:HE2  | 2.44                     | 0.48              |
| 1:A:395:TRP:HA    | 1:A:395:TRP:HE3  | 1.76                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:207:ASN:ND2  | 3:P:208:ASN:H    | 2.12                     | 0.48              |
| 7:T:29:ILE:O     | 7:T:33:ALA:HB3   | 2.13                     | 0.48              |
| 4:D:167:GLU:HG3  | 8:H:13:LEU:HD22  | 1.96                     | 0.48              |
| 5:E:142:LEU:HD12 | 5:E:161:HIS:CE1  | 2.48                     | 0.48              |
| 1:N:49:ASN:ND2   | 1:N:51:LYS:H     | 2.12                     | 0.48              |
| 1:N:222:THR:OG1  | 1:N:225:GLU:HG3  | 2.13                     | 0.48              |
| 2:O:248:ASN:HD22 | 2:O:249:GLY:N    | 2.12                     | 0.48              |
| 1:A:41:ILE:HD13  | 1:A:190:PHE:CD2  | 2.48                     | 0.48              |
| 2:B:89:ILE:HD13  | 2:B:96:LEU:HB2   | 1.96                     | 0.48              |
| 6:F:40:ASP:O     | 6:F:44:LYS:HG3   | 2.14                     | 0.48              |
| 1:N:106:MET:HE2  | 1:N:107:PRO:N    | 2.28                     | 0.48              |
| 3:P:156:TYR:C    | 3:P:158:GLY:H    | 2.19                     | 0.48              |
| 6:F:13:MET:O     | 6:F:17:ARG:HG3   | 2.12                     | 0.48              |
| 3:P:216:SER:CB   | 6:S:59:MET:HE2   | 2.43                     | 0.48              |
| 6:S:16:ILE:O     | 6:S:19:TRP:HB3   | 2.14                     | 0.48              |
| 10:W:49:GLY:N    | 10:W:54:HIS:ND1  | 2.61                     | 0.48              |
| 1:A:106:MET:HE3  | 1:A:110:VAL:CG2  | 2.42                     | 0.48              |
| 2:B:295:LEU:O    | 2:B:299:VAL:HG23 | 2.14                     | 0.48              |
| 2:B:325:TYR:CD1  | 9:I:60:ALA:HB3   | 2.49                     | 0.48              |
| 5:E:78:LEU:HD11  | 5:E:187:PHE:CE2  | 2.48                     | 0.48              |
| 5:E:185:TYR:O    | 5:E:186:GLN:HB3  | 2.14                     | 0.48              |
| 2:O:164:HIS:O    | 2:O:173:ALA:HA   | 2.14                     | 0.48              |
| 4:Q:195:GLU:OE1  | 4:Q:201:ARG:NH2  | 2.46                     | 0.48              |
| 3:C:6:ARG:HG2    | 3:C:16:ASN:HB2   | 1.95                     | 0.47              |
| 1:N:85:HIS:HB2   | 1:N:100:LYS:HB2  | 1.96                     | 0.47              |
| 1:N:433:ASP:OD1  | 1:N:436:ARG:HG2  | 2.13                     | 0.47              |
| 3:P:377:MET:HE2  | 6:S:20:TYR:CG    | 2.48                     | 0.47              |
| 4:Q:70:VAL:HG21  | 4:Q:83:ARG:NH2   | 2.28                     | 0.47              |
| 4:Q:149:TYR:CE1  | 4:Q:156:GLN:HB3  | 2.49                     | 0.47              |
| 7:T:80:ASP:HB3   | 8:U:47:ARG:HH11  | 1.78                     | 0.47              |
| 1:A:37:VAL:HG22  | 1:A:109:VAL:HG11 | 1.96                     | 0.47              |
| 1:A:85:HIS:HB2   | 1:A:100:LYS:HB2  | 1.95                     | 0.47              |
| 5:E:141:HIS:HB2  | 5:E:176:ALA:CB   | 2.42                     | 0.47              |
| 4:Q:171:TYR:OH   | 4:Q:182:ILE:HA   | 2.14                     | 0.47              |
| 1:A:95:THR:HG22  | 1:A:96:ALA:N     | 2.28                     | 0.47              |
| 1:A:178:THR:HG22 | 1:A:179:ARG:N    | 2.29                     | 0.47              |
| 4:D:186:VAL:O    | 4:D:190:LEU:HG   | 2.14                     | 0.47              |
| 4:D:220:TYR:O    | 4:D:224:ARG:HG2  | 2.14                     | 0.47              |
| 5:E:83:GLU:C     | 5:E:85:LYS:H     | 2.22                     | 0.47              |
| 5:E:102:THR:C    | 5:E:103:GLN:HG3  | 2.39                     | 0.47              |
| 5:E:116:LYS:HD2  | 5:E:116:LYS:H    | 1.78                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:141:HIS:HB3  | 19:E:501:FES:S2   | 2.54                     | 0.47              |
| 1:N:170:THR:CG2  | 1:N:171:THR:H     | 2.27                     | 0.47              |
| 3:P:28:ILE:HG12  | 3:P:225:TYR:OH    | 2.15                     | 0.47              |
| 1:A:382:HIS:HB3  | 1:A:388:ARG:O     | 2.13                     | 0.47              |
| 2:B:47:ILE:CD1   | 2:B:116:VAL:HG13  | 2.44                     | 0.47              |
| 3:C:28:ILE:CD1   | 14:C:2002:UQ:HM21 | 2.44                     | 0.47              |
| 1:N:53:ASN:HB3   | 1:N:173:ASN:ND2   | 2.29                     | 0.47              |
| 1:N:137:GLU:O    | 1:N:141:MET:HG3   | 2.13                     | 0.47              |
| 4:Q:186:VAL:O    | 4:Q:190:LEU:HG    | 2.14                     | 0.47              |
| 5:E:178:TYR:N    | 5:E:178:TYR:CD1   | 2.83                     | 0.47              |
| 8:H:43:ARG:O     | 8:H:47:ARG:HG3    | 2.15                     | 0.47              |
| 3:P:6:ARG:HD3    | 3:P:16:ASN:OD1    | 2.14                     | 0.47              |
| 4:Q:142:VAL:HG23 | 4:Q:142:VAL:O     | 2.14                     | 0.47              |
| 3:C:49:GLY:C     | 12:C:501:HEM:HAC  | 2.40                     | 0.47              |
| 5:E:77:LYS:HG3   | 5:E:191:ASP:O     | 2.13                     | 0.47              |
| 9:I:34:UNK:CG    | 9:I:35:UNK:N      | 2.70                     | 0.47              |
| 2:O:73:SER:N     | 2:O:74:PRO:HD2    | 2.29                     | 0.47              |
| 2:O:89:ILE:HD13  | 2:O:96:LEU:HB2    | 1.95                     | 0.47              |
| 2:O:295:LEU:O    | 2:O:299:VAL:HG23  | 2.14                     | 0.47              |
| 2:O:395:PRO:O    | 2:O:398:VAL:HG12  | 2.14                     | 0.47              |
| 1:A:264:ASP:HA   | 1:A:265:PRO:HD3   | 1.77                     | 0.47              |
| 2:B:361:LYS:HA   | 2:B:402:ILE:HD11  | 1.96                     | 0.47              |
| 3:C:117:GLY:O    | 12:C:502:HEM:HMC3 | 2.15                     | 0.47              |
| 5:E:41:ALA:O     | 5:E:45:VAL:HG23   | 2.15                     | 0.47              |
| 5:E:135:LEU:CD1  | 5:E:169:GLY:HA3   | 2.44                     | 0.47              |
| 5:E:155:GLY:HA3  | 5:E:166:ASP:O     | 2.15                     | 0.47              |
| 7:G:34:LEU:HB2   | 7:G:35:PRO:HD3    | 1.95                     | 0.47              |
| 7:G:50:PRO:HB2   | 7:G:51:PRO:CD     | 2.45                     | 0.47              |
| 10:J:58:LYS:HB2  | 10:J:59:TYR:CE1   | 2.49                     | 0.47              |
| 1:N:205:HIS:O    | 1:N:209:VAL:HG12  | 2.15                     | 0.47              |
| 1:N:342:TRP:O    | 1:N:345:LEU:HB2   | 2.15                     | 0.47              |
| 2:O:122:TYR:O    | 2:O:126:VAL:HG23  | 2.14                     | 0.47              |
| 2:O:374:THR:HG22 | 2:O:376:GLN:N     | 2.29                     | 0.47              |
| 2:O:402:ILE:HG23 | 2:O:403:ASP:N     | 2.29                     | 0.47              |
| 3:P:49:GLY:C     | 12:P:501:HEM:HAC  | 2.40                     | 0.47              |
| 6:S:73:ARG:NH1   | 7:T:32:ASP:OD2    | 2.47                     | 0.47              |
| 6:S:77:LYS:HA    | 6:S:80:TRP:CE2    | 2.50                     | 0.47              |
| 1:A:144:ASP:OD2  | 1:A:147:ASN:ND2   | 2.47                     | 0.47              |
| 1:A:158:PHE:O    | 1:A:164:ALA:HB2   | 2.15                     | 0.47              |
| 3:C:101:ARG:C    | 3:C:101:ARG:CD    | 2.88                     | 0.47              |
| 4:D:102:ARG:HA   | 4:D:108:ALA:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:28:GLU:CG    | 8:H:32:LYS:HE3   | 2.44                     | 0.47              |
| 1:N:178:THR:HG22 | 1:N:179:ARG:N    | 2.29                     | 0.47              |
| 2:O:31:ASN:N     | 2:O:31:ASN:ND2   | 2.63                     | 0.47              |
| 3:P:31:TRP:NE1   | 11:P:3007:PEE:O4 | 2.48                     | 0.47              |
| 3:P:350:ILE:O    | 3:P:354:MET:HG2  | 2.15                     | 0.47              |
| 5:R:112:VAL:HG21 | 5:R:170:ARG:NH2  | 2.29                     | 0.47              |
| 5:E:136:VAL:O    | 5:E:138:VAL:N    | 2.44                     | 0.47              |
| 9:I:61:ARG:C     | 9:I:62:ARG:HG3   | 2.40                     | 0.47              |
| 2:B:46:ARG:HD2   | 2:B:110:GLU:CD   | 2.40                     | 0.47              |
| 2:B:47:ILE:HD13  | 2:B:120:MET:HE2  | 1.94                     | 0.47              |
| 2:B:47:ILE:HD11  | 2:B:116:VAL:CG1  | 2.45                     | 0.47              |
| 2:B:122:TYR:O    | 2:B:126:VAL:HG23 | 2.15                     | 0.47              |
| 3:C:37:LEU:O     | 3:C:41:CYS:HB2   | 2.15                     | 0.47              |
| 3:C:198:LEU:HD21 | 12:C:502:HEM:CMA | 2.45                     | 0.47              |
| 5:E:130:PRO:C    | 5:E:132:TRP:H    | 2.22                     | 0.47              |
| 2:O:36:ALA:HB3   | 2:O:207:VAL:HG13 | 1.97                     | 0.47              |
| 2:O:59:THR:HG22  | 2:O:60:THR:N     | 2.30                     | 0.47              |
| 3:P:101:ARG:HD2  | 3:P:101:ARG:O    | 2.15                     | 0.47              |
| 3:P:155:PRO:O    | 3:P:156:TYR:HB2  | 2.15                     | 0.47              |
| 4:Q:3:LEU:HD12   | 4:Q:3:LEU:N      | 2.29                     | 0.47              |
| 7:T:80:ASP:OD1   | 8:U:47:ARG:HD3   | 2.14                     | 0.47              |
| 3:C:9:HIS:CD2    | 3:C:12:LEU:HG    | 2.50                     | 0.46              |
| 5:E:162:GLY:O    | 5:E:163:SER:C    | 2.58                     | 0.46              |
| 9:I:31:UNK:CA    | 9:I:73:PRO:HG2   | 2.44                     | 0.46              |
| 10:J:7:ARG:HH11  | 10:J:7:ARG:HB2   | 1.80                     | 0.46              |
| 1:N:219:VAL:CG1  | 1:N:220:SER:N    | 2.78                     | 0.46              |
| 3:P:247:SER:OG   | 3:P:250:LEU:HB2  | 2.15                     | 0.46              |
| 3:P:287:ASN:O    | 3:P:288:LYS:C    | 2.58                     | 0.46              |
| 5:R:77:LYS:HE2   | 5:R:79:SER:HB2   | 1.96                     | 0.46              |
| 2:B:54:GLY:C     | 2:B:56:ARG:H     | 2.22                     | 0.46              |
| 6:F:71:LYS:O     | 6:F:72:HIS:HB2   | 2.15                     | 0.46              |
| 1:N:122:LEU:HD11 | 1:N:186:ILE:HD12 | 1.98                     | 0.46              |
| 1:N:189:HIS:ND1  | 1:N:194:ARG:NH2  | 2.51                     | 0.46              |
| 4:Q:14:HIS:HB3   | 4:Q:21:LEU:HA    | 1.97                     | 0.46              |
| 4:Q:240:PRO:HD3  | 7:T:12:HIS:CE1   | 2.50                     | 0.46              |
| 10:W:4:ALA:O     | 10:W:8:GLN:HG3   | 2.15                     | 0.46              |
| 2:B:207:VAL:HG12 | 2:B:208:GLY:N    | 2.30                     | 0.46              |
| 4:D:70:VAL:HG21  | 4:D:83:ARG:NH2   | 2.30                     | 0.46              |
| 5:E:74:ILE:HG22  | 5:E:91:TRP:CD1   | 2.51                     | 0.46              |
| 1:N:130:GLU:O    | 1:N:134:ILE:HG13 | 2.16                     | 0.46              |
| 2:O:47:ILE:HD11  | 2:O:116:VAL:CG1  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:403:ASP:C     | 2:O:405:VAL:H     | 2.23                     | 0.46              |
| 15:Q:3003:CDL:OB3 | 6:S:73:ARG:NH2    | 2.48                     | 0.46              |
| 5:R:185:TYR:O     | 5:R:186:GLN:HB3   | 2.15                     | 0.46              |
| 2:O:259:THR:HG22  | 2:O:260:GLU:N     | 2.29                     | 0.46              |
| 6:S:17:ARG:HG2    | 6:S:17:ARG:NH1    | 2.29                     | 0.46              |
| 8:U:21:ARG:HG3    | 8:U:21:ARG:HH11   | 1.80                     | 0.46              |
| 1:A:433:ASP:OD1   | 1:A:436:ARG:HG2   | 2.16                     | 0.46              |
| 2:B:27:THR:CG2    | 2:B:28:LYS:H      | 2.24                     | 0.46              |
| 3:C:247:SER:N     | 3:C:248:PRO:HD3   | 2.30                     | 0.46              |
| 4:D:28:ARG:HD2    | 4:D:171:TYR:CD1   | 2.51                     | 0.46              |
| 5:E:96:LEU:HD12   | 5:E:135:LEU:O     | 2.16                     | 0.46              |
| 1:N:37:VAL:HG22   | 1:N:109:VAL:HG11  | 1.98                     | 0.46              |
| 5:R:107:ASN:C     | 5:R:109:GLU:N     | 2.73                     | 0.46              |
| 1:A:64:PHE:HE2    | 1:A:86:PHE:CE1    | 2.34                     | 0.46              |
| 2:B:21:ALA:O      | 2:B:22:GLU:HB3    | 2.15                     | 0.46              |
| 2:B:273:SER:O     | 2:B:276:GLN:HB3   | 2.16                     | 0.46              |
| 1:N:61:HIS:CE1    | 1:N:134:ILE:HG12  | 2.51                     | 0.46              |
| 1:N:134:ILE:CG2   | 1:N:174:ILE:HD13  | 2.46                     | 0.46              |
| 2:O:259:THR:CG2   | 2:O:260:GLU:N     | 2.79                     | 0.46              |
| 3:P:202:HIS:NE2   | 14:P:3002:UQ:O4   | 2.43                     | 0.46              |
| 12:P:502:HEM:HMB1 | 12:P:502:HEM:HBB2 | 1.97                     | 0.46              |
| 4:Q:240:PRO:O     | 4:Q:241:LYS:C     | 2.59                     | 0.46              |
| 5:R:179:ASN:O     | 5:R:180:LEU:C     | 2.59                     | 0.46              |
| 1:A:49:ASN:ND2    | 1:A:51:LYS:H      | 2.14                     | 0.46              |
| 1:A:402:VAL:HA    | 1:A:406:MET:HE2   | 1.98                     | 0.46              |
| 2:B:212:LYS:HB3   | 2:B:215:ASP:OD2   | 2.16                     | 0.46              |
| 4:D:102:ARG:HG2   | 4:D:102:ARG:HH11  | 1.80                     | 0.46              |
| 1:N:23:LEU:HD23   | 1:N:23:LEU:C      | 2.41                     | 0.46              |
| 1:N:288:LYS:HE3   | 1:N:289:HIS:CE1   | 2.51                     | 0.46              |
| 2:O:307:PHE:H     | 9:V:52:ARG:HG2    | 1.81                     | 0.46              |
| 1:A:45:SER:HA     | 1:A:48:GLU:CD     | 2.41                     | 0.46              |
| 2:B:50:PHE:N      | 2:B:50:PHE:CD1    | 2.83                     | 0.46              |
| 2:B:333:ALA:O     | 2:B:337:ILE:HG13  | 2.16                     | 0.46              |
| 3:C:90:PHE:CE1    | 3:C:236:MET:HB3   | 2.51                     | 0.46              |
| 5:E:189:GLY:O     | 5:E:192:LEU:O     | 2.34                     | 0.46              |
| 8:H:10:GLU:C      | 8:H:11:GLU:HG3    | 2.41                     | 0.46              |
| 2:O:24:LEU:HD12   | 2:O:37:SER:O      | 2.15                     | 0.46              |
| 4:Q:169:LEU:HD23  | 4:Q:169:LEU:C     | 2.41                     | 0.46              |
| 5:R:109:GLU:HG2   | 5:R:123:ASP:HB2   | 1.97                     | 0.46              |
| 9:V:70:LEU:CD2    | 9:V:71:ASN:OD1    | 2.64                     | 0.46              |
| 1:A:368:GLN:O     | 1:A:369:LEU:HD23  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:248:ASN:HD22   | 2:B:249:GLY:N     | 2.14                     | 0.46              |
| 2:B:259:THR:CG2    | 2:B:260:GLU:N     | 2.78                     | 0.46              |
| 5:E:133:VAL:O      | 5:E:133:VAL:HG13  | 2.16                     | 0.46              |
| 10:J:40:ASP:O      | 10:J:44:GLU:HG3   | 2.15                     | 0.46              |
| 1:N:264:ASP:HA     | 1:N:265:PRO:HD3   | 1.80                     | 0.46              |
| 2:O:385:GLU:O      | 2:O:389:SER:HB3   | 2.15                     | 0.46              |
| 3:P:305:ILE:HB     | 3:P:306:PRO:HD3   | 1.98                     | 0.46              |
| 5:R:141:HIS:HB3    | 19:R:501:FES:S2   | 2.56                     | 0.46              |
| 9:I:39:UNK:HA      | 9:V:40:UNK:O      | 2.16                     | 0.45              |
| 1:N:354:VAL:HG23   | 1:N:355:LYS:N     | 2.30                     | 0.45              |
| 2:O:286:LYS:HE2    | 2:O:287:ARG:NH1   | 2.31                     | 0.45              |
| 3:P:153:ALA:CB     | 3:P:288:LYS:HG2   | 2.45                     | 0.45              |
| 3:P:263:LEU:C      | 3:P:264:VAL:HG23  | 2.41                     | 0.45              |
| 5:R:99:ARG:HB3     | 5:R:133:VAL:CG1   | 2.46                     | 0.45              |
| 8:U:28:GLU:CG      | 8:U:32:LYS:HE3    | 2.46                     | 0.45              |
| 10:W:42:ILE:HG22   | 10:W:46:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:137:GLU:O      | 1:A:141:MET:HG3   | 2.16                     | 0.45              |
| 1:A:205:HIS:O      | 1:A:209:VAL:HG12  | 2.16                     | 0.45              |
| 2:B:168:TYR:HB2    | 2:B:173:ALA:HB2   | 1.98                     | 0.45              |
| 2:B:307:PHE:H      | 9:I:52:ARG:HG2    | 1.81                     | 0.45              |
| 2:B:403:ASP:C      | 2:B:405:VAL:H     | 2.24                     | 0.45              |
| 3:C:28:ILE:HG12    | 3:C:225:TYR:OH    | 2.17                     | 0.45              |
| 4:D:169:LEU:HD23   | 4:D:169:LEU:O     | 2.16                     | 0.45              |
| 4:D:171:TYR:OH     | 4:D:182:ILE:HA    | 2.16                     | 0.45              |
| 5:E:52:LYS:C       | 5:E:52:LYS:CD     | 2.85                     | 0.45              |
| 6:F:32:MET:O       | 6:F:33:ARG:C      | 2.58                     | 0.45              |
| 3:P:247:SER:N      | 3:P:248:PRO:HD3   | 2.31                     | 0.45              |
| 4:Q:102:ARG:HB3    | 4:Q:107:GLY:HA2   | 1.98                     | 0.45              |
| 2:O:31:ASN:ND2     | 2:O:31:ASN:H      | 2.13                     | 0.45              |
| 3:P:22:LEU:HD21    | 14:P:3002:UQ:CM3  | 2.47                     | 0.45              |
| 3:P:380:TYR:CZ     | 6:S:37:LEU:HD21   | 2.52                     | 0.45              |
| 1:A:70:ARG:HA      | 1:A:71:PRO:HD2    | 1.81                     | 0.45              |
| 1:A:418:LYS:O      | 1:A:420:PRO:HD3   | 2.16                     | 0.45              |
| 2:B:372:VAL:HG13   | 2:B:378:LEU:HA    | 1.99                     | 0.45              |
| 3:C:313:GLN:NE2    | 6:F:36:THR:OG1    | 2.44                     | 0.45              |
| 15:C:2004:CDL:H712 | 11:C:2007:PEE:H50 | 1.98                     | 0.45              |
| 15:D:2003:CDL:OB3  | 6:F:73:ARG:NH2    | 2.49                     | 0.45              |
| 2:O:54:GLY:C       | 2:O:56:ARG:H      | 2.23                     | 0.45              |
| 5:R:163:SER:HA     | 5:R:174:GLY:HA3   | 1.99                     | 0.45              |
| 2:B:34:ILE:HD13    | 2:B:390:GLY:HA2   | 1.97                     | 0.45              |
| 2:B:68:LEU:HD23    | 2:B:186:ILE:HG21  | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:170:THR:O      | 2:O:172:LEU:N      | 2.50                     | 0.45              |
| 2:O:367:THR:HA     | 2:O:370:MET:HE3    | 1.97                     | 0.45              |
| 4:Q:47:ALA:HA      | 4:Q:90:TYR:HA      | 1.99                     | 0.45              |
| 4:Q:220:TYR:O      | 4:Q:224:ARG:HG2    | 2.17                     | 0.45              |
| 6:S:52:GLU:OE2     | 7:T:11:ARG:NH1     | 2.49                     | 0.45              |
| 7:T:36:ASN:O       | 7:T:40:ARG:HG3     | 2.17                     | 0.45              |
| 1:A:255:LEU:O      | 1:A:321:GLY:HA3    | 2.16                     | 0.45              |
| 2:B:24:LEU:HD13    | 2:B:38:LEU:HB2     | 1.98                     | 0.45              |
| 2:B:96:LEU:HD12    | 2:B:97:SER:N       | 2.32                     | 0.45              |
| 5:E:144:CYS:CB     | 5:E:158:CYS:SG     | 3.05                     | 0.45              |
| 5:E:189:GLY:O      | 5:E:192:LEU:N      | 2.50                     | 0.45              |
| 6:F:91:GLU:HB3     | 6:F:92:PRO:HD3     | 1.99                     | 0.45              |
| 1:A:45:SER:HA      | 1:A:48:GLU:HG3     | 1.98                     | 0.45              |
| 2:B:101:THR:OG1    | 2:B:104:LYS:HG3    | 2.17                     | 0.45              |
| 15:D:2003:CDL:H721 | 15:D:2003:CDL:HA61 | 1.98                     | 0.45              |
| 2:O:46:ARG:NH2     | 2:O:376:GLN:HG3    | 2.32                     | 0.45              |
| 10:W:38:GLY:O      | 10:W:42:ILE:HG13   | 2.16                     | 0.45              |
| 2:B:27:THR:CG2     | 2:B:28:LYS:N       | 2.77                     | 0.45              |
| 2:B:110:GLU:O      | 2:B:111:CYS:HB3    | 2.16                     | 0.45              |
| 2:B:207:VAL:HG12   | 2:B:208:GLY:H      | 1.82                     | 0.45              |
| 2:B:318:ASP:O      | 2:B:319:SER:HB2    | 2.16                     | 0.45              |
| 3:C:328:LEU:HD12   | 3:C:328:LEU:HA     | 1.83                     | 0.45              |
| 1:N:45:SER:HA      | 1:N:48:GLU:CD      | 2.42                     | 0.45              |
| 2:O:34:ILE:HD13    | 2:O:390:GLY:HA2    | 1.99                     | 0.45              |
| 2:O:75:LEU:HD11    | 2:O:140:LEU:HD22   | 1.97                     | 0.45              |
| 5:R:140:THR:OG1    | 5:R:176:ALA:HB1    | 2.17                     | 0.45              |
| 9:V:69:SER:HB2     | 9:V:72:ALA:H       | 1.81                     | 0.45              |
| 2:B:43:PRO:O       | 2:B:113:ARG:HG3    | 2.17                     | 0.45              |
| 2:B:54:GLY:C       | 2:B:56:ARG:N       | 2.75                     | 0.45              |
| 11:C:2007:PEE:H11  | 6:F:29:TYR:OH      | 2.17                     | 0.45              |
| 4:D:167:GLU:CG     | 8:H:13:LEU:HD22    | 2.46                     | 0.45              |
| 5:E:127:VAL:CG1    | 5:E:128:LYS:H      | 2.15                     | 0.45              |
| 2:O:225:ASN:C      | 2:O:227:ARG:HG3    | 2.42                     | 0.45              |
| 3:P:263:LEU:O      | 3:P:264:VAL:CG2    | 2.65                     | 0.45              |
| 4:Q:8:PRO:HG2      | 4:Q:10:PHE:CE1     | 2.52                     | 0.45              |
| 6:S:82:LYS:O       | 6:S:83:TYR:C       | 2.59                     | 0.45              |
| 7:T:56:TYR:O       | 7:T:59:TYR:HB3     | 2.17                     | 0.45              |
| 1:A:27:SER:HA      | 1:A:199:ALA:O      | 2.16                     | 0.45              |
| 3:C:50:LEU:O       | 3:C:54:MET:HG3     | 2.17                     | 0.45              |
| 2:O:54:GLY:C       | 2:O:56:ARG:N       | 2.75                     | 0.45              |
| 3:P:92:PHE:O       | 3:P:95:ILE:HG22    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 9:V:55:MET:HA      | 9:V:58:ARG:HG3   | 1.99                     | 0.45              |
| 10:W:59:TYR:CD1    | 10:W:59:TYR:N    | 2.84                     | 0.45              |
| 2:B:395:PRO:O      | 2:B:398:VAL:CG1  | 2.65                     | 0.44              |
| 3:P:106:GLY:HA2    | 3:P:108:TYR:CZ   | 2.52                     | 0.44              |
| 15:P:3004:CDL:HA32 | 7:T:40:ARG:CB    | 2.46                     | 0.44              |
| 7:T:34:LEU:O       | 7:T:35:PRO:C     | 2.60                     | 0.44              |
| 2:B:164:HIS:O      | 2:B:173:ALA:HA   | 2.17                     | 0.44              |
| 5:E:73:LYS:HB2     | 5:E:195:VAL:O    | 2.16                     | 0.44              |
| 1:N:255:LEU:O      | 1:N:321:GLY:HA3  | 2.17                     | 0.44              |
| 3:P:19:LEU:C       | 3:P:20:ILE:HG13  | 2.42                     | 0.44              |
| 3:P:266:PRO:HA     | 3:P:267:PRO:HD3  | 1.85                     | 0.44              |
| 6:S:82:LYS:HD2     | 6:S:85:GLU:OE1   | 2.16                     | 0.44              |
| 2:B:46:ARG:NH2     | 2:B:376:GLN:HG3  | 2.33                     | 0.44              |
| 2:B:132:PHE:CE1    | 2:B:191:LEU:HB3  | 2.52                     | 0.44              |
| 4:D:57:THR:CG2     | 4:D:58:GLU:N     | 2.79                     | 0.44              |
| 6:F:77:LYS:HB3     | 6:F:77:LYS:HE2   | 1.81                     | 0.44              |
| 3:P:28:ILE:HD11    | 3:P:225:TYR:CE2  | 2.52                     | 0.44              |
| 4:Q:223:LYS:HD3    | 4:Q:223:LYS:C    | 2.43                     | 0.44              |
| 5:R:178:TYR:N      | 5:R:178:TYR:HD1  | 2.15                     | 0.44              |
| 6:S:77:LYS:HB3     | 6:S:77:LYS:HE2   | 1.80                     | 0.44              |
| 3:C:212:ILE:HD12   | 6:F:62:ILE:HG23  | 1.99                     | 0.44              |
| 9:I:68:ILE:HD13    | 9:I:68:ILE:HA    | 1.84                     | 0.44              |
| 1:N:191:LYS:CA     | 1:N:195:MET:HE2  | 2.47                     | 0.44              |
| 2:O:144:LEU:HB2    | 2:O:183:ILE:HD12 | 1.99                     | 0.44              |
| 2:O:221:GLU:O      | 2:O:223:PHE:N    | 2.50                     | 0.44              |
| 2:O:399:ALA:HA     | 2:O:402:ILE:HG22 | 1.99                     | 0.44              |
| 8:U:65:ARG:O       | 8:U:69:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:134:ILE:CG2    | 1:A:174:ILE:HD13 | 2.47                     | 0.44              |
| 1:A:170:THR:HG22   | 1:A:171:THR:H    | 1.80                     | 0.44              |
| 2:B:28:LYS:O       | 2:B:28:LYS:HG2   | 2.17                     | 0.44              |
| 2:B:46:ARG:HD2     | 2:B:110:GLU:OE2  | 2.18                     | 0.44              |
| 5:E:3:ASN:H        | 5:E:3:ASN:ND2    | 2.15                     | 0.44              |
| 7:G:48:VAL:O       | 7:G:51:PRO:HD2   | 2.17                     | 0.44              |
| 4:Q:134:TYR:CD2    | 4:Q:162:PRO:HG3  | 2.52                     | 0.44              |
| 4:Q:169:LEU:CD2    | 4:Q:182:ILE:HD11 | 2.48                     | 0.44              |
| 3:C:358:SER:O      | 3:C:362:ILE:HG13 | 2.16                     | 0.44              |
| 5:R:75:GLU:O       | 5:R:75:GLU:HG3   | 2.17                     | 0.44              |
| 5:R:102:THR:C      | 5:R:104:ALA:N    | 2.75                     | 0.44              |
| 3:C:323:GLN:OE1    | 7:G:47:LYS:HD3   | 2.18                     | 0.44              |
| 3:C:380:TYR:CZ     | 6:F:37:LEU:HD21  | 2.53                     | 0.44              |
| 5:E:119:ASP:O      | 5:E:121:GLN:N    | 2.49                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:161:HIS:HB2  | 19:E:501:FES:S1   | 2.58                     | 0.44              |
| 2:O:345:LYS:HG2  | 2:O:418:VAL:CG1   | 2.47                     | 0.44              |
| 3:P:150:LEU:HB3  | 3:P:292:VAL:HG22  | 1.99                     | 0.44              |
| 4:Q:28:ARG:HD2   | 4:Q:171:TYR:CD1   | 2.53                     | 0.44              |
| 4:Q:235:MET:HB3  | 7:T:15:THR:HG22   | 1.99                     | 0.44              |
| 5:R:133:VAL:O    | 5:R:133:VAL:HG13  | 2.17                     | 0.44              |
| 1:A:63:ALA:O     | 1:A:116:VAL:HG13  | 2.18                     | 0.44              |
| 1:A:112:LEU:O    | 1:A:116:VAL:HG23  | 2.18                     | 0.44              |
| 5:E:171:ILE:O    | 5:E:171:ILE:HG23  | 2.17                     | 0.44              |
| 1:N:62:LEU:HD11  | 1:N:127:ILE:HG12  | 1.98                     | 0.44              |
| 1:N:168:GLU:CD   | 1:N:168:GLU:H     | 2.26                     | 0.44              |
| 1:N:243:ALA:O    | 1:N:425:VAL:HA    | 2.17                     | 0.44              |
| 1:N:365:MET:HG3  | 1:N:366:VAL:N     | 2.33                     | 0.44              |
| 2:O:361:LYS:HD3  | 2:O:403:ASP:HA    | 2.00                     | 0.44              |
| 3:P:14:MET:HE2   | 18:P:2010:BOG:O4  | 2.18                     | 0.44              |
| 3:P:230:ILE:HG23 | 11:R:3005:PEE:H25 | 2.00                     | 0.44              |
| 5:R:110:ALA:HA   | 5:R:122:HIS:NE2   | 2.32                     | 0.44              |
| 1:A:168:GLU:H    | 1:A:168:GLU:CD    | 2.26                     | 0.44              |
| 2:B:59:THR:CG2   | 2:B:60:THR:N      | 2.80                     | 0.44              |
| 2:B:314:VAL:CG1  | 9:I:63:ASP:HB3    | 2.39                     | 0.44              |
| 3:C:263:LEU:C    | 3:C:264:VAL:HG23  | 2.43                     | 0.44              |
| 1:A:189:HIS:ND1  | 1:A:194:ARG:NH2   | 2.55                     | 0.43              |
| 1:A:191:LYS:N    | 1:A:195:MET:HE2   | 2.32                     | 0.43              |
| 1:A:281:ASP:OD1  | 9:I:33:UNK:HB2    | 2.18                     | 0.43              |
| 2:B:56:ARG:HH11  | 2:B:56:ARG:HG3    | 1.83                     | 0.43              |
| 2:B:353:THR:HG22 | 2:B:354:GLU:N     | 2.32                     | 0.43              |
| 4:D:143:VAL:HG21 | 4:D:149:TYR:HB2   | 1.99                     | 0.43              |
| 5:E:73:LYS:HB3   | 5:E:196:GLY:O     | 2.17                     | 0.43              |
| 5:E:97:PHE:O     | 5:E:134:ILE:HA    | 2.18                     | 0.43              |
| 5:E:136:VAL:HG23 | 5:E:181:GLU:O     | 2.17                     | 0.43              |
| 1:N:40:TRP:CZ2   | 1:N:377:GLU:HA    | 2.53                     | 0.43              |
| 2:O:227:ARG:HB3  | 2:O:228:SER:H     | 1.48                     | 0.43              |
| 3:P:377:MET:HE2  | 6:S:20:TYR:HB2    | 2.00                     | 0.43              |
| 4:Q:169:LEU:HD22 | 4:Q:182:ILE:CD1   | 2.48                     | 0.43              |
| 4:Q:215:LEU:HD13 | 5:R:46:ALA:HB3    | 1.99                     | 0.43              |
| 4:Q:238:ARG:CZ   | 5:R:5:VAL:HG22    | 2.48                     | 0.43              |
| 3:C:92:PHE:O     | 3:C:95:ILE:HG22   | 2.17                     | 0.43              |
| 3:C:98:HIS:CD2   | 12:C:502:HEM:NC   | 2.85                     | 0.43              |
| 4:D:223:LYS:HD3  | 4:D:223:LYS:C     | 2.43                     | 0.43              |
| 4:D:235:MET:HB3  | 7:G:15:THR:HG22   | 2.01                     | 0.43              |
| 6:F:73:ARG:NH1   | 7:G:32:ASP:OD2    | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:257:VAL:HG22  | 2:O:424:MET:HG3   | 2.00                     | 0.43              |
| 3:P:121:LEU:O     | 3:P:125:MET:HG3   | 2.18                     | 0.43              |
| 3:P:325:LEU:HD22  | 3:P:370:ILE:HG13  | 2.00                     | 0.43              |
| 3:P:380:TYR:OH    | 6:S:34:ASP:OD1    | 2.32                     | 0.43              |
| 4:Q:168:ILE:O     | 4:Q:168:ILE:HG12  | 2.17                     | 0.43              |
| 3:C:46:ILE:HA     | 12:C:501:HEM:HMC2 | 2.00                     | 0.43              |
| 5:E:125:ASP:C     | 5:E:126:ARG:HG3   | 2.44                     | 0.43              |
| 7:G:50:PRO:HB2    | 7:G:51:PRO:HD3    | 2.01                     | 0.43              |
| 9:I:71:ASN:N      | 9:I:71:ASN:HD22   | 2.16                     | 0.43              |
| 4:Q:69:GLU:OE1    | 4:Q:82:MET:HB3    | 2.18                     | 0.43              |
| 4:Q:181:GLN:HA    | 8:U:77:LEU:HD22   | 2.00                     | 0.43              |
| 8:U:36:ARG:HB3    | 8:U:36:ARG:NH1    | 2.33                     | 0.43              |
| 1:A:186:ILE:HG23  | 1:A:190:PHE:HD1   | 1.82                     | 0.43              |
| 2:O:76:THR:CG2    | 2:O:136:GLU:OE1   | 2.64                     | 0.43              |
| 2:O:345:LYS:HG2   | 2:O:418:VAL:HG13  | 2.01                     | 0.43              |
| 5:R:161:HIS:HB2   | 19:R:501:FES:S1   | 2.59                     | 0.43              |
| 1:A:53:ASN:HB3    | 1:A:173:ASN:ND2   | 2.34                     | 0.43              |
| 1:A:130:GLU:O     | 1:A:134:ILE:HG13  | 2.18                     | 0.43              |
| 2:B:280:GLY:HA3   | 2:B:293:SER:OG    | 2.19                     | 0.43              |
| 4:D:168:ILE:HG12  | 4:D:168:ILE:O     | 2.18                     | 0.43              |
| 11:E:2005:PEE:H58 | 10:J:24:VAL:HG11  | 2.01                     | 0.43              |
| 2:B:46:ARG:HD2    | 2:B:110:GLU:CG    | 2.48                     | 0.43              |
| 2:B:76:THR:HG23   | 2:B:82:SER:HB2    | 2.01                     | 0.43              |
| 1:N:280:TYR:CG    | 1:N:281:ASP:N     | 2.85                     | 0.43              |
| 2:O:402:ILE:HG23  | 2:O:403:ASP:H     | 1.83                     | 0.43              |
| 3:P:105:TYR:CD2   | 3:P:209:PRO:HA    | 2.53                     | 0.43              |
| 5:R:3:ASN:H       | 5:R:3:ASN:HD22    | 1.66                     | 0.43              |
| 5:R:170:ARG:HA    | 5:R:179:ASN:CB    | 2.45                     | 0.43              |
| 6:S:70:LEU:HD12   | 6:S:70:LEU:C      | 2.43                     | 0.43              |
| 4:D:197:GLU:O     | 4:D:198:HIS:C     | 2.61                     | 0.43              |
| 1:N:205:HIS:O     | 1:N:208:LEU:HB3   | 2.18                     | 0.43              |
| 1:N:274:ASN:ND2   | 1:N:309:THR:HB    | 2.34                     | 0.43              |
| 2:O:248:ASN:HD21  | 2:O:428:GLY:HA2   | 1.83                     | 0.43              |
| 2:B:170:THR:O     | 2:B:172:LEU:N     | 2.51                     | 0.43              |
| 4:D:79:GLU:HA     | 4:D:79:GLU:OE2    | 2.19                     | 0.43              |
| 1:N:351:GLU:HA    | 1:N:354:VAL:HG22  | 2.01                     | 0.43              |
| 2:O:39:GLU:OE2    | 2:O:113:ARG:NH2   | 2.50                     | 0.43              |
| 5:R:96:LEU:HD12   | 5:R:135:LEU:O     | 2.19                     | 0.43              |
| 3:C:146:VAL:HG21  | 3:C:269:ILE:HG21  | 2.00                     | 0.43              |
| 4:D:27:ARG:NH1    | 4:D:55:THR:O      | 2.52                     | 0.43              |
| 5:E:52:LYS:HD3    | 5:E:52:LYS:O      | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:O:162:ASN:O     | 2:O:244:ILE:HD12   | 2.18                     | 0.43              |
| 3:P:129:PHE:CE1   | 13:P:3001:JZV:HAFB | 2.54                     | 0.43              |
| 3:P:367:PHE:N     | 3:P:368:PRO:HD2    | 2.34                     | 0.43              |
| 5:R:78:LEU:HD22   | 5:R:132:TRP:CE2    | 2.54                     | 0.43              |
| 8:U:32:LYS:O      | 8:U:36:ARG:HG3     | 2.19                     | 0.43              |
| 8:U:67:HIS:C      | 8:U:67:HIS:HD1     | 2.27                     | 0.43              |
| 1:A:140:GLU:OE2   | 9:I:50:LEU:N       | 2.41                     | 0.43              |
| 3:C:155:PRO:O     | 3:C:157:ILE:N      | 2.50                     | 0.43              |
| 3:C:224:TYR:HB3   | 4:D:227:TRP:CZ2    | 2.54                     | 0.43              |
| 12:C:502:HEM:HBC2 | 12:C:502:HEM:CMC   | 2.49                     | 0.43              |
| 10:J:42:ILE:HG22  | 10:J:46:LEU:HD12   | 2.00                     | 0.43              |
| 1:N:103:SER:HB3   | 1:N:202:GLY:O      | 2.19                     | 0.43              |
| 2:O:73:SER:N      | 2:O:74:PRO:CD      | 2.82                     | 0.43              |
| 2:O:156:GLN:HE22  | 9:V:77:ARG:C       | 2.27                     | 0.43              |
| 2:O:221:GLU:HG3   | 2:O:222:GLN:N      | 2.26                     | 0.43              |
| 3:P:277:PHE:CG    | 3:P:278:ALA:N      | 2.86                     | 0.43              |
| 1:A:191:LYS:O     | 1:A:195:MET:HG3    | 2.18                     | 0.42              |
| 2:B:56:ARG:HB2    | 2:B:102:ARG:O      | 2.19                     | 0.42              |
| 4:D:161:ALA:O     | 4:D:162:PRO:C      | 2.62                     | 0.42              |
| 4:D:221:TYR:CD2   | 5:E:39:VAL:HG11    | 2.54                     | 0.42              |
| 5:E:137:GLY:O     | 5:E:145:VAL:HG13   | 2.19                     | 0.42              |
| 9:I:31:UNK:O      | 9:I:32:UNK:O       | 2.37                     | 0.42              |
| 1:N:281:ASP:O     | 1:N:283:THR:N      | 2.52                     | 0.42              |
| 1:N:436:ARG:HD2   | 1:N:436:ARG:HA     | 1.82                     | 0.42              |
| 3:P:208:ASN:HB2   | 3:P:209:PRO:HD2    | 2.01                     | 0.42              |
| 3:P:219:ILE:HD12  | 3:P:224:TYR:CD1    | 2.53                     | 0.42              |
| 5:R:122:HIS:O     | 5:R:123:ASP:C      | 2.62                     | 0.42              |
| 5:R:153:PHE:CD1   | 5:R:153:PHE:N      | 2.86                     | 0.42              |
| 5:R:155:GLY:HA3   | 5:R:166:ASP:O      | 2.19                     | 0.42              |
| 3:C:286:PRO:O     | 3:C:287:ASN:CB     | 2.67                     | 0.42              |
| 4:D:69:GLU:OE1    | 4:D:82:MET:HB3     | 2.18                     | 0.42              |
| 5:E:122:HIS:CE1   | 5:E:124:LEU:HB2    | 2.55                     | 0.42              |
| 2:B:257:VAL:HG22  | 2:B:424:MET:HG3    | 2.01                     | 0.42              |
| 2:B:345:LYS:HG2   | 2:B:418:VAL:HG13   | 2.02                     | 0.42              |
| 4:D:116:ILE:HG23  | 4:D:117:VAL:N      | 2.33                     | 0.42              |
| 5:E:179:ASN:O     | 5:E:180:LEU:C      | 2.60                     | 0.42              |
| 1:N:90:THR:O      | 1:N:167:VAL:HG11   | 2.19                     | 0.42              |
| 2:O:96:LEU:H      | 9:V:70:LEU:HD22    | 1.84                     | 0.42              |
| 2:O:286:LYS:C     | 2:O:288:GLY:H      | 2.27                     | 0.42              |
| 3:P:18:SER:CB     | 3:P:202:HIS:HE1    | 2.32                     | 0.42              |
| 6:S:99:ARG:HH11   | 6:S:99:ARG:HB3     | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:70:LEU:HD23   | 9:V:71:ASN:H      | 1.83                     | 0.42              |
| 2:B:52:LYS:O      | 2:B:203:ARG:NH2   | 2.46                     | 0.42              |
| 2:B:374:THR:HG22  | 2:B:376:GLN:N     | 2.33                     | 0.42              |
| 5:E:105:GLU:C     | 5:E:107:ASN:H     | 2.24                     | 0.42              |
| 5:E:191:ASP:OD2   | 5:E:191:ASP:N     | 2.52                     | 0.42              |
| 8:H:40:CYS:O      | 8:H:44:VAL:HG23   | 2.18                     | 0.42              |
| 1:N:27:SER:HA     | 1:N:199:ALA:O     | 2.19                     | 0.42              |
| 1:A:16:VAL:HA     | 1:A:25:VAL:O      | 2.19                     | 0.42              |
| 1:A:111:GLU:HG3   | 1:A:215:HIS:NE2   | 2.35                     | 0.42              |
| 12:C:502:HEM:HBC2 | 12:C:502:HEM:HMC1 | 2.00                     | 0.42              |
| 1:N:45:SER:HA     | 1:N:48:GLU:CG     | 2.49                     | 0.42              |
| 1:N:144:ASP:OD2   | 1:N:147:ASN:ND2   | 2.52                     | 0.42              |
| 1:N:418:LYS:O     | 1:N:420:PRO:HD3   | 2.19                     | 0.42              |
| 2:O:227:ARG:O     | 2:O:228:SER:O     | 2.38                     | 0.42              |
| 2:O:353:THR:HG22  | 2:O:354:GLU:N     | 2.35                     | 0.42              |
| 3:P:5:ILE:O       | 3:P:5:ILE:HG22    | 2.20                     | 0.42              |
| 5:E:99:ARG:HB3    | 5:E:133:VAL:CG1   | 2.48                     | 0.42              |
| 1:N:433:ASP:OD2   | 1:N:435:ASN:HB2   | 2.20                     | 0.42              |
| 4:Q:167:GLU:C     | 4:Q:169:LEU:N     | 2.75                     | 0.42              |
| 9:V:52:ARG:HG3    | 9:V:52:ARG:HH11   | 1.84                     | 0.42              |
| 1:A:274:ASN:HD22  | 1:A:274:ASN:HA    | 1.64                     | 0.42              |
| 2:B:22:GLU:O      | 2:B:23:ASP:OD2    | 2.38                     | 0.42              |
| 7:G:34:LEU:O      | 7:G:35:PRO:C      | 2.60                     | 0.42              |
| 2:O:209:ILE:HD11  | 2:O:379:LEU:N     | 2.35                     | 0.42              |
| 4:Q:167:GLU:HG2   | 8:U:13:LEU:HD12   | 2.01                     | 0.42              |
| 2:B:144:LEU:HB2   | 2:B:183:ILE:HD12  | 2.01                     | 0.42              |
| 2:B:287:ARG:NH1   | 2:B:287:ARG:HG3   | 2.34                     | 0.42              |
| 5:E:122:HIS:O     | 5:E:125:ASP:HB2   | 2.19                     | 0.42              |
| 10:J:4:ALA:O      | 10:J:8:GLN:HG3    | 2.20                     | 0.42              |
| 2:O:287:ARG:NH1   | 2:O:287:ARG:HG3   | 2.35                     | 0.42              |
| 3:P:263:LEU:O     | 3:P:264:VAL:HG23  | 2.20                     | 0.42              |
| 5:R:52:LYS:C      | 5:R:52:LYS:CD     | 2.87                     | 0.42              |
| 1:A:17:THR:CG2    | 1:A:205:HIS:NE2   | 2.83                     | 0.42              |
| 1:A:253:VAL:O     | 1:A:323:HIS:HA    | 2.20                     | 0.42              |
| 2:B:28:LYS:HG3    | 2:B:34:ILE:HG12   | 2.02                     | 0.42              |
| 2:B:292:THR:O     | 2:B:292:THR:CG2   | 2.66                     | 0.42              |
| 4:D:26:VAL:HG22   | 4:D:188:THR:HG22  | 2.01                     | 0.42              |
| 5:E:75:GLU:HA     | 5:E:193:VAL:O     | 2.20                     | 0.42              |
| 6:F:77:LYS:HA     | 6:F:80:TRP:CE2    | 2.55                     | 0.42              |
| 1:N:4:TYR:CB      | 2:O:114:ASP:OD2   | 2.67                     | 0.42              |
| 1:A:233:ARG:HH21  | 1:A:316:ASP:HB2   | 1.83                     | 0.42              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:B:38:LEU:HD12    | 2:B:38:LEU:C     | 2.45                     | 0.42              |
| 2:B:374:THR:HB     | 2:B:377:GLY:H    | 1.84                     | 0.42              |
| 3:C:150:LEU:HB3    | 3:C:292:VAL:HG22 | 2.02                     | 0.42              |
| 3:C:342:GLN:HB3    | 3:C:348:PHE:CD1  | 2.55                     | 0.42              |
| 5:E:103:GLN:O      | 5:E:107:ASN:ND2  | 2.51                     | 0.42              |
| 3:P:150:LEU:HB3    | 3:P:292:VAL:CG2  | 2.50                     | 0.42              |
| 5:R:77:LYS:HE2     | 5:R:79:SER:CB    | 2.49                     | 0.42              |
| 6:S:13:MET:O       | 6:S:17:ARG:HG3   | 2.19                     | 0.42              |
| 10:W:57:HIS:HA     | 10:W:60:GLU:HB3  | 2.01                     | 0.42              |
| 1:A:304:CYS:HB2    | 1:A:325:VAL:O    | 2.20                     | 0.41              |
| 7:G:81:GLN:OXT     | 7:G:81:GLN:HG3   | 2.20                     | 0.41              |
| 3:P:313:GLN:HE21   | 6:S:36:THR:HB    | 1.85                     | 0.41              |
| 4:Q:116:ILE:HG23   | 4:Q:117:VAL:N    | 2.35                     | 0.41              |
| 5:R:116:LYS:O      | 5:R:117:LEU:HD23 | 2.20                     | 0.41              |
| 2:B:59:THR:C       | 2:B:61:ALA:N     | 2.75                     | 0.41              |
| 15:C:2004:CDL:HA32 | 7:G:40:ARG:CB    | 2.50                     | 0.41              |
| 7:G:29:ILE:O       | 7:G:33:ALA:HB3   | 2.19                     | 0.41              |
| 8:H:50:THR:HG23    | 8:H:50:THR:O     | 2.19                     | 0.41              |
| 1:N:30:SER:O       | 1:N:202:GLY:HA2  | 2.19                     | 0.41              |
| 1:N:240:GLU:HA     | 1:N:422:LEU:O    | 2.20                     | 0.41              |
| 2:O:371:SER:C      | 2:O:372:VAL:HG23 | 2.45                     | 0.41              |
| 5:E:152:ASP:OD2    | 5:E:153:PHE:CE1  | 2.73                     | 0.41              |
| 3:P:219:ILE:HD12   | 3:P:224:TYR:CG   | 2.55                     | 0.41              |
| 5:R:184:THR:HG22   | 5:R:185:TYR:N    | 2.35                     | 0.41              |
| 1:A:209:VAL:O      | 1:A:212:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:351:GLU:HA     | 1:A:354:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:387:GLY:O      | 1:A:388:ARG:HB3  | 2.19                     | 0.41              |
| 3:C:5:ILE:O        | 3:C:5:ILE:HG22   | 2.21                     | 0.41              |
| 5:E:114:VAL:O      | 5:E:115:SER:C    | 2.63                     | 0.41              |
| 2:O:275:LEU:HG     | 2:O:279:LEU:HD12 | 2.02                     | 0.41              |
| 3:P:9:HIS:CD2      | 3:P:11:LEU:H     | 2.38                     | 0.41              |
| 3:P:98:HIS:CD2     | 12:P:502:HEM:NC  | 2.88                     | 0.41              |
| 5:R:134:ILE:HD12   | 5:R:185:TYR:HD1  | 1.85                     | 0.41              |
| 8:U:27:THR:HG22    | 8:U:29:LYS:N     | 2.33                     | 0.41              |
| 3:C:150:LEU:HB3    | 3:C:292:VAL:CG2  | 2.50                     | 0.41              |
| 10:J:56:LYS:HB3    | 10:J:56:LYS:HE2  | 1.77                     | 0.41              |
| 1:N:70:ARG:HA      | 1:N:71:PRO:HD2   | 1.80                     | 0.41              |
| 1:N:281:ASP:CB     | 9:V:33:UNK:HB1   | 2.50                     | 0.41              |
| 5:R:97:PHE:O       | 5:R:134:ILE:HA   | 2.21                     | 0.41              |
| 6:S:99:ARG:HB3     | 6:S:99:ARG:NH1   | 2.35                     | 0.41              |
| 6:F:51:PRO:HD2     | 6:F:54:LEU:HD12  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:65:ARG:O      | 8:H:69:VAL:HG23   | 2.20                     | 0.41              |
| 2:O:154:SER:O     | 2:O:155:PRO:C     | 2.64                     | 0.41              |
| 2:O:155:PRO:O     | 2:O:156:GLN:C     | 2.64                     | 0.41              |
| 2:O:169:LYS:HD2   | 2:O:238:THR:HG21  | 2.02                     | 0.41              |
| 2:O:306:PRO:HA    | 9:V:52:ARG:CG     | 2.51                     | 0.41              |
| 2:O:307:PHE:CD1   | 2:O:308:ASP:N     | 2.88                     | 0.41              |
| 2:O:395:PRO:O     | 2:O:398:VAL:CG1   | 2.69                     | 0.41              |
| 6:S:91:GLU:HB3    | 6:S:92:PRO:HD3    | 2.03                     | 0.41              |
| 2:B:399:ALA:O     | 2:B:402:ILE:CG2   | 2.65                     | 0.41              |
| 1:N:16:VAL:HA     | 1:N:25:VAL:O      | 2.21                     | 0.41              |
| 1:N:289:HIS:CD2   | 2:O:83:PHE:HD1    | 2.39                     | 0.41              |
| 1:N:383:LEU:HD23  | 1:N:388:ARG:HA    | 2.02                     | 0.41              |
| 2:O:72:ALA:C      | 2:O:74:PRO:HD2    | 2.45                     | 0.41              |
| 5:R:13:TYR:O      | 7:T:24:ARG:HG3    | 2.21                     | 0.41              |
| 1:A:26:ALA:O      | 1:A:198:ALA:HA    | 2.21                     | 0.41              |
| 3:C:367:PHE:N     | 3:C:368:PRO:HD2   | 2.36                     | 0.41              |
| 1:N:85:HIS:CE1    | 2:O:370:MET:HE1   | 2.55                     | 0.41              |
| 3:P:146:VAL:HG21  | 3:P:269:ILE:HG21  | 2.03                     | 0.41              |
| 13:P:3001:JZV:HAZ | 13:P:3001:JZV:HAY | 1.81                     | 0.41              |
| 5:R:171:ILE:CD1   | 5:R:176:ALA:HB3   | 2.50                     | 0.41              |
| 5:R:188:VAL:HG23  | 5:R:192:LEU:HB2   | 2.02                     | 0.41              |
| 1:A:243:ALA:O     | 1:A:425:VAL:HA    | 2.20                     | 0.41              |
| 1:A:342:TRP:O     | 1:A:345:LEU:HB2   | 2.20                     | 0.41              |
| 2:B:262:ALA:O     | 2:B:320:GLY:HA3   | 2.20                     | 0.41              |
| 2:B:399:ALA:HA    | 2:B:402:ILE:HG22  | 2.02                     | 0.41              |
| 3:C:38:LEU:HD23   | 3:C:38:LEU:HA     | 1.90                     | 0.41              |
| 3:C:271:PRO:HG2   | 3:C:276:LEU:HD23  | 2.03                     | 0.41              |
| 4:D:21:LEU:HD13   | 4:D:192:TRP:HB2   | 2.03                     | 0.41              |
| 4:D:165:TYR:CZ    | 4:D:168:ILE:HG13  | 2.55                     | 0.41              |
| 5:E:151:GLY:O     | 5:E:154:GLY:N     | 2.54                     | 0.41              |
| 5:E:171:ILE:HG12  | 5:E:176:ALA:O     | 2.20                     | 0.41              |
| 1:N:133:VAL:O     | 1:N:137:GLU:HG3   | 2.20                     | 0.41              |
| 1:N:422:LEU:HD22  | 1:N:437:ILE:CD1   | 2.51                     | 0.41              |
| 2:O:46:ARG:HD2    | 2:O:110:GLU:CD    | 2.46                     | 0.41              |
| 2:O:59:THR:CG2    | 2:O:60:THR:N      | 2.84                     | 0.41              |
| 2:O:169:LYS:CG    | 2:O:240:TRP:HB2   | 2.49                     | 0.41              |
| 2:O:212:LYS:HB3   | 2:O:215:ASP:OD2   | 2.21                     | 0.41              |
| 2:O:248:ASN:ND2   | 2:O:428:GLY:HA2   | 2.36                     | 0.41              |
| 2:O:318:ASP:O     | 2:O:319:SER:HB2   | 2.19                     | 0.41              |
| 3:P:45:GLN:CB     | 12:P:501:HEM:HAB  | 2.51                     | 0.41              |
| 3:P:138:GLN:HA    | 3:P:138:GLN:OE1   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:P:156:TYR:N    | 3:P:156:TYR:CD2   | 2.89                     | 0.41              |
| 3:P:286:PRO:O    | 3:P:287:ASN:CB    | 2.69                     | 0.41              |
| 3:P:342:GLN:HB3  | 3:P:348:PHE:CD1   | 2.56                     | 0.41              |
| 4:Q:70:VAL:CG2   | 4:Q:83:ARG:CZ     | 2.98                     | 0.41              |
| 4:Q:221:TYR:HD2  | 5:R:39:VAL:HG11   | 1.83                     | 0.41              |
| 1:A:114:ALA:HB2  | 1:A:216:PHE:CE2   | 2.55                     | 0.41              |
| 3:C:295:LEU:HD11 | 13:C:2001:JZV:HAZ | 2.02                     | 0.41              |
| 6:F:13:MET:HE2   | 6:F:16:ILE:HD12   | 2.03                     | 0.41              |
| 2:O:72:ALA:HB1   | 2:O:75:LEU:HD12   | 2.03                     | 0.41              |
| 3:P:37:LEU:O     | 3:P:41:CYS:HB2    | 2.20                     | 0.41              |
| 3:P:81:ARG:HD3   | 3:P:81:ARG:C      | 2.46                     | 0.41              |
| 5:R:95:PRO:HG2   | 5:R:145:VAL:CG1   | 2.51                     | 0.41              |
| 1:A:4:TYR:HE2    | 1:A:396:ASP:OD2   | 2.04                     | 0.40              |
| 1:A:140:GLU:HG2  | 9:I:50:LEU:HG     | 2.02                     | 0.40              |
| 1:A:276:ILE:HG12 | 1:A:357:ALA:HB2   | 2.02                     | 0.40              |
| 1:A:321:GLY:HA2  | 1:A:342:TRP:CZ2   | 2.55                     | 0.40              |
| 2:B:133:ARG:HD3  | 2:B:135:TRP:CZ2   | 2.56                     | 0.40              |
| 2:B:248:ASN:ND2  | 2:B:250:HIS:H     | 2.20                     | 0.40              |
| 5:E:75:GLU:HG3   | 5:E:75:GLU:O      | 2.21                     | 0.40              |
| 2:O:372:VAL:HG13 | 2:O:378:LEU:HA    | 2.03                     | 0.40              |
| 4:Q:26:VAL:HG22  | 4:Q:188:THR:HG22  | 2.02                     | 0.40              |
| 5:R:134:ILE:HB   | 5:R:185:TYR:CE1   | 2.56                     | 0.40              |
| 6:S:60:PHE:O     | 6:S:64:ARG:HB2    | 2.20                     | 0.40              |
| 4:D:70:VAL:CG2   | 4:D:83:ARG:CZ     | 2.99                     | 0.40              |
| 5:E:153:PHE:C    | 5:E:155:GLY:H     | 2.29                     | 0.40              |
| 7:G:73:ASN:HA    | 7:G:74:PRO:HD2    | 1.96                     | 0.40              |
| 2:O:56:ARG:HB2   | 2:O:102:ARG:O     | 2.21                     | 0.40              |
| 2:O:291:VAL:C    | 2:O:293:SER:H     | 2.30                     | 0.40              |
| 1:A:170:THR:CG2  | 1:A:171:THR:H     | 2.33                     | 0.40              |
| 1:A:354:VAL:HG23 | 1:A:355:LYS:N     | 2.35                     | 0.40              |
| 3:C:324:THR:O    | 3:C:325:LEU:C     | 2.64                     | 0.40              |
| 5:E:109:GLU:OE1  | 5:E:109:GLU:HA    | 2.21                     | 0.40              |
| 5:E:115:SER:CB   | 5:E:116:LYS:HD2   | 2.52                     | 0.40              |
| 7:G:60:SER:O     | 7:G:61:TRP:C      | 2.63                     | 0.40              |
| 1:N:62:LEU:O     | 1:N:64:PHE:N      | 2.55                     | 0.40              |
| 1:N:253:VAL:O    | 1:N:323:HIS:HA    | 2.20                     | 0.40              |
| 1:N:343:MET:O    | 1:N:347:THR:HG23  | 2.21                     | 0.40              |
| 2:O:124:LEU:HD23 | 2:O:124:LEU:C     | 2.46                     | 0.40              |
| 4:Q:54:VAL:HG11  | 4:Q:192:TRP:NE1   | 2.36                     | 0.40              |
| 4:Q:57:THR:CG2   | 4:Q:58:GLU:N      | 2.83                     | 0.40              |
| 4:Q:102:ARG:HA   | 4:Q:108:ALA:O     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:R:76:ILE:CD1    | 5:R:98:VAL:HG21   | 2.52                     | 0.40              |
| 5:R:121:GLN:O     | 5:R:170:ARG:NH1   | 2.45                     | 0.40              |
| 13:C:2001:JZV:HAZ | 13:C:2001:JZV:HAY | 1.80                     | 0.40              |
| 5:E:76:ILE:HB     | 5:E:193:VAL:CG1   | 2.51                     | 0.40              |
| 5:E:165:TYR:CE2   | 5:E:180:LEU:HG    | 2.57                     | 0.40              |
| 2:O:168:TYR:HB2   | 2:O:173:ALA:HB2   | 2.03                     | 0.40              |
| 3:P:27:ASN:ND2    | 3:P:209:PRO:HG2   | 2.36                     | 0.40              |
| 4:Q:79:GLU:OE2    | 4:Q:79:GLU:HA     | 2.22                     | 0.40              |
| 5:R:106:ILE:HG21  | 5:R:130:PRO:HB3   | 2.02                     | 0.40              |
| 5:R:194:VAL:O     | 5:R:194:VAL:HG12  | 2.21                     | 0.40              |
| 8:U:67:HIS:C      | 8:U:67:HIS:ND1    | 2.79                     | 0.40              |
| 2:B:217:LYS:HE2   | 2:B:221:GLU:OE2   | 2.21                     | 0.40              |
| 2:B:276:GLN:HG2   | 2:B:281:ALA:HB2   | 2.03                     | 0.40              |
| 2:B:370:MET:O     | 2:B:373:GLU:HG3   | 2.22                     | 0.40              |
| 1:N:394:GLU:O     | 1:N:395:TRP:C     | 2.64                     | 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     | 442/446 (99%)  | 414 (94%) | 22 (5%)  | 6 (1%)   | 9           | 17  |
| 1   | N     | 440/446 (99%)  | 414 (94%) | 19 (4%)  | 7 (2%)   | 7           | 14  |
| 2   | B     | 418/441 (95%)  | 358 (86%) | 46 (11%) | 14 (3%)  | 3           | 5   |
| 2   | O     | 420/441 (95%)  | 370 (88%) | 40 (10%) | 10 (2%)  | 4           | 9   |
| 3   | C     | 378/380 (100%) | 363 (96%) | 10 (3%)  | 5 (1%)   | 9           | 18  |
| 3   | P     | 377/380 (99%)  | 358 (95%) | 14 (4%)  | 5 (1%)   | 9           | 18  |
| 4   | D     | 239/241 (99%)  | 227 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 4   | Q     | 239/241 (99%)  | 223 (93%) | 15 (6%)  | 1 (0%)   | 30          | 50  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | E     | 194/196 (99%)   | 152 (78%)  | 28 (14%) | 14 (7%)  | 1           | 1   |
| 5   | R     | 194/196 (99%)   | 165 (85%)  | 22 (11%) | 7 (4%)   | 2           | 4   |
| 6   | F     | 99/110 (90%)    | 95 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 6   | S     | 99/110 (90%)    | 91 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 7   | G     | 78/81 (96%)     | 69 (88%)   | 6 (8%)   | 3 (4%)   | 2           | 4   |
| 7   | T     | 77/81 (95%)     | 69 (90%)   | 6 (8%)   | 2 (3%)   | 4           | 7   |
| 8   | H     | 68/77 (88%)     | 64 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 8   | U     | 65/77 (84%)     | 60 (92%)   | 3 (5%)   | 2 (3%)   | 3           | 6   |
| 9   | I     | 29/47 (62%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 9   | V     | 29/47 (62%)     | 28 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | J     | 59/61 (97%)     | 58 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 10  | W     | 58/61 (95%)     | 54 (93%)   | 3 (5%)   | 1 (2%)   | 7           | 14  |
| All | All   | 4002/4160 (96%) | 3659 (91%) | 266 (7%) | 77 (2%)  | 6           | 12  |

All (77) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | GLY  |
| 2   | B     | 21  | ALA  |
| 2   | B     | 24  | LEU  |
| 2   | B     | 26  | ILE  |
| 2   | B     | 29  | LEU  |
| 2   | B     | 171 | ALA  |
| 2   | B     | 226 | ILE  |
| 2   | B     | 228 | SER  |
| 3   | C     | 287 | ASN  |
| 5   | E     | 127 | VAL  |
| 5   | E     | 128 | LYS  |
| 5   | E     | 130 | PRO  |
| 5   | E     | 163 | SER  |
| 2   | O     | 26  | ILE  |
| 2   | O     | 171 | ALA  |
| 2   | O     | 228 | SER  |
| 3   | P     | 287 | ASN  |
| 4   | Q     | 3   | LEU  |
| 5   | R     | 163 | SER  |
| 8   | U     | 52  | GLU  |
| 10  | W     | 61  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 282 | ARG  |
| 2   | B     | 231 | GLY  |
| 5   | E     | 80  | ASP  |
| 5   | E     | 102 | THR  |
| 5   | E     | 115 | SER  |
| 5   | E     | 177 | PRO  |
| 5   | E     | 191 | ASP  |
| 1   | N     | 218 | GLY  |
| 1   | N     | 282 | ARG  |
| 2   | O     | 24  | LEU  |
| 2   | O     | 222 | GLN  |
| 5   | R     | 185 | TYR  |
| 5   | R     | 191 | ASP  |
| 8   | U     | 49  | HIS  |
| 1   | A     | 72  | CYS  |
| 2   | B     | 389 | SER  |
| 5   | E     | 137 | GLY  |
| 1   | N     | 63  | ALA  |
| 1   | N     | 72  | CYS  |
| 1   | N     | 262 | TRP  |
| 1   | N     | 433 | ASP  |
| 2   | O     | 372 | VAL  |
| 2   | O     | 389 | SER  |
| 3   | P     | 156 | TYR  |
| 5   | R     | 186 | GLN  |
| 7   | T     | 33  | ALA  |
| 1   | A     | 262 | TRP  |
| 1   | A     | 433 | ASP  |
| 2   | B     | 372 | VAL  |
| 2   | B     | 386 | ALA  |
| 3   | C     | 3   | PRO  |
| 5   | E     | 154 | GLY  |
| 2   | O     | 19  | PRO  |
| 3   | P     | 3   | PRO  |
| 3   | P     | 157 | ILE  |
| 5   | R     | 154 | GLY  |
| 2   | B     | 201 | SER  |
| 2   | B     | 221 | GLU  |
| 2   | B     | 371 | SER  |
| 3   | C     | 156 | TYR  |
| 5   | E     | 166 | ASP  |
| 7   | G     | 33  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 443 | TRP  |
| 5   | E     | 120 | PRO  |
| 5   | E     | 150 | SER  |
| 7   | G     | 61  | TRP  |
| 2   | O     | 55  | SER  |
| 2   | O     | 330 | ALA  |
| 3   | C     | 158 | GLY  |
| 1   | A     | 71  | PRO  |
| 3   | C     | 264 | VAL  |
| 5   | R     | 137 | GLY  |
| 3   | P     | 264 | VAL  |
| 5   | R     | 127 | VAL  |
| 7   | T     | 50  | PRO  |
| 7   | G     | 50  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |    |
|-----|-------|----------------|------------|----------|-------------|----|
| 1   | A     | 365/368 (99%)  | 355 (97%)  | 10 (3%)  | 39          | 62 |
| 1   | N     | 365/368 (99%)  | 354 (97%)  | 11 (3%)  | 36          | 60 |
| 2   | B     | 331/347 (95%)  | 319 (96%)  | 12 (4%)  | 31          | 55 |
| 2   | O     | 333/347 (96%)  | 320 (96%)  | 13 (4%)  | 28          | 51 |
| 3   | C     | 328/329 (100%) | 326 (99%)  | 2 (1%)   | 78          | 88 |
| 3   | P     | 328/329 (100%) | 327 (100%) | 1 (0%)   | 86          | 93 |
| 4   | D     | 200/200 (100%) | 196 (98%)  | 4 (2%)   | 48          | 69 |
| 4   | Q     | 200/200 (100%) | 197 (98%)  | 3 (2%)   | 57          | 74 |
| 5   | E     | 166/166 (100%) | 164 (99%)  | 2 (1%)   | 63          | 78 |
| 5   | R     | 165/166 (99%)  | 162 (98%)  | 3 (2%)   | 51          | 71 |
| 6   | F     | 93/96 (97%)    | 86 (92%)   | 7 (8%)   | 12          | 24 |
| 6   | S     | 93/96 (97%)    | 87 (94%)   | 6 (6%)   | 15          | 29 |
| 7   | G     | 71/71 (100%)   | 70 (99%)   | 1 (1%)   | 59          | 75 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 7   | T     | 70/71 (99%)     | 70 (100%)  | 0        | 100         | 100 |
| 8   | H     | 65/71 (92%)     | 65 (100%)  | 0        | 100         | 100 |
| 8   | U     | 63/71 (89%)     | 62 (98%)   | 1 (2%)   | 55          | 73  |
| 9   | I     | 23/26 (88%)     | 21 (91%)   | 2 (9%)   | 9           | 18  |
| 9   | V     | 23/26 (88%)     | 21 (91%)   | 2 (9%)   | 9           | 18  |
| 10  | J     | 49/49 (100%)    | 48 (98%)   | 1 (2%)   | 48          | 69  |
| 10  | W     | 47/49 (96%)     | 46 (98%)   | 1 (2%)   | 47          | 67  |
| All | All   | 3378/3446 (98%) | 3296 (98%) | 82 (2%)  | 43          | 65  |

All (82) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | VAL  |
| 1   | A     | 106 | MET  |
| 1   | A     | 108 | LYS  |
| 1   | A     | 228 | VAL  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 281 | ASP  |
| 1   | A     | 352 | SER  |
| 1   | A     | 395 | TRP  |
| 1   | A     | 432 | LEU  |
| 1   | A     | 443 | TRP  |
| 2   | B     | 23  | ASP  |
| 2   | B     | 26  | ILE  |
| 2   | B     | 31  | ASN  |
| 2   | B     | 150 | VAL  |
| 2   | B     | 170 | THR  |
| 2   | B     | 225 | ASN  |
| 2   | B     | 248 | ASN  |
| 2   | B     | 250 | HIS  |
| 2   | B     | 291 | VAL  |
| 2   | B     | 338 | ARG  |
| 2   | B     | 341 | MET  |
| 2   | B     | 402 | ILE  |
| 3   | C     | 216 | SER  |
| 3   | C     | 223 | PRO  |
| 4   | D     | 57  | THR  |
| 4   | D     | 70  | VAL  |
| 4   | D     | 169 | LEU  |
| 4   | D     | 203 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 178 | TYR  |
| 5   | E     | 185 | TYR  |
| 6   | F     | 52  | GLU  |
| 6   | F     | 58  | ARG  |
| 6   | F     | 64  | ARG  |
| 6   | F     | 70  | LEU  |
| 6   | F     | 73  | ARG  |
| 6   | F     | 78  | GLU  |
| 6   | F     | 84  | GLU  |
| 7   | G     | 50  | PRO  |
| 9   | I     | 68  | ILE  |
| 9   | I     | 71  | ASN  |
| 10  | J     | 59  | TYR  |
| 1   | N     | 3   | THR  |
| 1   | N     | 18  | THR  |
| 1   | N     | 50  | GLU  |
| 1   | N     | 106 | MET  |
| 1   | N     | 108 | LYS  |
| 1   | N     | 228 | VAL  |
| 1   | N     | 281 | ASP  |
| 1   | N     | 352 | SER  |
| 1   | N     | 395 | TRP  |
| 1   | N     | 432 | LEU  |
| 1   | N     | 443 | TRP  |
| 2   | O     | 18  | CYS  |
| 2   | O     | 19  | PRO  |
| 2   | O     | 26  | ILE  |
| 2   | O     | 31  | ASN  |
| 2   | O     | 150 | VAL  |
| 2   | O     | 170 | THR  |
| 2   | O     | 248 | ASN  |
| 2   | O     | 250 | HIS  |
| 2   | O     | 260 | GLU  |
| 2   | O     | 291 | VAL  |
| 2   | O     | 341 | MET  |
| 2   | O     | 402 | ILE  |
| 2   | O     | 418 | VAL  |
| 3   | P     | 216 | SER  |
| 4   | Q     | 70  | VAL  |
| 4   | Q     | 169 | LEU  |
| 4   | Q     | 203 | ARG  |
| 5   | R     | 31  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | R     | 178 | TYR  |
| 5   | R     | 185 | TYR  |
| 6   | S     | 52  | GLU  |
| 6   | S     | 64  | ARG  |
| 6   | S     | 70  | LEU  |
| 6   | S     | 73  | ARG  |
| 6   | S     | 78  | GLU  |
| 6   | S     | 84  | GLU  |
| 8   | U     | 49  | HIS  |
| 9   | V     | 68  | ILE  |
| 9   | V     | 75  | SER  |
| 10  | W     | 59  | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | GLN  |
| 1   | A     | 176 | HIS  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 289 | HIS  |
| 1   | A     | 301 | HIS  |
| 1   | A     | 311 | ASN  |
| 1   | A     | 339 | GLN  |
| 1   | A     | 385 | ASN  |
| 2   | B     | 31  | ASN  |
| 2   | B     | 115 | HIS  |
| 2   | B     | 153 | GLN  |
| 2   | B     | 156 | GLN  |
| 2   | B     | 197 | ASN  |
| 2   | B     | 198 | ASN  |
| 2   | B     | 222 | GLN  |
| 2   | B     | 247 | GLN  |
| 2   | B     | 248 | ASN  |
| 2   | B     | 270 | ASN  |
| 2   | B     | 276 | GLN  |
| 2   | B     | 297 | GLN  |
| 2   | B     | 315 | ASN  |
| 2   | B     | 342 | ASN  |
| 2   | B     | 343 | GLN  |
| 2   | B     | 362 | ASN  |
| 2   | B     | 363 | GLN  |
| 3   | C     | 9   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 17  | ASN  |
| 3   | C     | 55  | HIS  |
| 3   | C     | 69  | HIS  |
| 3   | C     | 73  | ASN  |
| 3   | C     | 82  | ASN  |
| 3   | C     | 207 | ASN  |
| 3   | C     | 313 | GLN  |
| 3   | C     | 342 | GLN  |
| 4   | D     | 35  | GLN  |
| 4   | D     | 50  | ASN  |
| 4   | D     | 148 | HIS  |
| 4   | D     | 225 | HIS  |
| 5   | E     | 3   | ASN  |
| 5   | E     | 53  | ASN  |
| 5   | E     | 57  | GLN  |
| 5   | E     | 121 | GLN  |
| 5   | E     | 122 | HIS  |
| 5   | E     | 149 | ASN  |
| 5   | E     | 164 | HIS  |
| 5   | E     | 179 | ASN  |
| 7   | G     | 23  | GLN  |
| 7   | G     | 44  | GLN  |
| 7   | G     | 73  | ASN  |
| 9   | I     | 71  | ASN  |
| 1   | N     | 10  | ASN  |
| 1   | N     | 32  | GLN  |
| 1   | N     | 85  | HIS  |
| 1   | N     | 118 | GLN  |
| 1   | N     | 143 | ASN  |
| 1   | N     | 173 | ASN  |
| 1   | N     | 176 | HIS  |
| 1   | N     | 274 | ASN  |
| 1   | N     | 289 | HIS  |
| 1   | N     | 311 | ASN  |
| 1   | N     | 339 | GLN  |
| 2   | O     | 31  | ASN  |
| 2   | O     | 115 | HIS  |
| 2   | O     | 156 | GLN  |
| 2   | O     | 197 | ASN  |
| 2   | O     | 198 | ASN  |
| 2   | O     | 247 | GLN  |
| 2   | O     | 248 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 276 | GLN  |
| 2   | O     | 297 | GLN  |
| 2   | O     | 315 | ASN  |
| 2   | O     | 342 | ASN  |
| 2   | O     | 343 | GLN  |
| 2   | O     | 362 | ASN  |
| 2   | O     | 363 | GLN  |
| 3   | P     | 9   | HIS  |
| 3   | P     | 17  | ASN  |
| 3   | P     | 27  | ASN  |
| 3   | P     | 69  | HIS  |
| 3   | P     | 73  | ASN  |
| 3   | P     | 82  | ASN  |
| 3   | P     | 207 | ASN  |
| 3   | P     | 313 | GLN  |
| 3   | P     | 342 | GLN  |
| 4   | Q     | 35  | GLN  |
| 4   | Q     | 50  | ASN  |
| 4   | Q     | 148 | HIS  |
| 5   | R     | 3   | ASN  |
| 5   | R     | 57  | GLN  |
| 5   | R     | 107 | ASN  |
| 5   | R     | 121 | GLN  |
| 5   | R     | 164 | HIS  |
| 5   | R     | 186 | GLN  |
| 6   | S     | 72  | HIS  |
| 7   | T     | 23  | GLN  |
| 7   | T     | 44  | GLN  |
| 7   | T     | 73  | ASN  |
| 7   | T     | 79  | ASN  |
| 8   | U     | 71  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

29 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$ |
| 18  | BOG  | D     | 2009 | -    | 20,20,20     | 0.94 | 2 (10%)     | 25,25,25    | 0.83 | 2 (8%)      |
| 14  | UQ   | C     | 2002 | -    | 19,19,63     | 2.67 | 10 (52%)    | 24,26,79    | 1.28 | 3 (12%)     |
| 16  | GOL  | C     | 2011 | -    | 5,5,5        | 1.32 | 0           | 5,5,5       | 0.62 | 0           |
| 11  | PEE  | P     | 3007 | -    | 48,48,50     | 1.43 | 7 (14%)     | 51,53,55    | 0.81 | 2 (3%)      |
| 18  | BOG  | Q     | 3091 | -    | 13,13,20     | 1.39 | 2 (15%)     | 18,18,25    | 1.15 | 2 (11%)     |
| 15  | CDL  | D     | 2003 | -    | 41,41,99     | 1.21 | 4 (9%)      | 47,53,111   | 1.06 | 2 (4%)      |
| 13  | JZV  | C     | 2001 | -    | 30,30,30     | 2.00 | 5 (16%)     | 41,41,41    | 3.47 | 11 (26%)    |
| 11  | PEE  | C     | 2007 | -    | 48,48,50     | 1.46 | 7 (14%)     | 51,53,55    | 0.84 | 2 (3%)      |
| 11  | PEE  | R     | 3005 | -    | 49,49,50     | 1.55 | 10 (20%)    | 52,54,55    | 0.87 | 3 (5%)      |
| 11  | PEE  | E     | 2005 | -    | 49,49,50     | 1.57 | 11 (22%)    | 52,54,55    | 0.88 | 3 (5%)      |
| 19  | FES  | E     | 501  | 5    | 0,4,4        | -    | -           | -           | -    | -           |
| 15  | CDL  | Q     | 3003 | -    | 41,41,99     | 1.21 | 2 (4%)      | 47,53,111   | 1.07 | 2 (4%)      |
| 12  | HEM  | P     | 502  | 3    | 50,50,50     | 1.53 | 8 (16%)     | 67,82,82    | 1.42 | 8 (11%)     |
| 13  | JZV  | P     | 3001 | -    | 30,30,30     | 2.05 | 5 (16%)     | 41,41,41    | 3.58 | 11 (26%)    |
| 12  | HEM  | P     | 501  | 3    | 50,50,50     | 1.44 | 4 (8%)      | 67,82,82    | 1.32 | 8 (11%)     |
| 11  | PEE  | N     | 3008 | -    | 4,4,50       | 3.72 | 4 (100%)    | 6,6,55      | 0.69 | 0           |
| 15  | CDL  | P     | 3004 | -    | 39,39,99     | 1.22 | 2 (5%)      | 45,51,111   | 1.14 | 4 (8%)      |
| 19  | FES  | R     | 501  | 5    | 0,4,4        | -    | -           | -           | -    | -           |
| 12  | HEM  | C     | 502  | 3    | 50,50,50     | 1.55 | 7 (14%)     | 67,82,82    | 1.65 | 13 (19%)    |
| 14  | UQ   | P     | 3002 | -    | 19,19,63     | 2.64 | 10 (52%)    | 24,26,79    | 1.28 | 3 (12%)     |
| 11  | PEE  | A     | 2008 | -    | 20,20,50     | 1.87 | 6 (30%)     | 23,25,55    | 0.69 | 0           |
| 12  | HEM  | C     | 501  | 3    | 50,50,50     | 1.47 | 6 (12%)     | 67,82,82    | 1.45 | 11 (16%)    |
| 15  | CDL  | C     | 2004 | -    | 39,39,99     | 1.21 | 2 (5%)      | 45,51,111   | 1.12 | 4 (8%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | HEC  | Q     | 501  | 4    | 46,50,50     | 1.76 | 8 (17%)  | 58,82,82    | 2.14 | 8 (13%)  |
| 17  | HEC  | D     | 501  | 4    | 46,50,50     | 1.69 | 8 (17%)  | 58,82,82    | 2.21 | 8 (13%)  |
| 18  | BOG  | D     | 2091 | -    | 13,13,20     | 1.30 | 2 (15%)  | 18,18,25    | 1.11 | 2 (11%)  |
| 18  | BOG  | P     | 2010 | -    | 12,12,20     | 1.37 | 3 (25%)  | 17,17,25    | 0.58 | 0        |
| 18  | BOG  | Q     | 3009 | -    | 20,20,20     | 0.97 | 1 (5%)   | 25,25,25    | 0.90 | 1 (4%)   |
| 16  | GOL  | P     | 3011 | -    | 5,5,5        | 1.43 | 1 (20%)  | 5,5,5       | 0.67 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 18  | BOG  | D     | 2009 | -    | -       | 5/11/31/31   | 0/1/1/1 |
| 14  | UQ   | C     | 2002 | -    | -       | 4/11/35/87   | 0/1/1/1 |
| 16  | GOL  | C     | 2011 | -    | -       | 4/4/4/4      | -       |
| 11  | PEE  | P     | 3007 | -    | -       | 26/52/52/54  | -       |
| 18  | BOG  | Q     | 3091 | -    | -       | 4/4/24/31    | 0/1/1/1 |
| 15  | CDL  | D     | 2003 | -    | -       | 22/51/51/110 | -       |
| 13  | JZV  | C     | 2001 | -    | -       | 3/29/29/29   | 0/2/2/2 |
| 11  | PEE  | C     | 2007 | -    | -       | 23/52/52/54  | -       |
| 11  | PEE  | R     | 3005 | -    | -       | 27/53/53/54  | -       |
| 11  | PEE  | E     | 2005 | -    | -       | 27/53/53/54  | -       |
| 19  | FES  | E     | 501  | 5    | -       | -            | 0/1/1/1 |
| 15  | CDL  | Q     | 3003 | -    | -       | 21/51/51/110 | -       |
| 12  | HEM  | P     | 502  | 3    | -       | 6/14/54/54   | -       |
| 13  | JZV  | P     | 3001 | -    | -       | 3/29/29/29   | 0/2/2/2 |
| 12  | HEM  | P     | 501  | 3    | -       | 5/14/54/54   | -       |
| 15  | CDL  | P     | 3004 | -    | -       | 21/49/49/110 | -       |
| 19  | FES  | R     | 501  | 5    | -       | -            | 0/1/1/1 |
| 12  | HEM  | C     | 502  | 3    | -       | 5/14/54/54   | -       |
| 14  | UQ   | P     | 3002 | -    | -       | 4/11/35/87   | 0/1/1/1 |
| 11  | PEE  | A     | 2008 | -    | -       | 12/24/24/54  | -       |
| 12  | HEM  | C     | 501  | 3    | -       | 7/14/54/54   | -       |
| 15  | CDL  | C     | 2004 | -    | -       | 21/49/49/110 | -       |
| 17  | HEC  | Q     | 501  | 4    | -       | 10/14/54/54  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 17  | HEC  | D     | 501  | 4    | -       | 10/14/54/54 | -       |
| 18  | BOG  | D     | 2091 | -    | -       | 2/4/24/31   | 0/1/1/1 |
| 18  | BOG  | P     | 2010 | -    | -       | 0/2/22/31   | 0/1/1/1 |
| 18  | BOG  | Q     | 3009 | -    | -       | 5/11/31/31  | 0/1/1/1 |
| 16  | GOL  | P     | 3011 | -    | -       | 3/4/4/4     | -       |

All (137) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | P     | 3001 | JZV  | CAT-CAS | -6.50 | 1.39        | 1.49     |
| 13  | C     | 2001 | JZV  | CAT-CAS | -6.28 | 1.39        | 1.49     |
| 17  | Q     | 501  | HEC  | CAC-C3C | 5.76  | 1.53        | 1.35     |
| 17  | Q     | 501  | HEC  | CAB-C3B | 5.58  | 1.53        | 1.35     |
| 17  | D     | 501  | HEC  | CAC-C3C | 5.55  | 1.53        | 1.35     |
| 13  | C     | 2001 | JZV  | CAI-CAJ | -5.27 | 1.39        | 1.48     |
| 13  | P     | 3001 | JZV  | CAI-CAJ | -5.22 | 1.39        | 1.48     |
| 14  | C     | 2002 | UQ   | C6-C5   | 5.18  | 1.44        | 1.35     |
| 14  | P     | 3002 | UQ   | C7-C6   | 5.15  | 1.60        | 1.51     |
| 11  | N     | 3008 | PEE  | P-O1P   | 5.07  | 1.62        | 1.50     |
| 17  | D     | 501  | HEC  | CAB-C3B | 5.04  | 1.51        | 1.35     |
| 14  | C     | 2002 | UQ   | C7-C6   | 5.01  | 1.60        | 1.51     |
| 12  | C     | 501  | HEM  | CBC-CAC | 4.89  | 1.53        | 1.30     |
| 14  | P     | 3002 | UQ   | C6-C5   | 4.84  | 1.43        | 1.35     |
| 12  | P     | 501  | HEM  | CBC-CAC | 4.62  | 1.52        | 1.30     |
| 11  | C     | 2007 | PEE  | C39-C38 | 4.42  | 1.56        | 1.31     |
| 12  | P     | 501  | HEM  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 13  | P     | 3001 | JZV  | CAS-NAR | 4.31  | 1.33        | 1.28     |
| 11  | P     | 3007 | PEE  | C39-C38 | 4.26  | 1.55        | 1.31     |
| 12  | C     | 502  | HEM  | CBB-CAB | 4.22  | 1.50        | 1.30     |
| 11  | E     | 2005 | PEE  | C39-C38 | 4.16  | 1.55        | 1.31     |
| 11  | R     | 3005 | PEE  | C39-C38 | 4.08  | 1.54        | 1.31     |
| 12  | P     | 502  | HEM  | CBC-CAC | 4.01  | 1.49        | 1.30     |
| 13  | C     | 2001 | JZV  | CAS-NAR | 3.98  | 1.33        | 1.28     |
| 12  | C     | 502  | HEM  | CBC-CAC | 3.93  | 1.49        | 1.30     |
| 12  | P     | 502  | HEM  | CBB-CAB | 3.82  | 1.48        | 1.30     |
| 14  | P     | 3002 | UQ   | C6-C1   | 3.81  | 1.57        | 1.46     |
| 12  | C     | 501  | HEM  | CBB-CAB | 3.81  | 1.48        | 1.30     |
| 14  | C     | 2002 | UQ   | C6-C1   | 3.74  | 1.57        | 1.46     |
| 11  | R     | 3005 | PEE  | O2-C10  | 3.62  | 1.44        | 1.34     |
| 11  | N     | 3008 | PEE  | P-O4P   | 3.55  | 1.65        | 1.54     |
| 11  | E     | 2005 | PEE  | O3-C30  | 3.55  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | P     | 501  | HEM  | CAB-C3B | -3.47 | 1.38        | 1.47     |
| 11  | P     | 3007 | PEE  | O3-C30  | 3.44  | 1.43        | 1.33     |
| 12  | C     | 501  | HEM  | CAB-C3B | -3.42 | 1.38        | 1.47     |
| 11  | C     | 2007 | PEE  | C21-C22 | -3.41 | 1.34        | 1.51     |
| 11  | P     | 3007 | PEE  | C21-C22 | -3.39 | 1.34        | 1.51     |
| 11  | C     | 2007 | PEE  | O3-C30  | 3.39  | 1.43        | 1.33     |
| 11  | A     | 2008 | PEE  | O2-C10  | 3.37  | 1.43        | 1.34     |
| 11  | E     | 2005 | PEE  | O2-C10  | 3.35  | 1.43        | 1.34     |
| 14  | P     | 3002 | UQ   | O3-C3   | 3.33  | 1.44        | 1.36     |
| 11  | C     | 2007 | PEE  | P-O1P   | 3.33  | 1.62        | 1.50     |
| 11  | R     | 3005 | PEE  | C21-C22 | -3.29 | 1.35        | 1.51     |
| 11  | A     | 2008 | PEE  | O3-C30  | 3.28  | 1.42        | 1.33     |
| 12  | C     | 502  | HEM  | C4D-C3D | 3.27  | 1.50        | 1.45     |
| 11  | A     | 2008 | PEE  | P-O1P   | 3.27  | 1.62        | 1.50     |
| 11  | N     | 3008 | PEE  | P-O3P   | 3.26  | 1.64        | 1.54     |
| 14  | C     | 2002 | UQ   | O3-C3   | 3.25  | 1.44        | 1.36     |
| 11  | R     | 3005 | PEE  | P-O1P   | 3.25  | 1.62        | 1.50     |
| 11  | R     | 3005 | PEE  | O3-C30  | 3.24  | 1.42        | 1.33     |
| 11  | E     | 2005 | PEE  | C21-C22 | -3.24 | 1.35        | 1.51     |
| 11  | E     | 2005 | PEE  | P-O1P   | 3.23  | 1.62        | 1.50     |
| 12  | C     | 502  | HEM  | CAB-C3B | -3.22 | 1.38        | 1.47     |
| 13  | C     | 2001 | JZV  | OAQ-NAR | -3.19 | 1.36        | 1.42     |
| 12  | P     | 502  | HEM  | CAB-C3B | -3.13 | 1.39        | 1.47     |
| 13  | P     | 3001 | JZV  | OAQ-NAR | -3.10 | 1.36        | 1.42     |
| 11  | P     | 3007 | PEE  | P-O1P   | 3.05  | 1.61        | 1.50     |
| 13  | P     | 3001 | JZV  | CAJ-NAD | 3.01  | 1.33        | 1.29     |
| 14  | C     | 2002 | UQ   | C2-C1   | 2.99  | 1.57        | 1.48     |
| 14  | C     | 2002 | UQ   | CM5-C5  | 2.97  | 1.56        | 1.50     |
| 12  | P     | 502  | HEM  | CAC-C3C | -2.97 | 1.39        | 1.47     |
| 14  | P     | 3002 | UQ   | C7-C8   | 2.87  | 1.55        | 1.50     |
| 13  | C     | 2001 | JZV  | CAJ-NAD | 2.85  | 1.33        | 1.29     |
| 14  | C     | 2002 | UQ   | O2-C2   | 2.83  | 1.43        | 1.36     |
| 11  | P     | 3007 | PEE  | O2-C10  | 2.74  | 1.42        | 1.34     |
| 14  | P     | 3002 | UQ   | C2-C1   | 2.74  | 1.56        | 1.48     |
| 14  | C     | 2002 | UQ   | C7-C8   | 2.72  | 1.54        | 1.50     |
| 11  | C     | 2007 | PEE  | O2-C10  | 2.70  | 1.41        | 1.34     |
| 14  | P     | 3002 | UQ   | CM5-C5  | 2.70  | 1.56        | 1.50     |
| 12  | C     | 501  | HEM  | CAC-C3C | -2.68 | 1.40        | 1.47     |
| 14  | P     | 3002 | UQ   | C5-C4   | 2.64  | 1.56        | 1.47     |
| 12  | P     | 501  | HEM  | CAC-C3C | -2.64 | 1.40        | 1.47     |
| 14  | P     | 3002 | UQ   | O2-C2   | 2.62  | 1.43        | 1.36     |
| 14  | C     | 2002 | UQ   | C5-C4   | 2.59  | 1.56        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | P     | 3002 | UQ   | C3-C4   | 2.56  | 1.56        | 1.48     |
| 11  | N     | 3008 | PEE  | P-O2P   | 2.56  | 1.62        | 1.54     |
| 11  | E     | 2005 | PEE  | C31-C30 | 2.55  | 1.58        | 1.50     |
| 17  | D     | 501  | HEC  | C4D-C3D | 2.54  | 1.49        | 1.44     |
| 11  | E     | 2005 | PEE  | C3-C2   | 2.51  | 1.58        | 1.50     |
| 18  | Q     | 3091 | BOG  | O5-C1   | 2.48  | 1.48        | 1.41     |
| 12  | C     | 502  | HEM  | CMB-C2B | 2.46  | 1.55        | 1.50     |
| 11  | R     | 3005 | PEE  | C11-C10 | 2.45  | 1.57        | 1.50     |
| 17  | D     | 501  | HEC  | C3C-C4C | -2.44 | 1.41        | 1.46     |
| 18  | P     | 2010 | BOG  | C4-C5   | 2.44  | 1.58        | 1.53     |
| 17  | Q     | 501  | HEC  | C3B-C2B | -2.41 | 1.33        | 1.41     |
| 12  | C     | 502  | HEM  | CAC-C3C | -2.40 | 1.41        | 1.47     |
| 11  | E     | 2005 | PEE  | C1-C2   | 2.39  | 1.58        | 1.50     |
| 14  | C     | 2002 | UQ   | C3-C4   | 2.39  | 1.55        | 1.48     |
| 11  | C     | 2007 | PEE  | C31-C30 | 2.39  | 1.57        | 1.50     |
| 15  | P     | 3004 | CDL  | O1-C1   | 2.38  | 1.50        | 1.43     |
| 17  | Q     | 501  | HEC  | C3C-C2C | -2.38 | 1.33        | 1.41     |
| 11  | A     | 2008 | PEE  | C3-C2   | 2.37  | 1.58        | 1.50     |
| 18  | D     | 2091 | BOG  | C4-C5   | 2.36  | 1.58        | 1.53     |
| 11  | R     | 3005 | PEE  | C31-C30 | 2.35  | 1.57        | 1.50     |
| 15  | C     | 2004 | CDL  | O1-C1   | 2.35  | 1.50        | 1.43     |
| 18  | Q     | 3091 | BOG  | C4-C5   | 2.34  | 1.58        | 1.53     |
| 11  | R     | 3005 | PEE  | C3-C2   | 2.34  | 1.58        | 1.50     |
| 11  | E     | 2005 | PEE  | C11-C10 | 2.33  | 1.57        | 1.50     |
| 17  | D     | 501  | HEC  | C4C-NC  | -2.31 | 1.35        | 1.39     |
| 12  | P     | 502  | HEM  | C1C-NC  | -2.30 | 1.35        | 1.39     |
| 18  | D     | 2091 | BOG  | O5-C1   | 2.30  | 1.47        | 1.41     |
| 11  | R     | 3005 | PEE  | C1-C2   | 2.30  | 1.58        | 1.50     |
| 15  | D     | 2003 | CDL  | OA6-CA5 | 2.28  | 1.40        | 1.34     |
| 17  | Q     | 501  | HEC  | C4C-NC  | -2.28 | 1.35        | 1.39     |
| 17  | D     | 501  | HEC  | CHD-C4C | -2.26 | 1.33        | 1.38     |
| 11  | P     | 3007 | PEE  | C31-C30 | 2.25  | 1.57        | 1.50     |
| 17  | Q     | 501  | HEC  | CHC-C4B | -2.24 | 1.33        | 1.38     |
| 18  | Q     | 3009 | BOG  | O5-C1   | 2.24  | 1.47        | 1.41     |
| 11  | A     | 2008 | PEE  | C1-C2   | 2.22  | 1.57        | 1.50     |
| 11  | A     | 2008 | PEE  | C11-C10 | 2.22  | 1.57        | 1.50     |
| 12  | P     | 502  | HEM  | C4D-C3D | 2.22  | 1.48        | 1.45     |
| 18  | P     | 2010 | BOG  | C1-C2   | 2.22  | 1.57        | 1.52     |
| 11  | R     | 3005 | PEE  | O2-C2   | 2.22  | 1.51        | 1.46     |
| 15  | Q     | 3003 | CDL  | O1-C1   | 2.22  | 1.49        | 1.43     |
| 17  | Q     | 501  | HEC  | C1D-ND  | -2.19 | 1.35        | 1.39     |
| 15  | C     | 2004 | CDL  | CB3-CB4 | 2.17  | 1.57        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | D     | 2003 | CDL  | O1-C1   | 2.15  | 1.49        | 1.43     |
| 17  | Q     | 501  | HEC  | C3C-C4C | -2.14 | 1.42        | 1.46     |
| 11  | C     | 2007 | PEE  | C3-C2   | 2.13  | 1.57        | 1.50     |
| 11  | E     | 2005 | PEE  | P-O4P   | 2.12  | 1.67        | 1.59     |
| 12  | C     | 501  | HEM  | C4A-NA  | -2.11 | 1.35        | 1.39     |
| 17  | D     | 501  | HEC  | C3C-C2C | -2.11 | 1.34        | 1.41     |
| 16  | P     | 3011 | GOL  | O2-C2   | 2.09  | 1.49        | 1.43     |
| 18  | D     | 2009 | BOG  | O5-C1   | 2.08  | 1.47        | 1.41     |
| 15  | P     | 3004 | CDL  | OB2-CB2 | -2.07 | 1.36        | 1.44     |
| 12  | P     | 502  | HEM  | C4B-NB  | -2.05 | 1.34        | 1.38     |
| 11  | E     | 2005 | PEE  | O2-C2   | 2.05  | 1.51        | 1.46     |
| 17  | D     | 501  | HEC  | C3B-C4B | -2.05 | 1.42        | 1.46     |
| 15  | D     | 2003 | CDL  | OB8-CB7 | 2.04  | 1.39        | 1.33     |
| 11  | P     | 3007 | PEE  | C3-C2   | 2.04  | 1.57        | 1.50     |
| 18  | D     | 2009 | BOG  | C1-C2   | 2.03  | 1.58        | 1.52     |
| 12  | C     | 502  | HEM  | CHD-C4C | -2.03 | 1.34        | 1.38     |
| 15  | Q     | 3003 | CDL  | OB2-CB2 | -2.02 | 1.37        | 1.44     |
| 12  | P     | 502  | HEM  | C3B-C4B | 2.02  | 1.48        | 1.44     |
| 15  | D     | 2003 | CDL  | CA3-CA4 | 2.01  | 1.57        | 1.50     |
| 18  | P     | 2010 | BOG  | O5-C1   | 2.00  | 1.47        | 1.42     |
| 12  | C     | 501  | HEM  | C2A-C3A | -2.00 | 1.33        | 1.38     |

All (113) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | P     | 3001 | JZV  | OAQ-NAR-CAS | 14.37 | 133.72      | 111.94   |
| 13  | C     | 2001 | JZV  | OAQ-NAR-CAS | 12.58 | 131.00      | 111.94   |
| 17  | Q     | 501  | HEC  | CBB-CAB-C3B | -9.51 | 108.43      | 127.43   |
| 17  | D     | 501  | HEC  | CBB-CAB-C3B | -9.50 | 108.44      | 127.43   |
| 13  | P     | 3001 | JZV  | CAT-CAS-NAR | 8.27  | 133.75      | 115.30   |
| 13  | C     | 2001 | JZV  | CAT-CAS-NAR | 8.17  | 133.53      | 115.30   |
| 13  | C     | 2001 | JZV  | CAY-CAS-NAR | -7.90 | 108.61      | 123.95   |
| 17  | Q     | 501  | HEC  | CBC-CAC-C3C | -7.81 | 111.83      | 127.43   |
| 13  | P     | 3001 | JZV  | OAE-NAD-CAJ | 7.68  | 119.95      | 111.50   |
| 13  | P     | 3001 | JZV  | CAY-CAS-NAR | -7.47 | 109.46      | 123.95   |
| 13  | C     | 2001 | JZV  | OAE-NAD-CAJ | 7.29  | 119.53      | 111.50   |
| 17  | D     | 501  | HEC  | CBC-CAC-C3C | -7.22 | 113.00      | 127.43   |
| 13  | C     | 2001 | JZV  | OAL-CAK-CAJ | 7.05  | 119.30      | 111.75   |
| 13  | P     | 3001 | JZV  | OAL-CAK-CAJ | 6.97  | 119.21      | 111.75   |
| 13  | C     | 2001 | JZV  | CAP-OAQ-NAR | 5.56  | 114.91      | 107.92   |
| 12  | C     | 502  | HEM  | CAD-C3D-C4D | 4.87  | 133.19      | 124.70   |
| 13  | C     | 2001 | JZV  | OAQ-CAP-CAH | 4.80  | 122.17      | 109.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Q     | 501  | HEC  | CAA-C2A-C1A | 4.73  | 134.46      | 124.85   |
| 12  | C     | 502  | HEM  | C3B-C2B-C1B | -4.66 | 102.91      | 106.41   |
| 17  | Q     | 501  | HEC  | CAA-C2A-C3A | -4.58 | 119.28      | 127.87   |
| 17  | D     | 501  | HEC  | CAA-C2A-C1A | 4.45  | 133.90      | 124.85   |
| 13  | P     | 3001 | JZV  | CAP-OAQ-NAR | 4.42  | 113.48      | 107.92   |
| 12  | P     | 502  | HEM  | CAD-C3D-C4D | 4.29  | 132.17      | 124.70   |
| 14  | P     | 3002 | UQ   | C8-C7-C6    | 4.12  | 122.23      | 112.08   |
| 12  | C     | 501  | HEM  | C3B-C4B-NB  | 4.05  | 112.38      | 109.47   |
| 14  | C     | 2002 | UQ   | C8-C7-C6    | 4.05  | 122.06      | 112.08   |
| 17  | D     | 501  | HEC  | CAA-C2A-C3A | -3.84 | 120.68      | 127.87   |
| 13  | P     | 3001 | JZV  | OAQ-CAP-CAH | 3.82  | 119.66      | 109.91   |
| 12  | P     | 502  | HEM  | C3B-C2B-C1B | -3.74 | 103.60      | 106.41   |
| 12  | P     | 501  | HEM  | CAD-C3D-C4D | 3.73  | 131.20      | 124.70   |
| 18  | Q     | 3091 | BOG  | C1'-O1-C1   | 3.67  | 118.83      | 113.26   |
| 12  | P     | 502  | HEM  | C4C-C3C-C2C | -3.45 | 103.82      | 106.81   |
| 12  | C     | 502  | HEM  | C2D-C1D-ND  | 3.42  | 113.86      | 109.90   |
| 12  | C     | 502  | HEM  | C2B-C1B-NB  | 3.42  | 113.78      | 109.84   |
| 18  | D     | 2091 | BOG  | C1'-O1-C1   | 3.40  | 118.43      | 113.26   |
| 18  | Q     | 3009 | BOG  | C1'-O1-C1   | 3.28  | 119.29      | 113.68   |
| 15  | P     | 3004 | CDL  | CB4-OB6-CB5 | -3.26 | 109.98      | 117.80   |
| 12  | C     | 501  | HEM  | C2D-C1D-ND  | 3.24  | 113.65      | 109.90   |
| 12  | P     | 501  | HEM  | CAD-C3D-C2D | -3.22 | 121.83      | 127.87   |
| 12  | C     | 501  | HEM  | CAD-C3D-C4D | 3.22  | 130.31      | 124.70   |
| 14  | C     | 2002 | UQ   | C7-C6-C1    | -3.11 | 114.90      | 118.52   |
| 12  | C     | 502  | HEM  | C4C-C3C-C2C | -3.11 | 104.12      | 106.81   |
| 17  | D     | 501  | HEC  | CAD-C3D-C4D | 3.10  | 130.99      | 124.94   |
| 12  | P     | 501  | HEM  | C3B-C4B-NB  | 3.08  | 111.68      | 109.47   |
| 17  | Q     | 501  | HEC  | CMB-C2B-C1B | 3.04  | 130.06      | 125.42   |
| 13  | C     | 2001 | JZV  | OAN-CAK-CAJ | -3.04 | 119.51      | 123.53   |
| 15  | C     | 2004 | CDL  | CA4-OA6-CA5 | -3.03 | 110.55      | 117.80   |
| 15  | C     | 2004 | CDL  | CB4-OB6-CB5 | -3.03 | 110.56      | 117.80   |
| 12  | C     | 502  | HEM  | C3B-C4B-NB  | 3.02  | 111.64      | 109.47   |
| 17  | D     | 501  | HEC  | CMA-C3A-C4A | 2.99  | 129.99      | 124.73   |
| 12  | C     | 501  | HEM  | CAD-C3D-C2D | -2.99 | 122.27      | 127.87   |
| 14  | P     | 3002 | UQ   | C7-C6-C1    | -2.94 | 115.10      | 118.52   |
| 17  | D     | 501  | HEC  | CMC-C2C-C1C | 2.93  | 129.87      | 125.42   |
| 12  | C     | 502  | HEM  | CAD-C3D-C2D | -2.91 | 122.42      | 127.87   |
| 12  | P     | 502  | HEM  | C3B-C4B-NB  | 2.90  | 111.55      | 109.47   |
| 12  | C     | 501  | HEM  | C3B-C2B-C1B | -2.90 | 104.23      | 106.41   |
| 13  | P     | 3001 | JZV  | CAP-CAH-CAI | 2.86  | 126.23      | 122.06   |
| 15  | P     | 3004 | CDL  | CA4-OA6-CA5 | -2.85 | 110.99      | 117.80   |
| 11  | E     | 2005 | PEE  | C22-C21-C20 | 2.83  | 127.44      | 113.86   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | P     | 502  | HEM  | C2B-C1B-NB  | 2.81  | 113.07      | 109.84   |
| 11  | R     | 3005 | PEE  | C22-C21-C20 | 2.80  | 127.34      | 113.86   |
| 12  | C     | 502  | HEM  | C4D-ND-C1D  | -2.80 | 101.89      | 105.21   |
| 11  | C     | 2007 | PEE  | C22-C21-C20 | 2.79  | 127.27      | 113.86   |
| 12  | P     | 501  | HEM  | C2D-C1D-ND  | 2.76  | 113.09      | 109.90   |
| 11  | P     | 3007 | PEE  | C22-C21-C20 | 2.73  | 126.98      | 113.86   |
| 11  | C     | 2007 | PEE  | C21-C22-C23 | 2.68  | 127.92      | 114.37   |
| 17  | Q     | 501  | HEC  | CBA-CAA-C2A | 2.66  | 119.88      | 112.53   |
| 12  | C     | 502  | HEM  | C3D-C4D-ND  | 2.64  | 113.07      | 110.17   |
| 13  | P     | 3001 | JZV  | CAM-OAL-CAK | -2.62 | 110.99      | 115.85   |
| 13  | P     | 3001 | JZV  | CAP-CAH-CAG | -2.60 | 113.89      | 119.51   |
| 12  | P     | 502  | HEM  | C2D-C1D-ND  | 2.58  | 112.89      | 109.90   |
| 11  | P     | 3007 | PEE  | C21-C22-C23 | 2.56  | 127.32      | 114.37   |
| 13  | P     | 3001 | JZV  | OAN-CAK-CAJ | -2.56 | 120.15      | 123.53   |
| 12  | C     | 501  | HEM  | CBD-CAD-C3D | 2.55  | 119.58      | 112.53   |
| 12  | C     | 502  | HEM  | C2A-C1A-NA  | 2.54  | 112.97      | 110.15   |
| 12  | C     | 501  | HEM  | C3C-C2C-C1C | -2.54 | 104.64      | 107.05   |
| 18  | D     | 2091 | BOG  | O1-C1-C2    | 2.51  | 111.04      | 108.14   |
| 18  | Q     | 3091 | BOG  | O1-C1-C2    | 2.50  | 111.02      | 108.14   |
| 18  | D     | 2009 | BOG  | C1'-O1-C1   | 2.49  | 117.94      | 113.68   |
| 11  | E     | 2005 | PEE  | C21-C22-C23 | 2.48  | 126.90      | 114.37   |
| 15  | D     | 2003 | CDL  | CB4-OB6-CB5 | -2.47 | 111.87      | 117.80   |
| 12  | P     | 502  | HEM  | CAD-C3D-C2D | -2.47 | 123.25      | 127.87   |
| 12  | C     | 502  | HEM  | CAA-C2A-C1A | 2.46  | 129.75      | 124.94   |
| 17  | Q     | 501  | HEC  | CAD-C3D-C4D | 2.46  | 129.74      | 124.94   |
| 15  | D     | 2003 | CDL  | CA6-CA4-CA3 | -2.45 | 106.06      | 111.78   |
| 15  | Q     | 3003 | CDL  | CB4-OB6-CB5 | -2.44 | 111.95      | 117.80   |
| 15  | P     | 3004 | CDL  | CA6-CA4-CA3 | -2.41 | 106.16      | 111.78   |
| 11  | R     | 3005 | PEE  | C21-C22-C23 | 2.41  | 126.55      | 114.37   |
| 12  | C     | 501  | HEM  | CMD-C2D-C1D | 2.40  | 128.79      | 125.03   |
| 13  | C     | 2001 | JZV  | CAM-OAL-CAK | -2.38 | 111.44      | 115.85   |
| 13  | C     | 2001 | JZV  | CAP-CAH-CAI | 2.37  | 125.53      | 122.06   |
| 12  | P     | 502  | HEM  | CAA-C2A-C1A | 2.37  | 129.57      | 124.94   |
| 15  | Q     | 3003 | CDL  | CA6-CA4-CA3 | -2.36 | 106.28      | 111.78   |
| 17  | D     | 501  | HEC  | CMD-C2D-C1D | 2.36  | 129.01      | 125.42   |
| 11  | E     | 2005 | PEE  | O3-C3-C2    | 2.35  | 115.16      | 108.40   |
| 11  | R     | 3005 | PEE  | O3-C3-C2    | 2.33  | 115.11      | 108.40   |
| 12  | C     | 502  | HEM  | C4D-C3D-C2D | -2.32 | 103.51      | 106.89   |
| 18  | D     | 2009 | BOG  | O1-C1-C2    | 2.31  | 111.78      | 108.27   |
| 12  | P     | 501  | HEM  | CBD-CAD-C3D | 2.30  | 118.89      | 112.53   |
| 12  | P     | 501  | HEM  | CMD-C2D-C1D | 2.27  | 128.59      | 125.03   |
| 12  | P     | 501  | HEM  | C3C-C2C-C1C | -2.25 | 104.91      | 107.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | C     | 2004 | CDL  | CA6-CA4-CA3 | -2.25 | 106.53      | 111.78   |
| 13  | C     | 2001 | JZV  | CAP-CAH-CAG | -2.21 | 114.73      | 119.51   |
| 14  | C     | 2002 | UQ   | C10-C9-C8   | -2.17 | 118.05      | 123.63   |
| 12  | C     | 501  | HEM  | C2B-C1B-NB  | 2.17  | 112.33      | 109.84   |
| 14  | P     | 3002 | UQ   | C10-C9-C8   | -2.14 | 118.14      | 123.63   |
| 17  | Q     | 501  | HEC  | CMA-C3A-C4A | 2.13  | 128.47      | 124.73   |
| 12  | C     | 501  | HEM  | CMB-C2B-C1B | 2.08  | 128.28      | 125.03   |
| 12  | P     | 501  | HEM  | CMB-C2B-C1B | 2.07  | 128.27      | 125.03   |
| 15  | P     | 3004 | CDL  | OB6-CB4-CB3 | 2.06  | 115.73      | 108.34   |
| 12  | C     | 502  | HEM  | CHA-C4D-ND  | -2.05 | 121.83      | 124.37   |
| 12  | C     | 501  | HEM  | C4D-ND-C1D  | -2.03 | 102.81      | 105.21   |
| 15  | C     | 2004 | CDL  | OB6-CB4-CB3 | 2.01  | 115.56      | 108.34   |

There are no chirality outliers.

All (280) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | C     | 2007 | PEE  | C4-O4P-P-O3P    |
| 11  | C     | 2007 | PEE  | C4-O4P-P-O2P    |
| 11  | C     | 2007 | PEE  | C4-O4P-P-O1P    |
| 11  | E     | 2005 | PEE  | C11-C10-O2-C2   |
| 11  | E     | 2005 | PEE  | C4-O4P-P-O3P    |
| 11  | E     | 2005 | PEE  | C4-O4P-P-O2P    |
| 11  | E     | 2005 | PEE  | C4-O4P-P-O1P    |
| 11  | E     | 2005 | PEE  | O4P-C4-C5-N     |
| 11  | P     | 3007 | PEE  | C4-O4P-P-O3P    |
| 11  | P     | 3007 | PEE  | C4-O4P-P-O2P    |
| 11  | P     | 3007 | PEE  | C4-O4P-P-O1P    |
| 11  | R     | 3005 | PEE  | C11-C10-O2-C2   |
| 11  | R     | 3005 | PEE  | C4-O4P-P-O3P    |
| 11  | R     | 3005 | PEE  | C4-O4P-P-O2P    |
| 11  | R     | 3005 | PEE  | C4-O4P-P-O1P    |
| 12  | C     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 14  | C     | 2002 | UQ   | C1-C6-C7-C8     |
| 14  | C     | 2002 | UQ   | C5-C6-C7-C8     |
| 14  | C     | 2002 | UQ   | C12-C11-C9-C8   |
| 14  | P     | 3002 | UQ   | C1-C6-C7-C8     |
| 14  | P     | 3002 | UQ   | C5-C6-C7-C8     |
| 14  | P     | 3002 | UQ   | C12-C11-C9-C8   |
| 15  | C     | 2004 | CDL  | CB2-C1-CA2-OA2  |
| 15  | C     | 2004 | CDL  | CA3-OA5-PA1-OA2 |
| 15  | C     | 2004 | CDL  | CA3-OA5-PA1-OA3 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | C     | 2004 | CDL  | CA3-OA5-PA1-OA4 |
| 15  | C     | 2004 | CDL  | CB3-OB5-PB2-OB2 |
| 15  | C     | 2004 | CDL  | CB3-OB5-PB2-OB3 |
| 15  | C     | 2004 | CDL  | C51-CB5-OB6-CB4 |
| 15  | D     | 2003 | CDL  | CA2-OA2-PA1-OA5 |
| 15  | D     | 2003 | CDL  | CA3-OA5-PA1-OA2 |
| 15  | D     | 2003 | CDL  | CA3-OA5-PA1-OA4 |
| 15  | D     | 2003 | CDL  | OA6-CA4-CA6-OA8 |
| 15  | D     | 2003 | CDL  | CB2-OB2-PB2-OB4 |
| 15  | D     | 2003 | CDL  | CB2-OB2-PB2-OB5 |
| 15  | D     | 2003 | CDL  | CB3-OB5-PB2-OB2 |
| 15  | D     | 2003 | CDL  | CB3-OB5-PB2-OB4 |
| 15  | P     | 3004 | CDL  | CB2-C1-CA2-OA2  |
| 15  | P     | 3004 | CDL  | CA2-C1-CB2-OB2  |
| 15  | P     | 3004 | CDL  | CA3-OA5-PA1-OA2 |
| 15  | P     | 3004 | CDL  | CA3-OA5-PA1-OA3 |
| 15  | P     | 3004 | CDL  | CA3-OA5-PA1-OA4 |
| 15  | P     | 3004 | CDL  | CB3-OB5-PB2-OB2 |
| 15  | P     | 3004 | CDL  | CB3-OB5-PB2-OB3 |
| 15  | P     | 3004 | CDL  | C51-CB5-OB6-CB4 |
| 15  | Q     | 3003 | CDL  | CA2-OA2-PA1-OA5 |
| 15  | Q     | 3003 | CDL  | CA3-OA5-PA1-OA2 |
| 15  | Q     | 3003 | CDL  | CA3-OA5-PA1-OA4 |
| 15  | Q     | 3003 | CDL  | OA6-CA4-CA6-OA8 |
| 15  | Q     | 3003 | CDL  | CB2-OB2-PB2-OB4 |
| 15  | Q     | 3003 | CDL  | CB2-OB2-PB2-OB5 |
| 15  | Q     | 3003 | CDL  | CB3-OB5-PB2-OB2 |
| 15  | Q     | 3003 | CDL  | CB3-OB5-PB2-OB4 |
| 16  | C     | 2011 | GOL  | O1-C1-C2-C3     |
| 16  | C     | 2011 | GOL  | C1-C2-C3-O3     |
| 16  | P     | 3011 | GOL  | C1-C2-C3-O3     |
| 17  | D     | 501  | HEC  | C2B-C3B-CAB-CBB |
| 17  | D     | 501  | HEC  | C4B-C3B-CAB-CBB |
| 17  | D     | 501  | HEC  | C2C-C3C-CAC-CBC |
| 17  | Q     | 501  | HEC  | C3A-C2A-CAA-CBA |
| 17  | Q     | 501  | HEC  | C2B-C3B-CAB-CBB |
| 17  | Q     | 501  | HEC  | C4B-C3B-CAB-CBB |
| 17  | Q     | 501  | HEC  | C2C-C3C-CAC-CBC |
| 17  | Q     | 501  | HEC  | C4C-C3C-CAC-CBC |
| 18  | Q     | 3009 | BOG  | C2-C1-O1-C1'    |
| 18  | Q     | 3091 | BOG  | C2-C1-O1-C1'    |
| 18  | Q     | 3091 | BOG  | O5-C1-O1-C1'    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | R     | 3005 | PEE  | O5-C30-O3-C3    |
| 11  | E     | 2005 | PEE  | O5-C30-O3-C3    |
| 15  | C     | 2004 | CDL  | OB9-CB7-OB8-CB6 |
| 15  | P     | 3004 | CDL  | OB9-CB7-OB8-CB6 |
| 11  | A     | 2008 | PEE  | O5-C30-O3-C3    |
| 11  | E     | 2005 | PEE  | O4-C10-O2-C2    |
| 11  | R     | 3005 | PEE  | O4-C10-O2-C2    |
| 15  | C     | 2004 | CDL  | OB7-CB5-OB6-CB4 |
| 15  | P     | 3004 | CDL  | OB7-CB5-OB6-CB4 |
| 11  | E     | 2005 | PEE  | C31-C30-O3-C3   |
| 11  | R     | 3005 | PEE  | C31-C30-O3-C3   |
| 15  | D     | 2003 | CDL  | C31-CA7-OA8-CA6 |
| 15  | Q     | 3003 | CDL  | C31-CA7-OA8-CA6 |
| 15  | C     | 2004 | CDL  | OA9-CA7-OA8-CA6 |
| 15  | P     | 3004 | CDL  | OA9-CA7-OA8-CA6 |
| 11  | A     | 2008 | PEE  | C31-C30-O3-C3   |
| 15  | C     | 2004 | CDL  | C71-CB7-OB8-CB6 |
| 15  | P     | 3004 | CDL  | C71-CB7-OB8-CB6 |
| 15  | C     | 2004 | CDL  | C31-CA7-OA8-CA6 |
| 15  | P     | 3004 | CDL  | C31-CA7-OA8-CA6 |
| 11  | C     | 2007 | PEE  | C37-C38-C39-C40 |
| 11  | P     | 3007 | PEE  | C37-C38-C39-C40 |
| 15  | C     | 2004 | CDL  | O1-C1-CA2-OA2   |
| 15  | P     | 3004 | CDL  | O1-C1-CA2-OA2   |
| 18  | Q     | 3091 | BOG  | O5-C5-C6-O6     |
| 15  | Q     | 3003 | CDL  | C71-CB7-OB8-CB6 |
| 15  | D     | 2003 | CDL  | OA9-CA7-OA8-CA6 |
| 15  | Q     | 3003 | CDL  | OA9-CA7-OA8-CA6 |
| 17  | Q     | 501  | HEC  | C1A-C2A-CAA-CBA |
| 15  | D     | 2003 | CDL  | C71-CB7-OB8-CB6 |
| 18  | D     | 2091 | BOG  | C2-C1-O1-C1'    |
| 18  | D     | 2009 | BOG  | C2-C1-O1-C1'    |
| 15  | D     | 2003 | CDL  | O1-C1-CA2-OA2   |
| 15  | Q     | 3003 | CDL  | O1-C1-CA2-OA2   |
| 11  | C     | 2007 | PEE  | C10-C11-C12-C13 |
| 11  | P     | 3007 | PEE  | C10-C11-C12-C13 |
| 15  | P     | 3004 | CDL  | C11-CA5-OA6-CA4 |
| 18  | D     | 2091 | BOG  | O5-C1-O1-C1'    |
| 15  | D     | 2003 | CDL  | CB7-C71-C72-C73 |
| 18  | Q     | 3091 | BOG  | C4-C5-C6-O6     |
| 15  | Q     | 3003 | CDL  | CB7-C71-C72-C73 |
| 15  | D     | 2003 | CDL  | OB9-CB7-OB8-CB6 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | C     | 2004 | CDL  | C11-CA5-OA6-CA4 |
| 18  | D     | 2009 | BOG  | O5-C1-O1-C1'    |
| 18  | Q     | 3009 | BOG  | O5-C1-O1-C1'    |
| 15  | Q     | 3003 | CDL  | OB9-CB7-OB8-CB6 |
| 11  | C     | 2007 | PEE  | C17-C18-C19-C20 |
| 11  | P     | 3007 | PEE  | C17-C18-C19-C20 |
| 18  | Q     | 3009 | BOG  | O1-C1'-C2'-C3'  |
| 17  | D     | 501  | HEC  | C3A-C2A-CAA-CBA |
| 18  | D     | 2009 | BOG  | O1-C1'-C2'-C3'  |
| 15  | C     | 2004 | CDL  | OA7-CA5-OA6-CA4 |
| 15  | P     | 3004 | CDL  | OA7-CA5-OA6-CA4 |
| 12  | C     | 502  | HEM  | C4D-C3D-CAD-CBD |
| 16  | C     | 2011 | GOL  | O1-C1-C2-O2     |
| 11  | C     | 2007 | PEE  | C35-C36-C37-C38 |
| 11  | R     | 3005 | PEE  | C34-C35-C36-C37 |
| 11  | E     | 2005 | PEE  | C34-C35-C36-C37 |
| 11  | P     | 3007 | PEE  | C40-C41-C42-C43 |
| 15  | C     | 2004 | CDL  | CA2-C1-CB2-OB2  |
| 11  | C     | 2007 | PEE  | C40-C41-C42-C43 |
| 18  | D     | 2009 | BOG  | C1'-C2'-C3'-C4' |
| 18  | Q     | 3009 | BOG  | C1'-C2'-C3'-C4' |
| 11  | P     | 3007 | PEE  | C21-C22-C23-C24 |
| 15  | D     | 2003 | CDL  | C51-CB5-OB6-CB4 |
| 15  | Q     | 3003 | CDL  | C51-CB5-OB6-CB4 |
| 17  | D     | 501  | HEC  | C1A-C2A-CAA-CBA |
| 11  | E     | 2005 | PEE  | C39-C40-C41-C42 |
| 11  | P     | 3007 | PEE  | C20-C21-C22-C23 |
| 15  | D     | 2003 | CDL  | OB7-CB5-OB6-CB4 |
| 11  | P     | 3007 | PEE  | C33-C34-C35-C36 |
| 11  | C     | 2007 | PEE  | C15-C16-C17-C18 |
| 11  | P     | 3007 | PEE  | C15-C16-C17-C18 |
| 11  | P     | 3007 | PEE  | C35-C36-C37-C38 |
| 11  | C     | 2007 | PEE  | C33-C34-C35-C36 |
| 15  | Q     | 3003 | CDL  | OB7-CB5-OB6-CB4 |
| 11  | C     | 2007 | PEE  | C20-C21-C22-C23 |
| 11  | E     | 2005 | PEE  | C20-C21-C22-C23 |
| 16  | C     | 2011 | GOL  | O2-C2-C3-O3     |
| 16  | P     | 3011 | GOL  | O2-C2-C3-O3     |
| 11  | R     | 3005 | PEE  | C39-C40-C41-C42 |
| 11  | E     | 2005 | PEE  | O3P-C1-C2-C3    |
| 11  | R     | 3005 | PEE  | O3P-C1-C2-C3    |
| 11  | R     | 3005 | PEE  | C30-C31-C32-C33 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 12  | P     | 502  | HEM  | C4D-C3D-CAD-CBD |
| 15  | D     | 2003 | CDL  | CA3-CA4-CA6-OA8 |
| 15  | Q     | 3003 | CDL  | CA3-CA4-CA6-OA8 |
| 15  | C     | 2004 | CDL  | O1-C1-CB2-OB2   |
| 11  | R     | 3005 | PEE  | C20-C21-C22-C23 |
| 11  | P     | 3007 | PEE  | C31-C32-C33-C34 |
| 13  | P     | 3001 | JZV  | CAS-NAR-OAQ-CAP |
| 15  | C     | 2004 | CDL  | OB5-CB3-CB4-OB6 |
| 15  | P     | 3004 | CDL  | OB5-CB3-CB4-OB6 |
| 11  | P     | 3007 | PEE  | C11-C12-C13-C14 |
| 11  | P     | 3007 | PEE  | C43-C44-C45-C46 |
| 11  | E     | 2005 | PEE  | C30-C31-C32-C33 |
| 11  | E     | 2005 | PEE  | C41-C42-C43-C44 |
| 15  | D     | 2003 | CDL  | C71-C72-C73-C74 |
| 15  | P     | 3004 | CDL  | O1-C1-CB2-OB2   |
| 11  | C     | 2007 | PEE  | C31-C32-C33-C34 |
| 11  | C     | 2007 | PEE  | C43-C44-C45-C46 |
| 15  | Q     | 3003 | CDL  | C71-C72-C73-C74 |
| 11  | C     | 2007 | PEE  | C34-C35-C36-C37 |
| 11  | C     | 2007 | PEE  | C21-C22-C23-C24 |
| 11  | C     | 2007 | PEE  | C11-C12-C13-C14 |
| 11  | E     | 2005 | PEE  | C23-C24-C25-C26 |
| 11  | R     | 3005 | PEE  | C23-C24-C25-C26 |
| 11  | A     | 2008 | PEE  | O3P-C1-C2-C3    |
| 15  | D     | 2003 | CDL  | OB5-CB3-CB4-CB6 |
| 15  | Q     | 3003 | CDL  | OB5-CB3-CB4-CB6 |
| 15  | C     | 2004 | CDL  | CB5-C51-C52-C53 |
| 14  | C     | 2002 | UQ   | C12-C11-C9-C10  |
| 14  | P     | 3002 | UQ   | C12-C11-C9-C10  |
| 11  | C     | 2007 | PEE  | C42-C43-C44-C45 |
| 11  | R     | 3005 | PEE  | C41-C42-C43-C44 |
| 11  | A     | 2008 | PEE  | C11-C10-O2-C2   |
| 11  | P     | 3007 | PEE  | C42-C43-C44-C45 |
| 11  | A     | 2008 | PEE  | O2-C2-C3-O3     |
| 13  | C     | 2001 | JZV  | CAS-NAR-OAQ-CAP |
| 11  | P     | 3007 | PEE  | C34-C35-C36-C37 |
| 11  | E     | 2005 | PEE  | C10-C11-C12-C13 |
| 16  | P     | 3011 | GOL  | O1-C1-C2-O2     |
| 11  | E     | 2005 | PEE  | C43-C44-C45-C46 |
| 13  | C     | 2001 | JZV  | CAY-CAS-NAR-OAQ |
| 13  | P     | 3001 | JZV  | CAY-CAS-NAR-OAQ |
| 13  | C     | 2001 | JZV  | CAT-CAS-NAR-OAQ |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | P     | 3001 | JZV  | CAT-CAS-NAR-OAQ |
| 12  | P     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 11  | R     | 3005 | PEE  | C43-C44-C45-C46 |
| 11  | A     | 2008 | PEE  | O4-C10-O2-C2    |
| 11  | R     | 3005 | PEE  | O3P-C1-C2-O2    |
| 15  | D     | 2003 | CDL  | OB5-CB3-CB4-OB6 |
| 15  | Q     | 3003 | CDL  | OB5-CB3-CB4-OB6 |
| 12  | C     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 11  | R     | 3005 | PEE  | C31-C32-C33-C34 |
| 11  | R     | 3005 | PEE  | C10-C11-C12-C13 |
| 17  | D     | 501  | HEC  | C4C-C3C-CAC-CBC |
| 11  | A     | 2008 | PEE  | O3P-C1-C2-O2    |
| 11  | E     | 2005 | PEE  | O3P-C1-C2-O2    |
| 12  | P     | 502  | HEM  | C2D-C3D-CAD-CBD |
| 11  | E     | 2005 | PEE  | C31-C32-C33-C34 |
| 11  | E     | 2005 | PEE  | C35-C36-C37-C38 |
| 11  | E     | 2005 | PEE  | C11-C12-C13-C14 |
| 11  | A     | 2008 | PEE  | C4-O4P-P-O2P    |
| 11  | R     | 3005 | PEE  | O4P-C4-C5-N     |
| 15  | C     | 2004 | CDL  | CB3-OB5-PB2-OB4 |
| 15  | D     | 2003 | CDL  | CA2-OA2-PA1-OA4 |
| 15  | P     | 3004 | CDL  | CB3-OB5-PB2-OB4 |
| 11  | R     | 3005 | PEE  | C11-C12-C13-C14 |
| 11  | R     | 3005 | PEE  | C19-C20-C21-C22 |
| 15  | C     | 2004 | CDL  | OB5-CB3-CB4-CB6 |
| 15  | P     | 3004 | CDL  | OB5-CB3-CB4-CB6 |
| 11  | P     | 3007 | PEE  | C12-C13-C14-C15 |
| 11  | A     | 2008 | PEE  | C10-C11-C12-C13 |
| 11  | E     | 2005 | PEE  | C14-C15-C16-C17 |
| 11  | C     | 2007 | PEE  | C12-C13-C14-C15 |
| 11  | E     | 2005 | PEE  | C19-C20-C21-C22 |
| 11  | R     | 3005 | PEE  | C14-C15-C16-C17 |
| 12  | P     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 12  | C     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 12  | P     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 11  | E     | 2005 | PEE  | C1-C2-O2-C10    |
| 11  | R     | 3005 | PEE  | C1-C2-O2-C10    |
| 12  | C     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 12  | P     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 12  | C     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 11  | A     | 2008 | PEE  | O3-C30-C31-C32  |
| 12  | P     | 502  | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | R     | 3005 | PEE  | C35-C36-C37-C38 |
| 12  | P     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 12  | C     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 12  | P     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 17  | D     | 501  | HEC  | CAD-CBD-CGD-O2D |
| 11  | E     | 2005 | PEE  | C22-C23-C24-C25 |
| 11  | E     | 2005 | PEE  | C37-C38-C39-C40 |
| 11  | R     | 3005 | PEE  | C37-C38-C39-C40 |
| 12  | C     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 11  | P     | 3007 | PEE  | C38-C39-C40-C41 |
| 17  | Q     | 501  | HEC  | CAA-CBA-CGA-O2A |
| 11  | A     | 2008 | PEE  | O5-C30-C31-C32  |
| 12  | C     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 11  | C     | 2007 | PEE  | C38-C39-C40-C41 |
| 11  | E     | 2005 | PEE  | C40-C41-C42-C43 |
| 15  | P     | 3004 | CDL  | CB5-C51-C52-C53 |
| 11  | P     | 3007 | PEE  | C19-C20-C21-C22 |
| 17  | D     | 501  | HEC  | CAD-CBD-CGD-O1D |
| 17  | Q     | 501  | HEC  | CAD-CBD-CGD-O2D |
| 11  | A     | 2008 | PEE  | C1-C2-C3-O3     |
| 12  | P     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 11  | R     | 3005 | PEE  | C22-C23-C24-C25 |
| 11  | P     | 3007 | PEE  | O2-C10-C11-C12  |
| 17  | Q     | 501  | HEC  | CAA-CBA-CGA-O1A |
| 17  | Q     | 501  | HEC  | CAD-CBD-CGD-O1D |
| 11  | C     | 2007 | PEE  | O2-C10-C11-C12  |
| 11  | P     | 3007 | PEE  | C22-C23-C24-C25 |
| 12  | C     | 501  | HEM  | CAD-CBD-CGD-O2D |
| 17  | D     | 501  | HEC  | CAA-CBA-CGA-O2A |
| 11  | P     | 3007 | PEE  | O5-C30-O3-C3    |
| 11  | C     | 2007 | PEE  | O2-C2-C3-O3     |
| 11  | P     | 3007 | PEE  | O2-C2-C3-O3     |
| 17  | D     | 501  | HEC  | CAA-CBA-CGA-O1A |
| 18  | D     | 2009 | BOG  | C4'-C5'-C6'-C7' |
| 11  | C     | 2007 | PEE  | O4-C10-C11-C12  |
| 15  | Q     | 3003 | CDL  | C72-C71-CB7-OB8 |
| 12  | C     | 501  | HEM  | CAD-CBD-CGD-O1D |
| 11  | P     | 3007 | PEE  | O4-C10-C11-C12  |
| 11  | P     | 3007 | PEE  | C31-C30-O3-C3   |
| 11  | R     | 3005 | PEE  | C40-C41-C42-C43 |
| 12  | C     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 12  | P     | 501  | HEM  | C2C-C3C-CAC-CBC |

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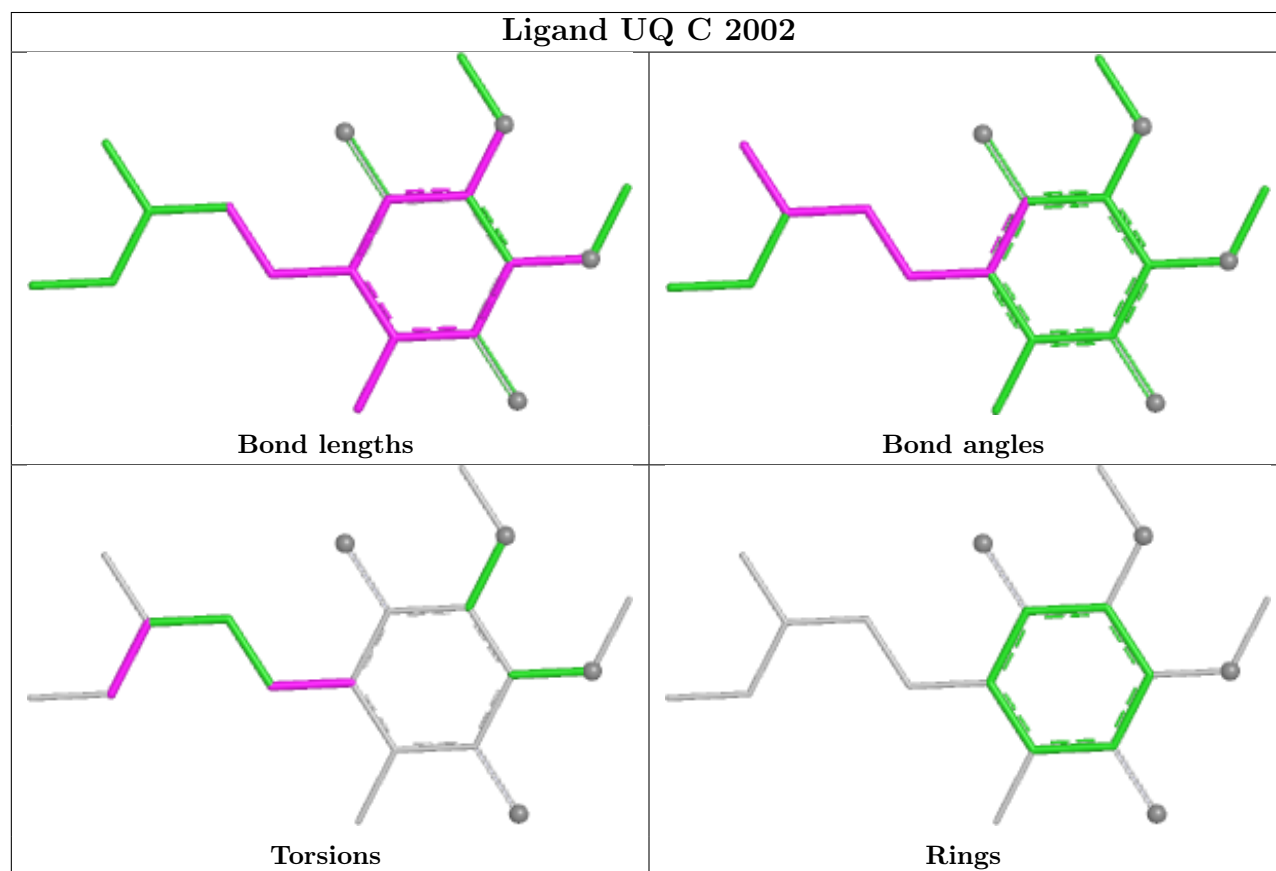
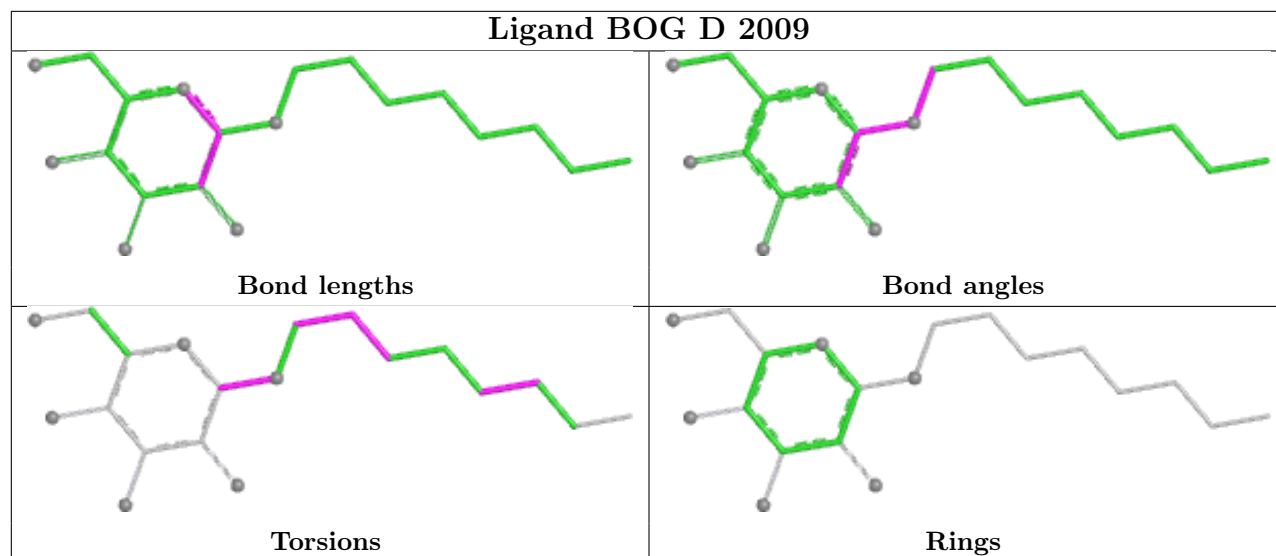
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Q     | 3009 | BOG  | C4'-C5'-C6'-C7' |
| 11  | C     | 2007 | PEE  | C32-C33-C34-C35 |
| 15  | D     | 2003 | CDL  | C72-C71-CB7-OB8 |

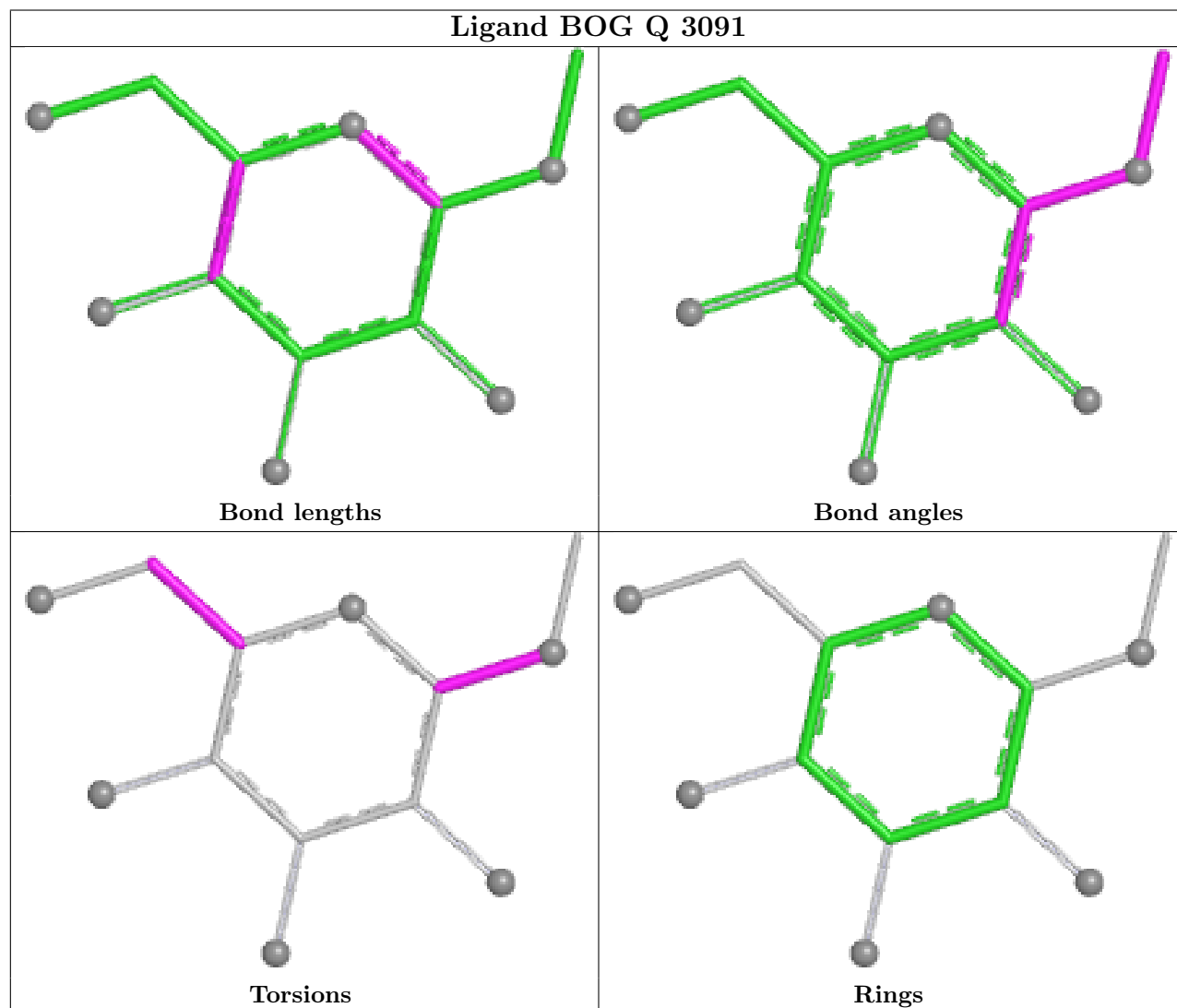
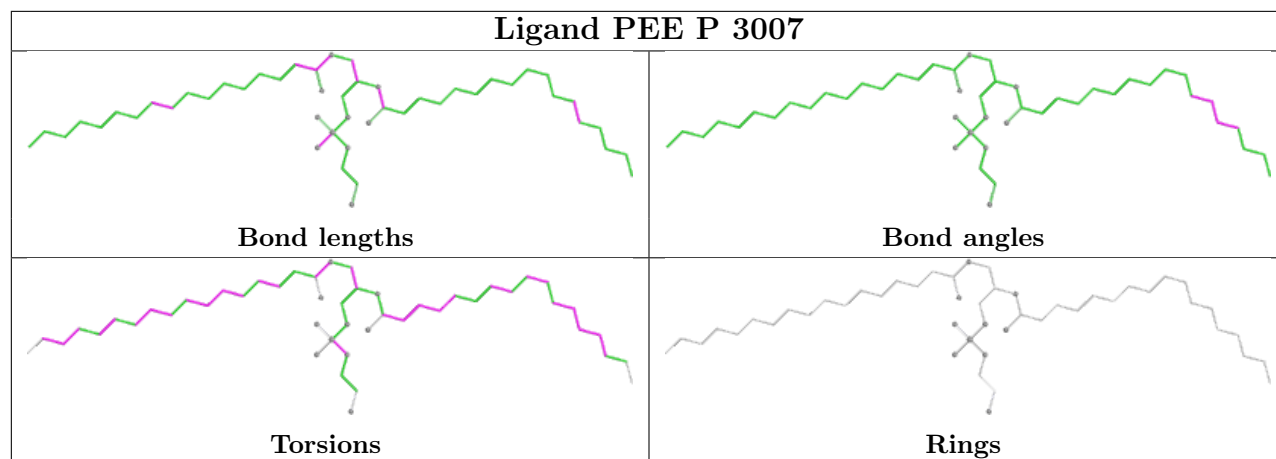
There are no ring outliers.

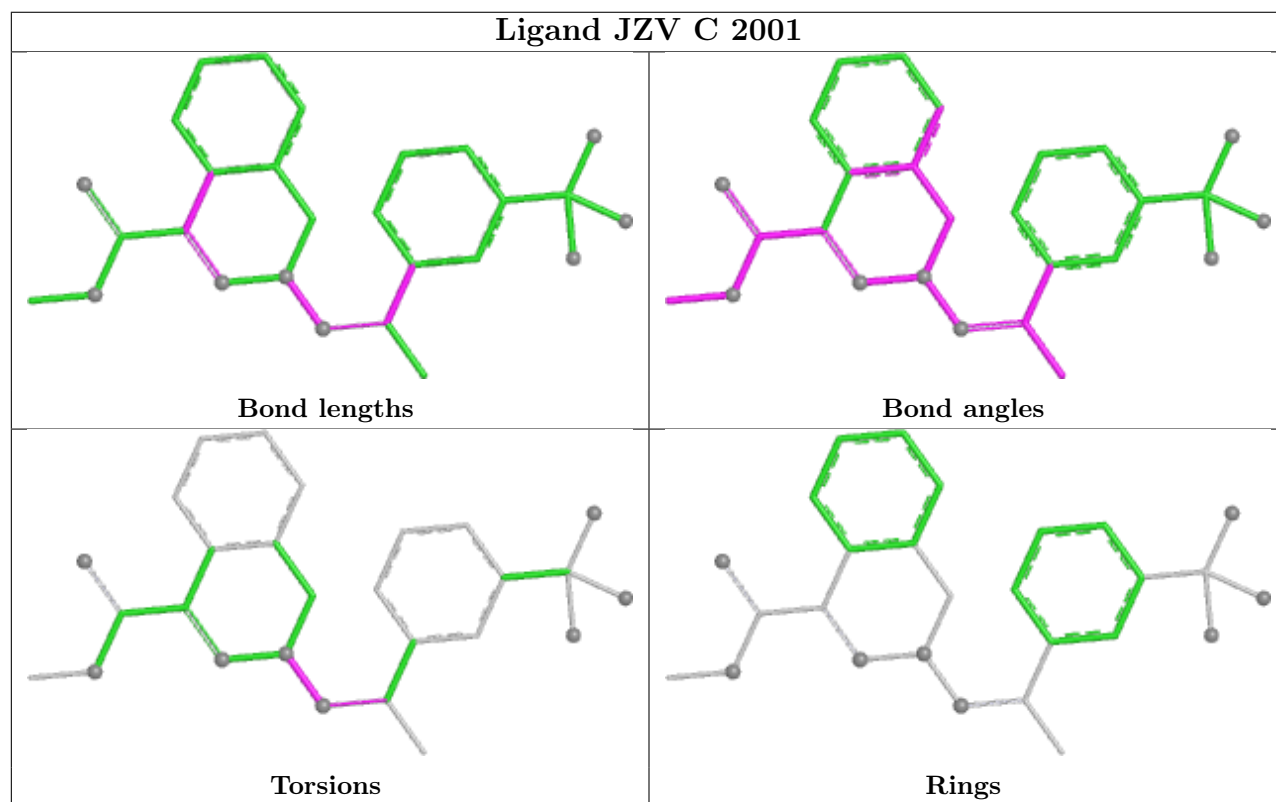
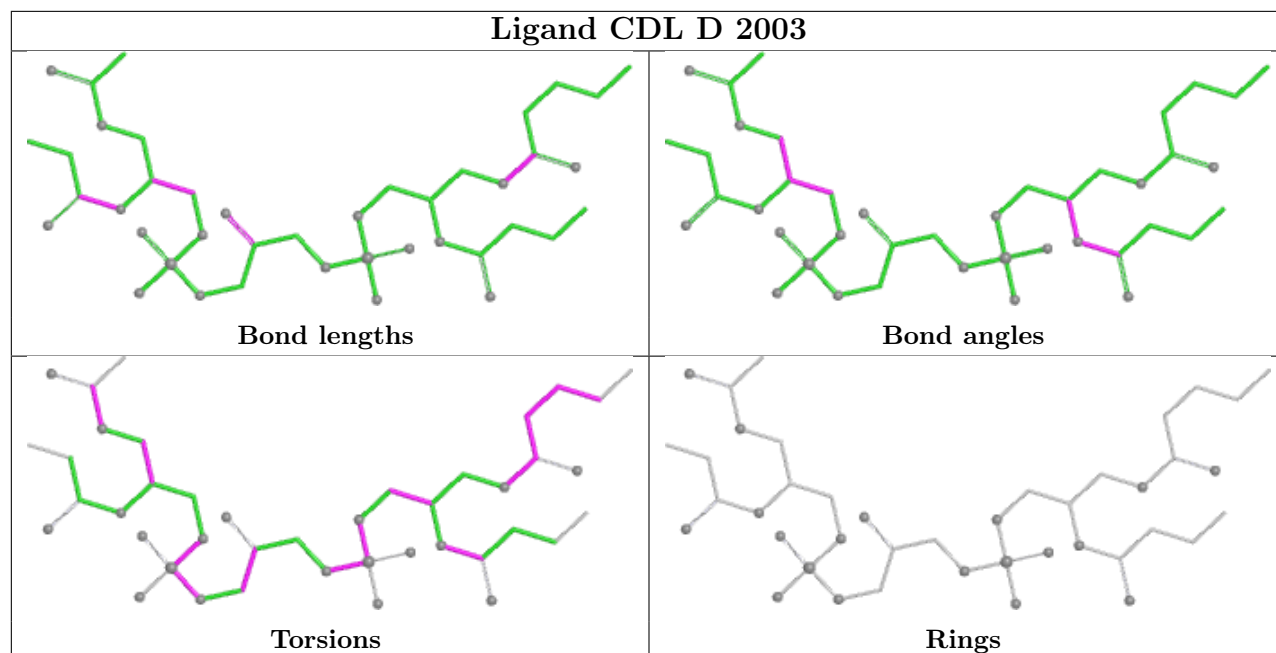
20 monomers are involved in 61 short contacts:

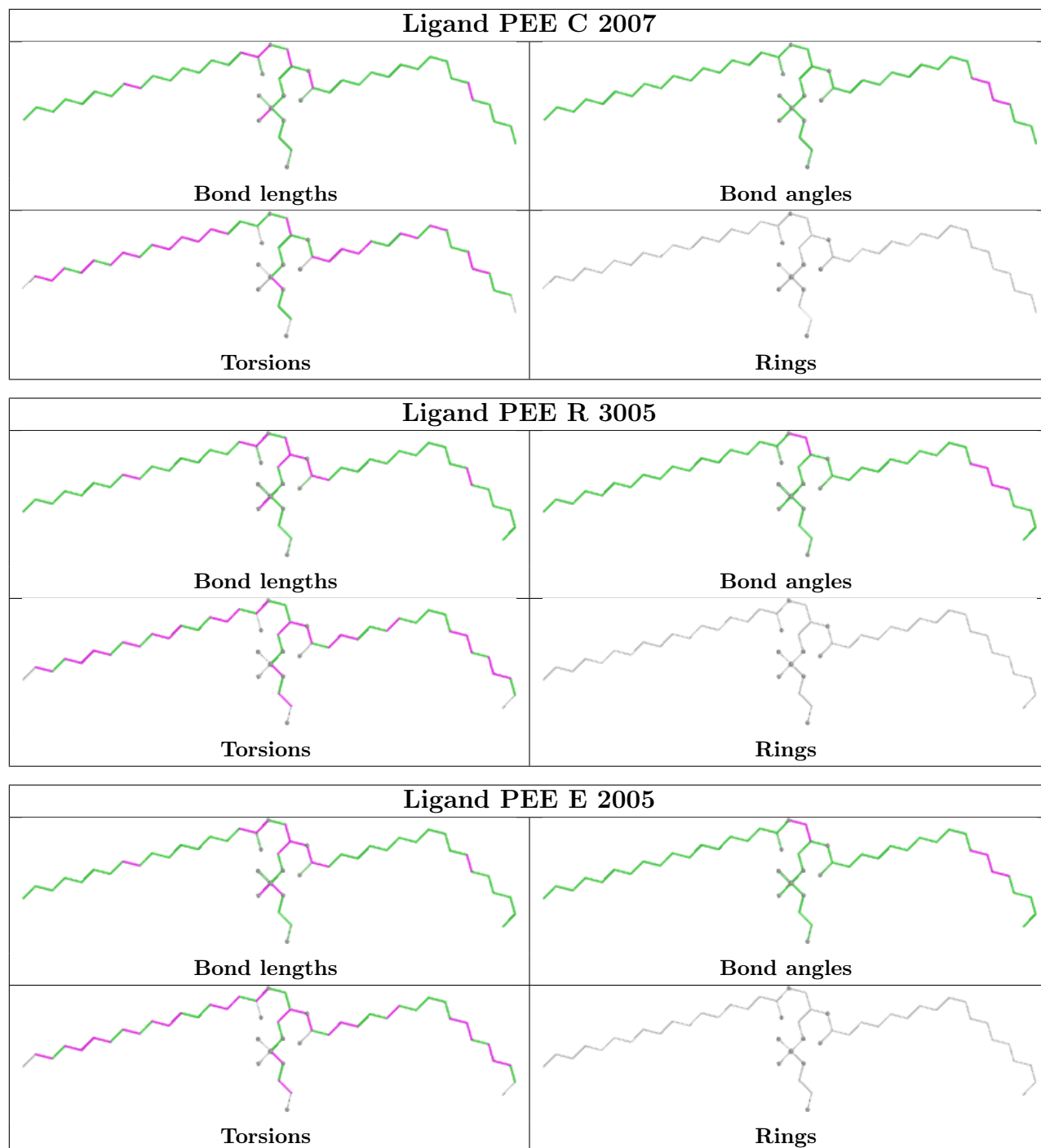
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | C     | 2002 | UQ   | 2       | 0            |
| 11  | P     | 3007 | PEE  | 3       | 0            |
| 18  | Q     | 3091 | BOG  | 1       | 0            |
| 15  | D     | 2003 | CDL  | 4       | 0            |
| 13  | C     | 2001 | JZV  | 4       | 0            |
| 11  | C     | 2007 | PEE  | 4       | 0            |
| 11  | R     | 3005 | PEE  | 2       | 0            |
| 11  | E     | 2005 | PEE  | 1       | 0            |
| 19  | E     | 501  | FES  | 2       | 0            |
| 15  | Q     | 3003 | CDL  | 3       | 0            |
| 12  | P     | 502  | HEM  | 4       | 0            |
| 13  | P     | 3001 | JZV  | 4       | 0            |
| 12  | P     | 501  | HEM  | 4       | 0            |
| 15  | P     | 3004 | CDL  | 4       | 0            |
| 19  | R     | 501  | FES  | 2       | 0            |
| 12  | C     | 502  | HEM  | 5       | 0            |
| 14  | P     | 3002 | UQ   | 3       | 0            |
| 12  | C     | 501  | HEM  | 5       | 0            |
| 15  | C     | 2004 | CDL  | 4       | 0            |
| 18  | P     | 2010 | BOG  | 2       | 0            |

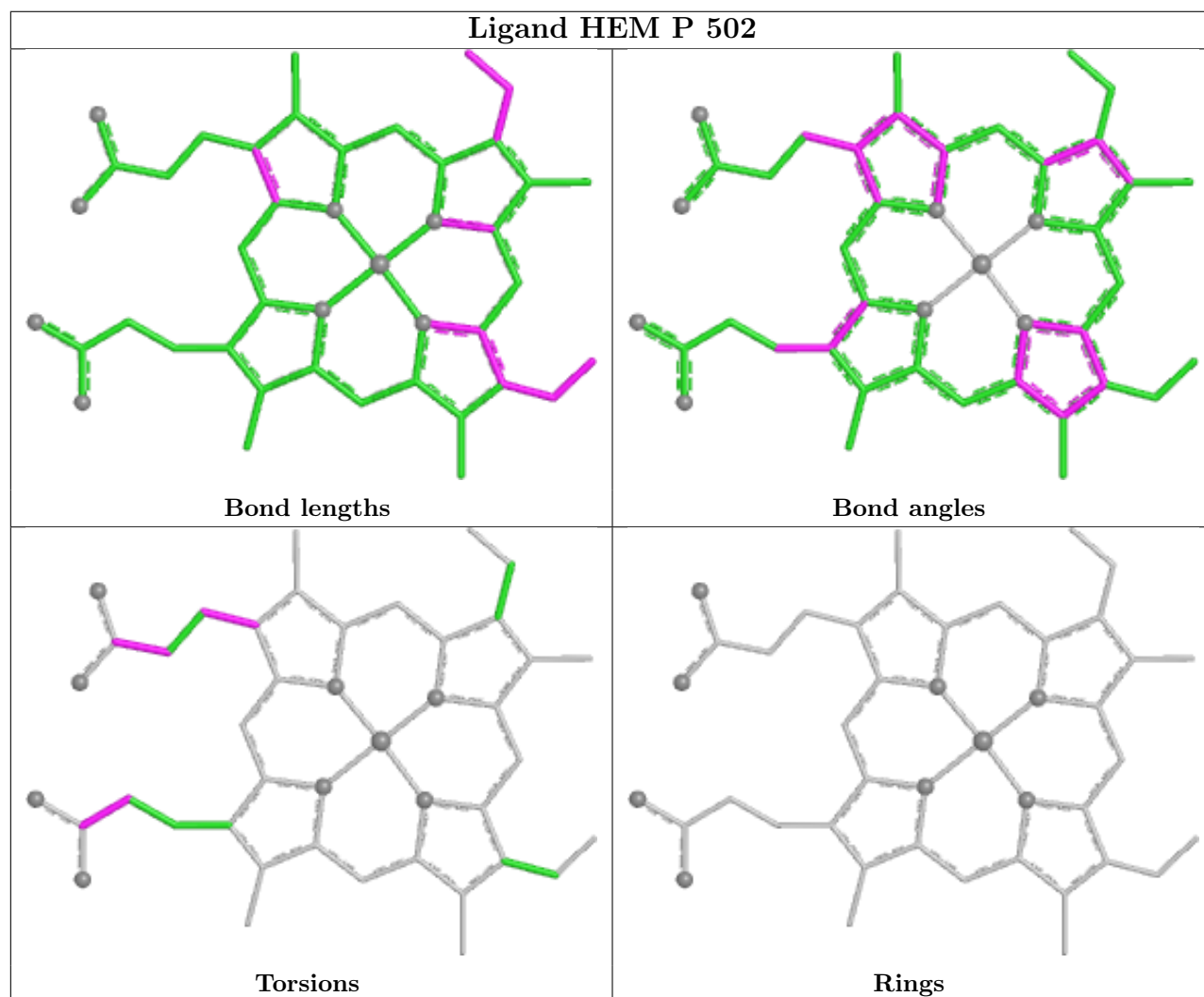
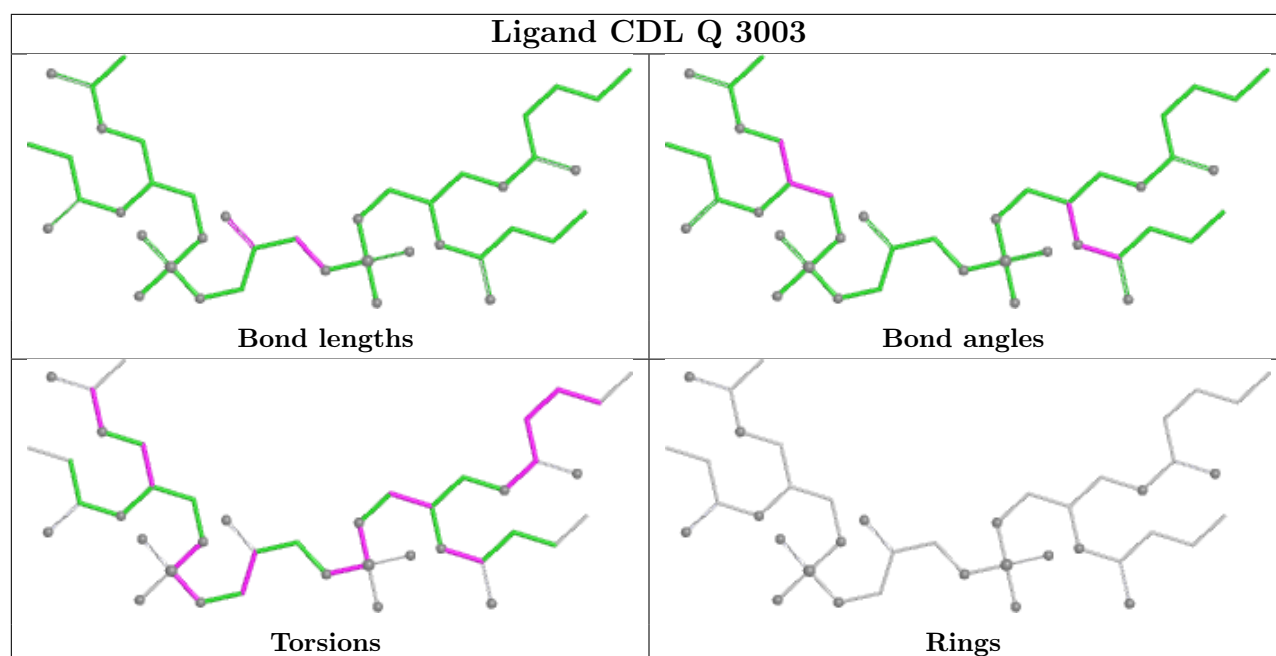
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

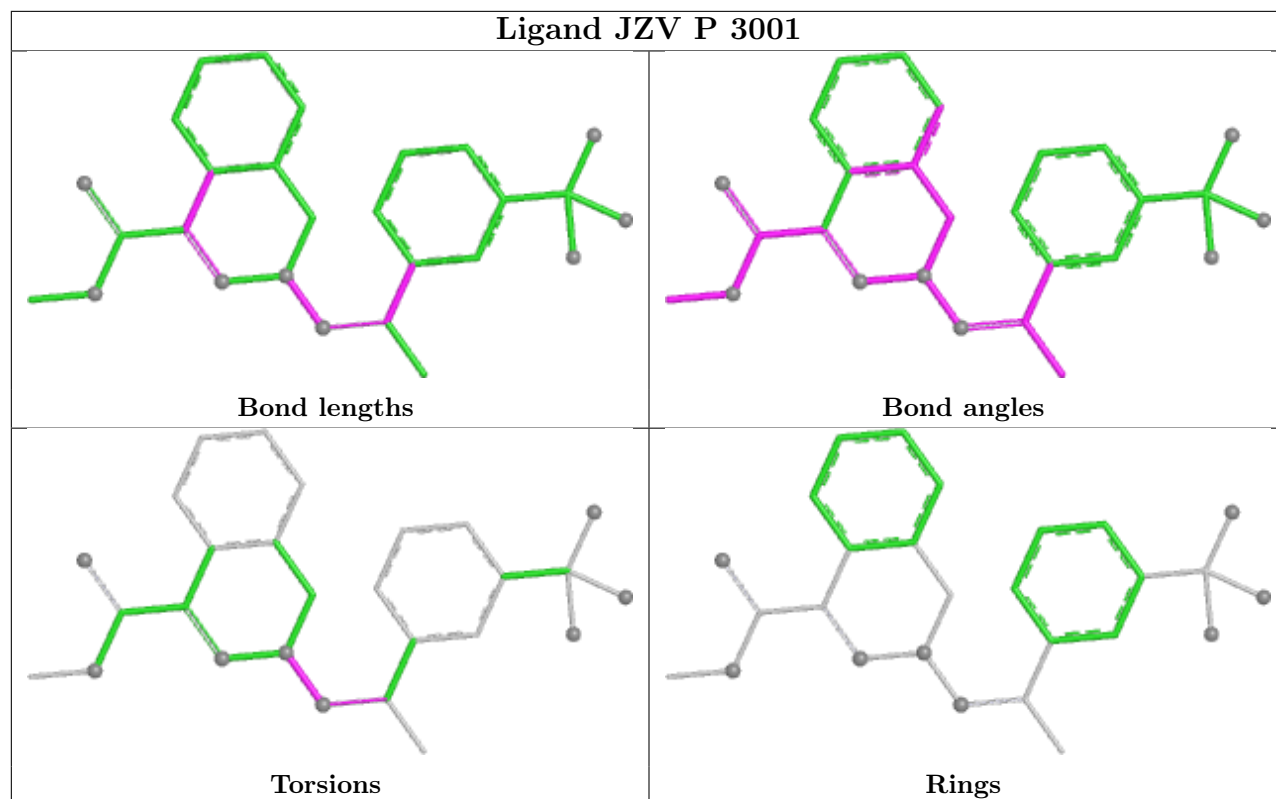


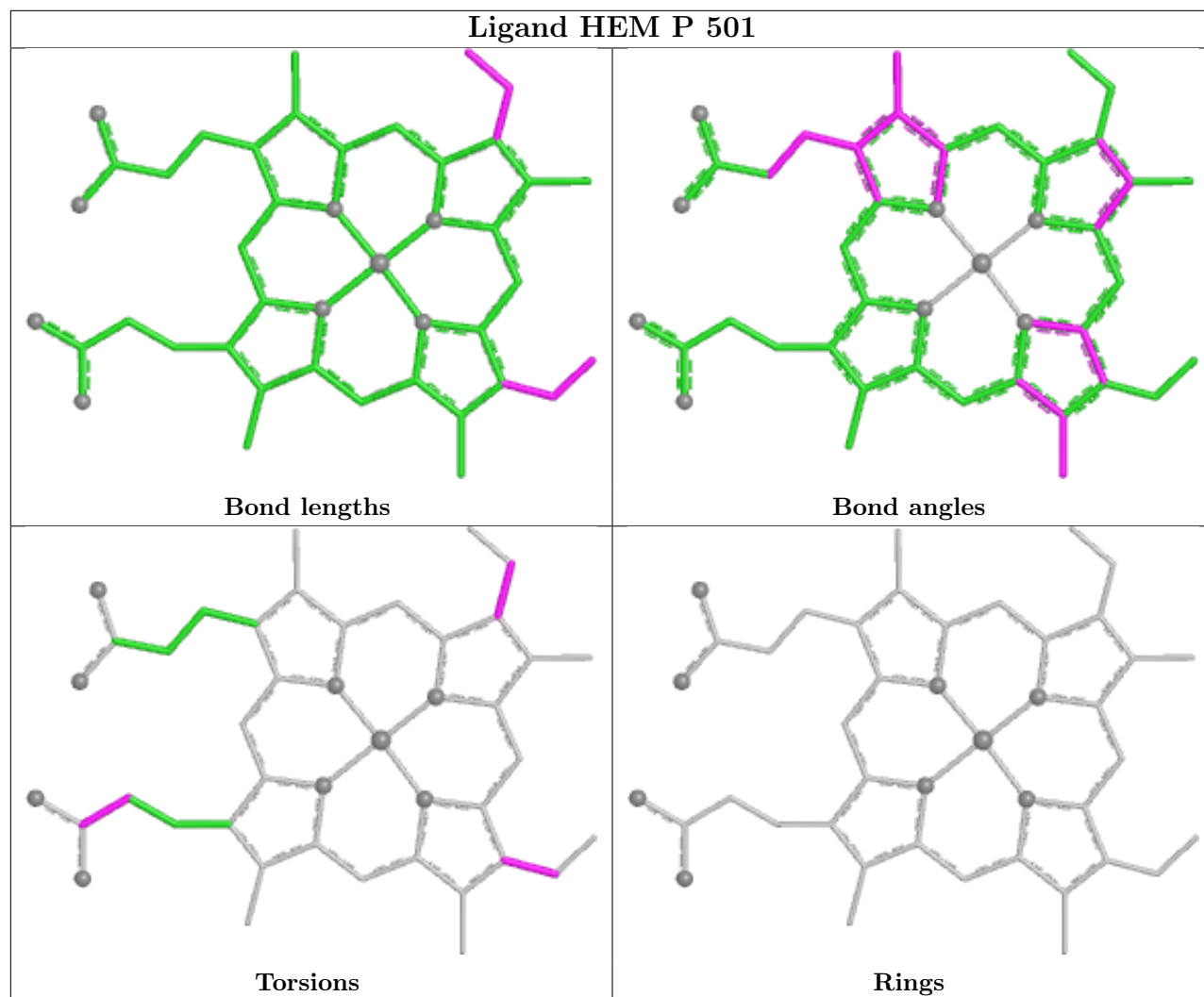


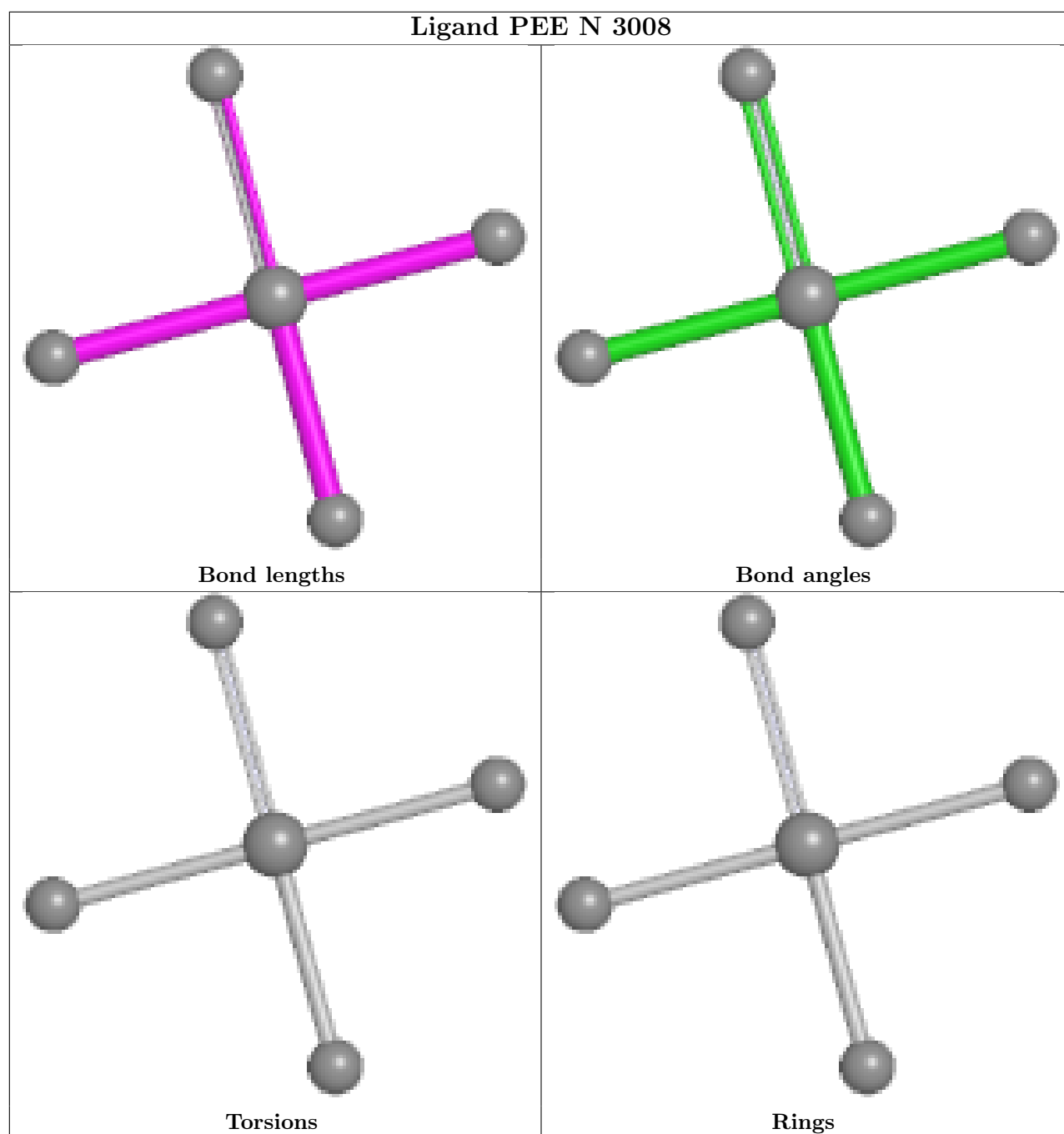




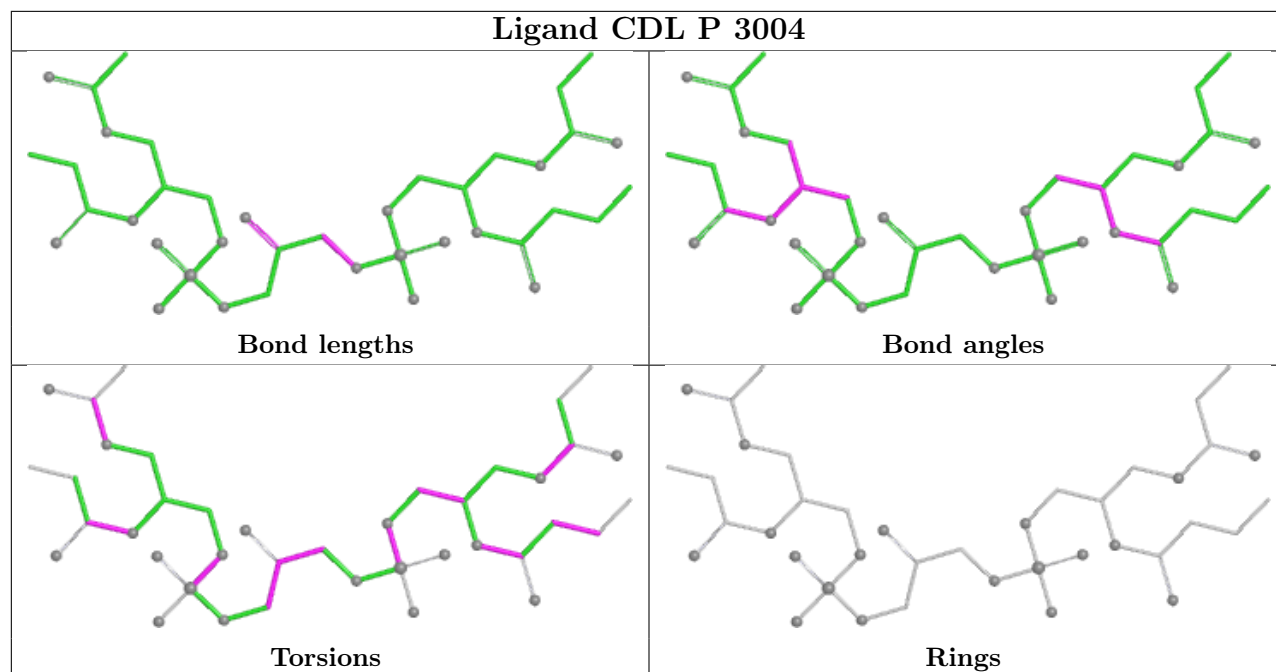




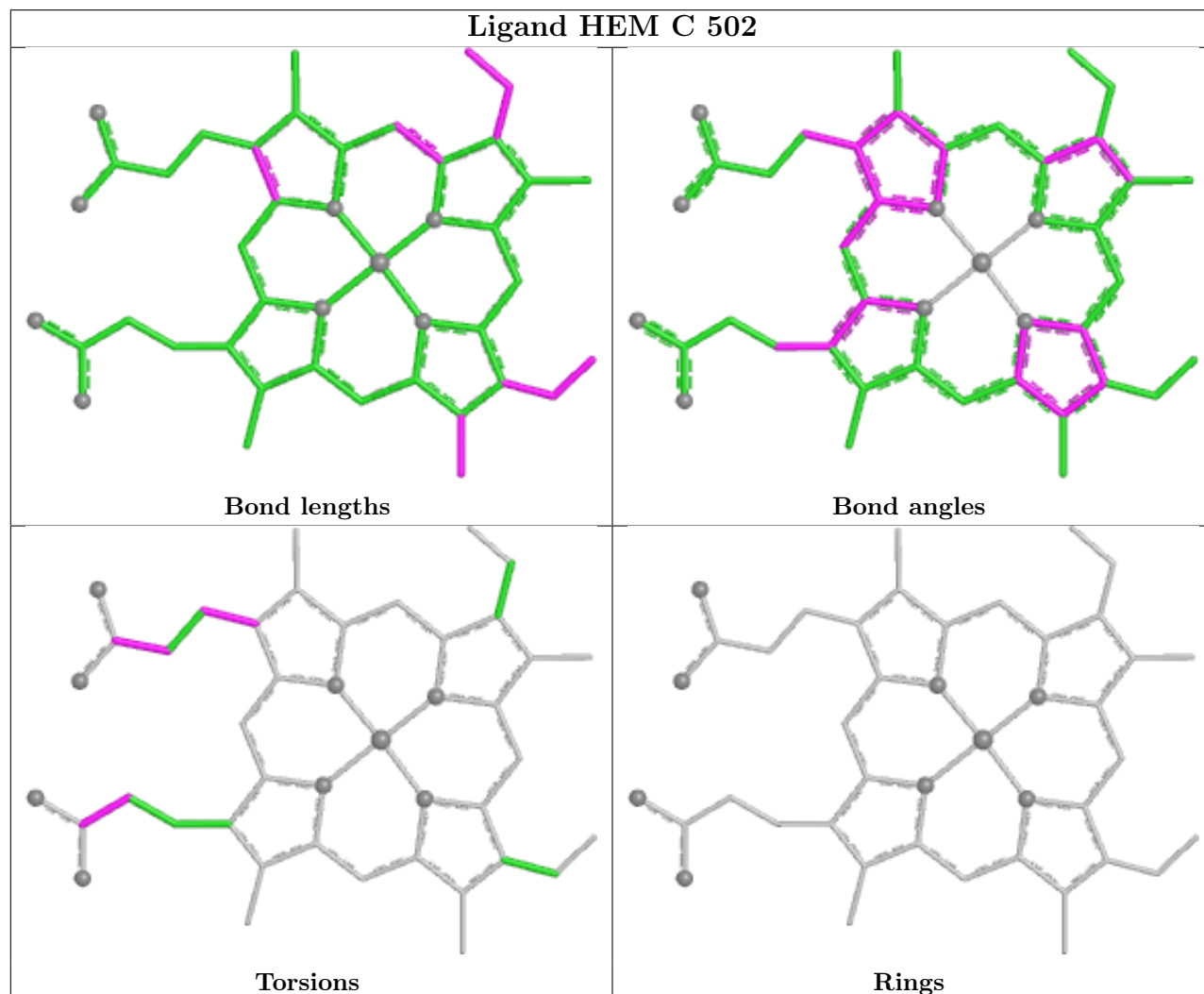


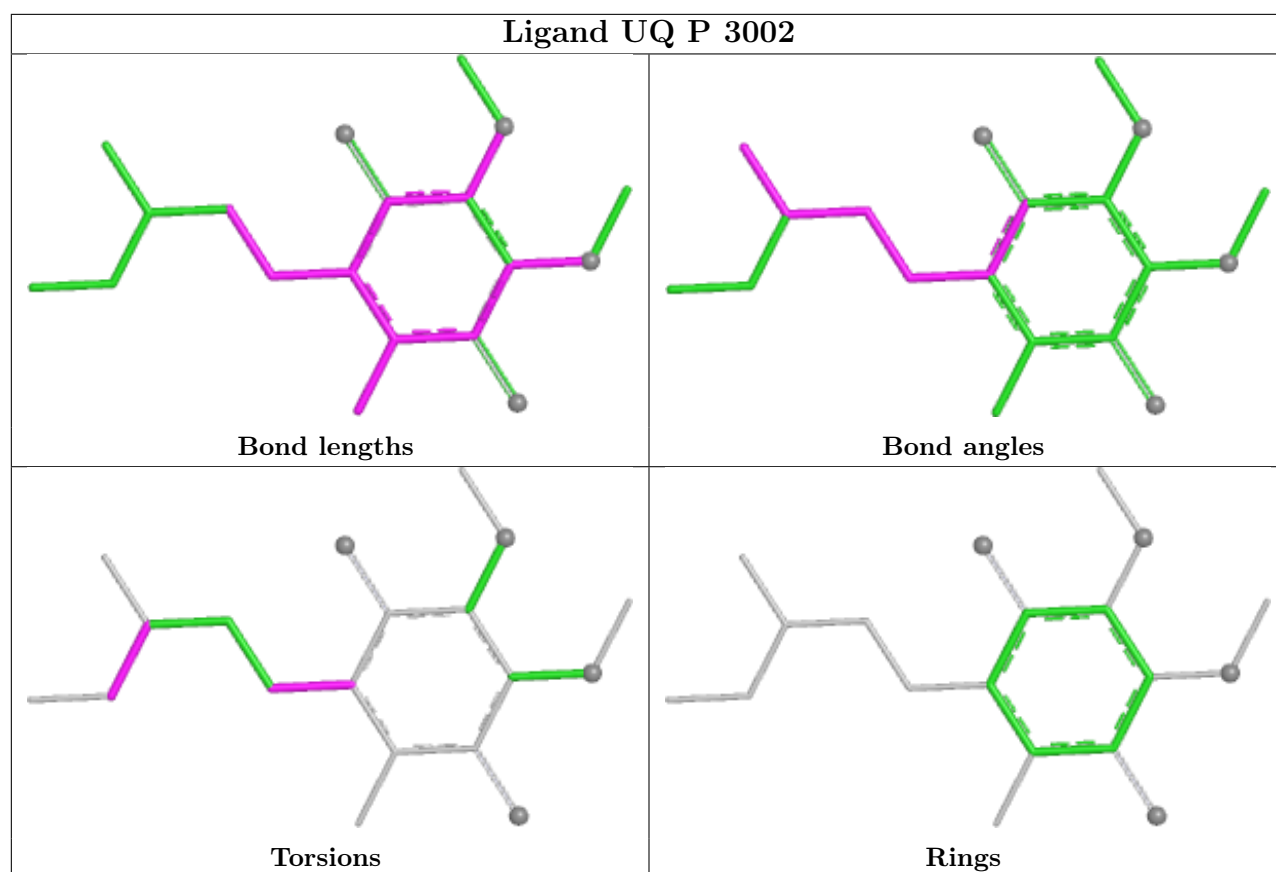


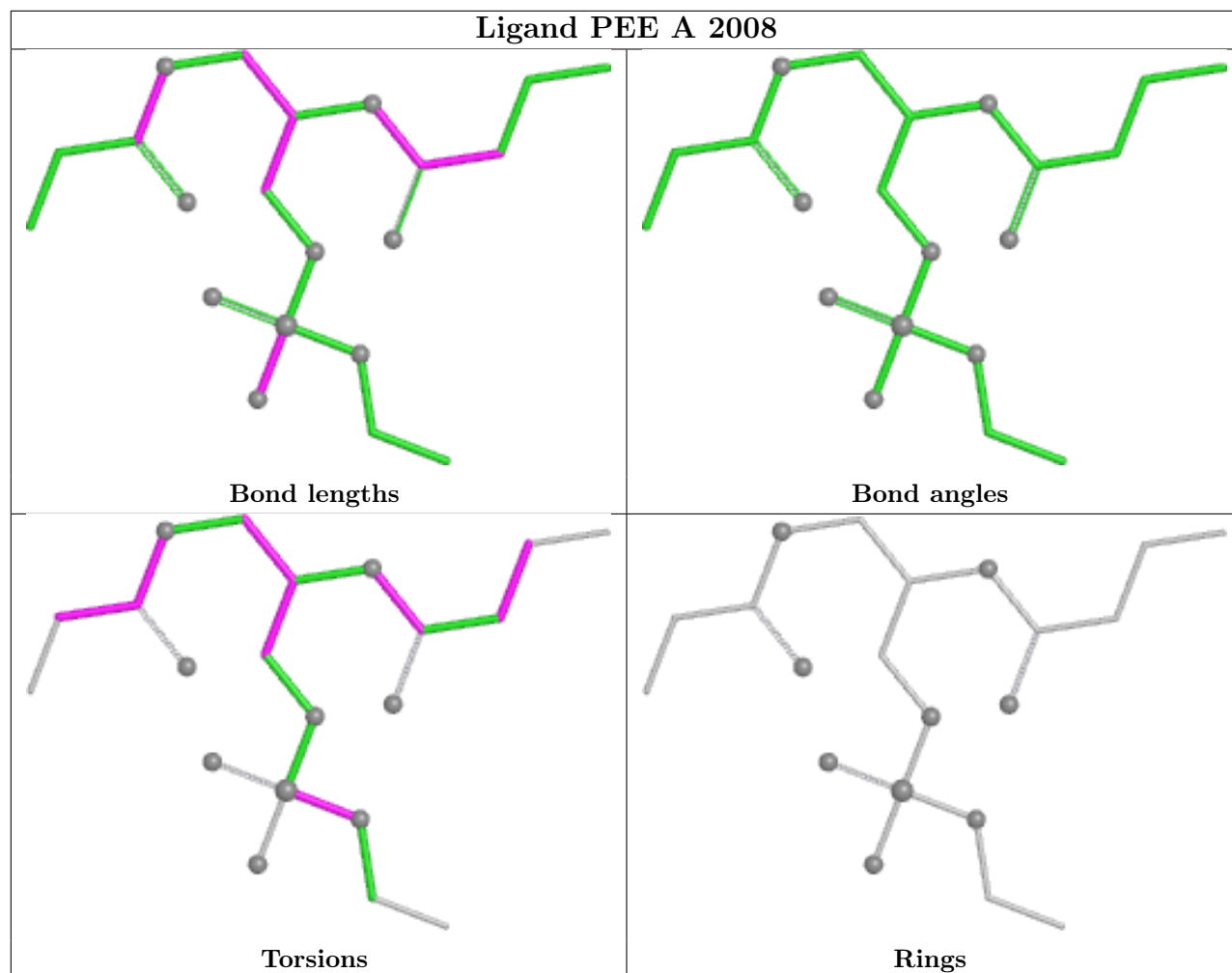
## Ligand CDL P 3004

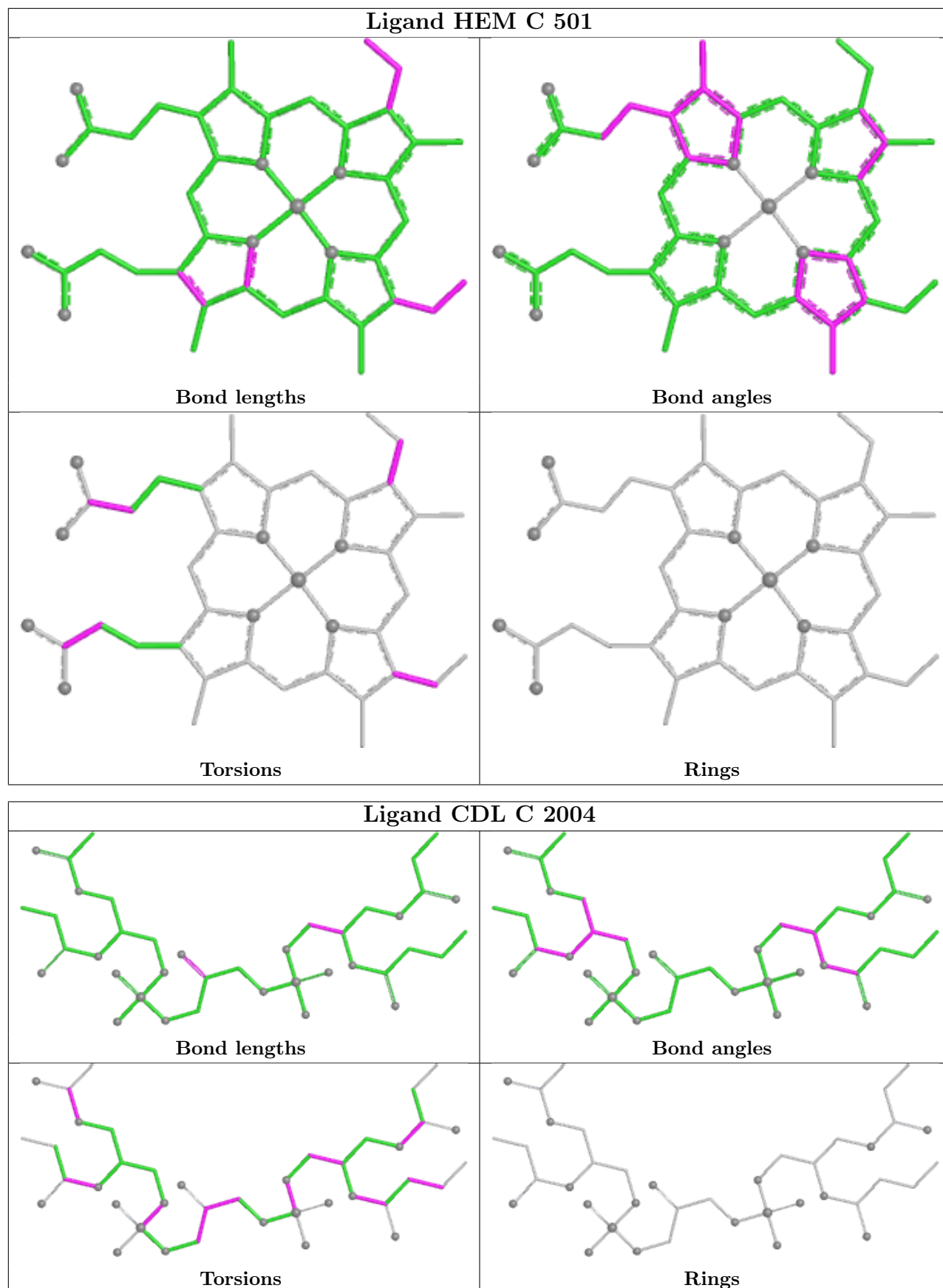


## Ligand HEM C 502

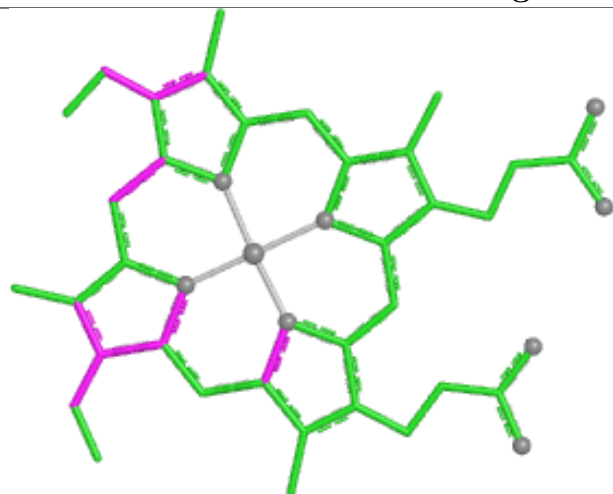




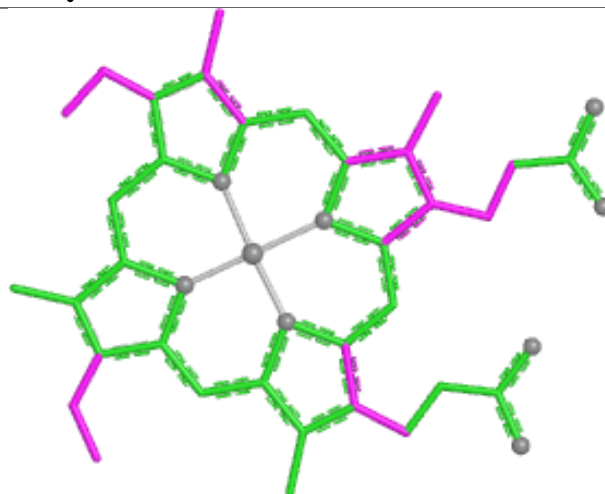




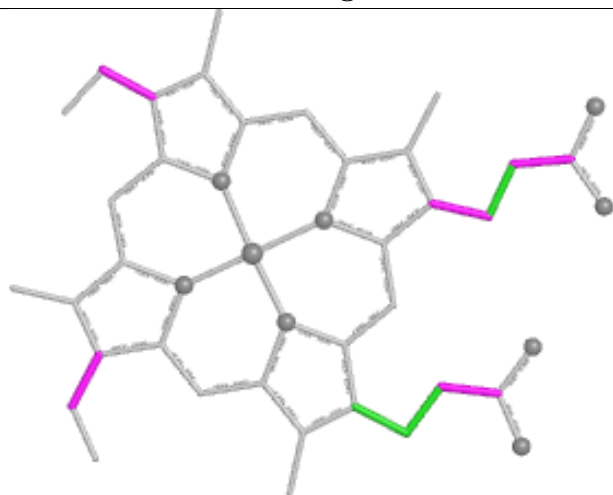
## Ligand HEC Q 501



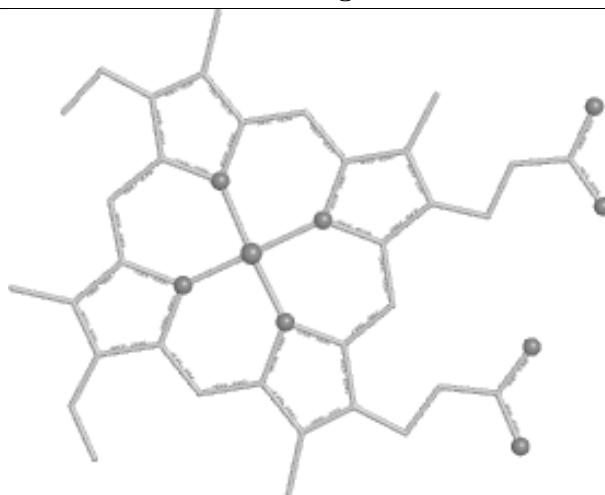
Bond lengths



Bond angles

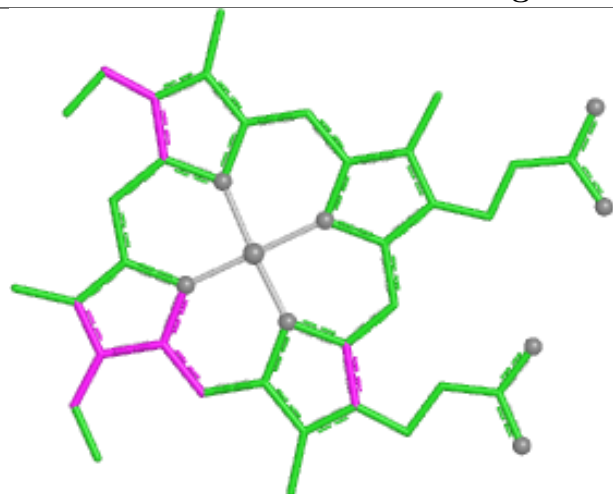


Torsions

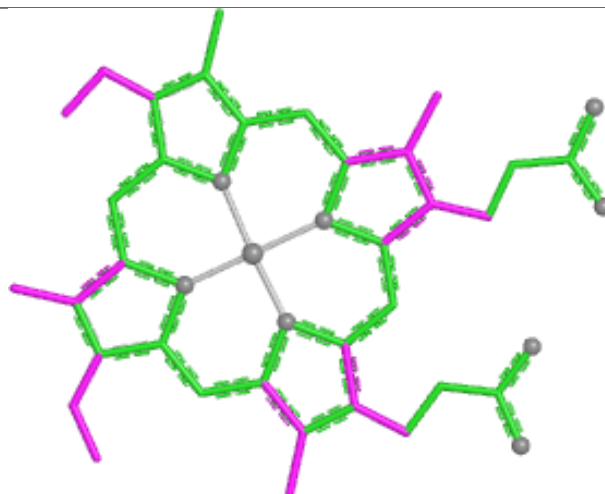


Rings

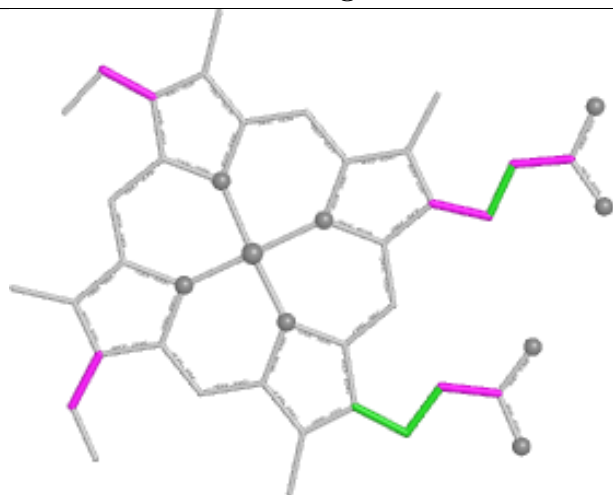
## Ligand HEC D 501



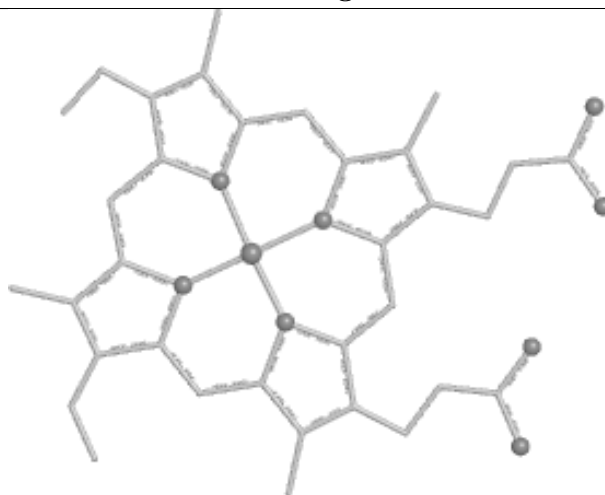
Bond lengths



Bond angles

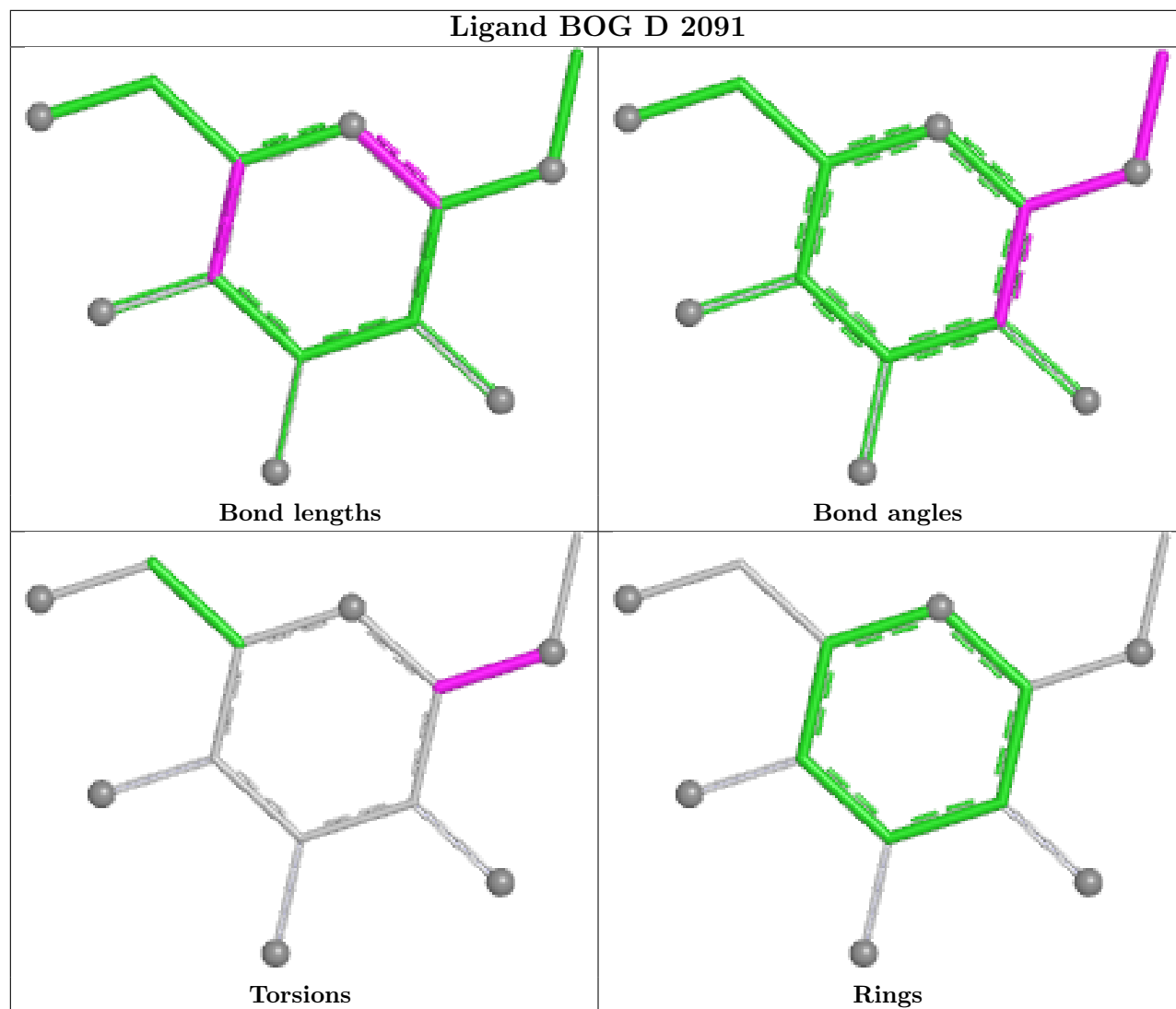


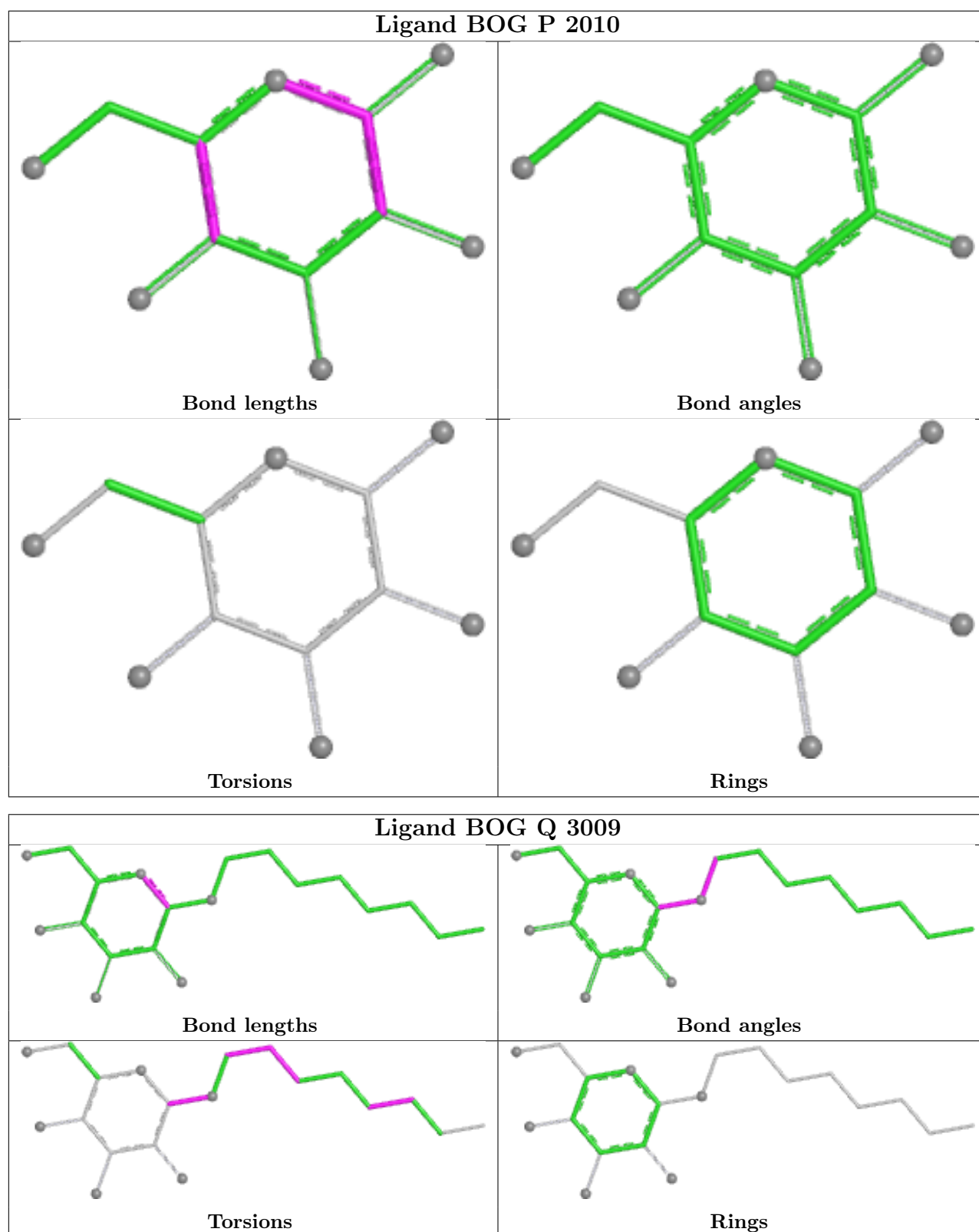
Torsions



Rings

## Ligand BOG D 2091





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 444/446 (99%)   | 0.43   | 15 (3%) 48 46  | 32, 58, 86, 100       | 0     |
| 1   | N     | 442/446 (99%)   | 0.89   | 45 (10%) 12 11 | 41, 68, 93, 100       | 0     |
| 2   | B     | 420/441 (95%)   | 1.08   | 49 (11%) 9 7   | 48, 76, 111, 133      | 0     |
| 2   | O     | 422/441 (95%)   | 1.01   | 53 (12%) 8 6   | 39, 74, 103, 122      | 0     |
| 3   | C     | 380/380 (100%)  | -0.11  | 17 (4%) 38 37  | 21, 39, 83, 123       | 0     |
| 3   | P     | 379/380 (99%)   | 0.36   | 16 (4%) 40 39  | 29, 58, 88, 125       | 0     |
| 4   | D     | 241/241 (100%)  | -0.18  | 5 (2%) 63 61   | 29, 41, 81, 103       | 0     |
| 4   | Q     | 241/241 (100%)  | 0.66   | 11 (4%) 37 36  | 46, 67, 97, 120       | 0     |
| 5   | E     | 196/196 (100%)  | 2.14   | 107 (54%) 0 0  | 34, 125, 156, 163     | 0     |
| 5   | R     | 196/196 (100%)  | 1.31   | 49 (25%) 2 1   | 40, 85, 129, 144      | 0     |
| 6   | F     | 101/110 (91%)   | -0.25  | 1 (0%) 79 79   | 26, 43, 61, 94        | 0     |
| 6   | S     | 101/110 (91%)   | 0.66   | 5 (4%) 34 34   | 50, 65, 102, 121      | 0     |
| 7   | G     | 80/81 (98%)     | 0.41   | 7 (8%) 15 15   | 33, 52, 97, 111       | 0     |
| 7   | T     | 79/81 (97%)     | 1.33   | 19 (24%) 2 1   | 46, 78, 139, 149      | 0     |
| 8   | H     | 70/77 (90%)     | 0.47   | 1 (1%) 73 73   | 34, 58, 80, 119       | 0     |
| 8   | U     | 67/77 (87%)     | 1.82   | 23 (34%) 1 0   | 82, 108, 128, 130     | 0     |
| 9   | I     | 31/47 (65%)     | 3.20   | 24 (77%) 0 0   | 72, 107, 133, 134     | 0     |
| 9   | V     | 31/47 (65%)     | 3.23   | 22 (70%) 0 0   | 66, 107, 132, 136     | 0     |
| 10  | J     | 61/61 (100%)    | 0.28   | 3 (4%) 35 34   | 43, 54, 95, 139       | 0     |
| 10  | W     | 60/61 (98%)     | 0.67   | 2 (3%) 49 47   | 55, 68, 99, 107       | 0     |
| All | All   | 4042/4160 (97%) | 0.73   | 474 (11%) 9 7  | 21, 64, 121, 163      | 0     |

All (474) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 106 | ILE  | 8.6  |
| 9   | V     | 56  | SER  | 8.2  |
| 5   | E     | 120 | PRO  | 7.8  |
| 2   | B     | 226 | ILE  | 7.5  |
| 1   | N     | 444 | ILE  | 7.3  |
| 5   | E     | 180 | LEU  | 7.3  |
| 9   | V     | 63  | ASP  | 7.2  |
| 9   | I     | 47  | ARG  | 6.9  |
| 9   | I     | 61  | ARG  | 6.7  |
| 5   | E     | 124 | LEU  | 6.7  |
| 5   | E     | 143 | GLY  | 6.6  |
| 5   | E     | 167 | ALA  | 6.1  |
| 7   | G     | 2   | ILE  | 6.0  |
| 5   | E     | 147 | ILE  | 6.0  |
| 7   | T     | 2   | ILE  | 5.9  |
| 8   | H     | 9   | GLU  | 5.9  |
| 5   | E     | 98  | VAL  | 5.9  |
| 5   | E     | 168 | SER  | 5.8  |
| 9   | I     | 63  | ASP  | 5.7  |
| 2   | O     | 226 | ILE  | 5.6  |
| 5   | E     | 109 | GLU  | 5.6  |
| 2   | B     | 20  | GLY  | 5.5  |
| 9   | V     | 59  | SER  | 5.5  |
| 9   | V     | 61  | ARG  | 5.5  |
| 5   | E     | 112 | VAL  | 5.5  |
| 5   | E     | 121 | GLN  | 5.4  |
| 9   | I     | 49  | LEU  | 5.4  |
| 5   | E     | 177 | PRO  | 5.3  |
| 5   | E     | 157 | TYR  | 5.3  |
| 5   | E     | 187 | PHE  | 5.2  |
| 5   | E     | 117 | LEU  | 5.2  |
| 1   | A     | 444 | ILE  | 5.2  |
| 5   | E     | 97  | PHE  | 5.1  |
| 5   | E     | 173 | LYS  | 5.0  |
| 2   | O     | 21  | ALA  | 4.9  |
| 9   | V     | 50  | LEU  | 4.9  |
| 5   | E     | 169 | GLY  | 4.9  |
| 9   | I     | 51  | CYS  | 4.8  |
| 3   | C     | 4   | ASN  | 4.8  |
| 9   | I     | 77  | ARG  | 4.8  |
| 5   | E     | 182 | VAL  | 4.8  |
| 9   | V     | 49  | LEU  | 4.7  |
| 5   | E     | 135 | LEU  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 142 | LEU  | 4.7  |
| 5   | E     | 178 | TYR  | 4.7  |
| 3   | P     | 2   | ALA  | 4.7  |
| 5   | R     | 124 | LEU  | 4.6  |
| 5   | E     | 79  | SER  | 4.6  |
| 9   | I     | 50  | LEU  | 4.6  |
| 5   | R     | 114 | VAL  | 4.5  |
| 9   | V     | 58  | ARG  | 4.5  |
| 3   | C     | 5   | ILE  | 4.4  |
| 5   | E     | 188 | VAL  | 4.4  |
| 5   | E     | 175 | PRO  | 4.4  |
| 7   | T     | 77  | TYR  | 4.4  |
| 2   | O     | 224 | LEU  | 4.4  |
| 5   | E     | 118 | ARG  | 4.3  |
| 5   | R     | 154 | GLY  | 4.3  |
| 5   | E     | 156 | TYR  | 4.3  |
| 5   | R     | 155 | GLY  | 4.3  |
| 9   | I     | 53  | GLU  | 4.3  |
| 5   | E     | 133 | VAL  | 4.3  |
| 9   | V     | 60  | ALA  | 4.3  |
| 5   | E     | 183 | PRO  | 4.3  |
| 5   | E     | 181 | GLU  | 4.3  |
| 5   | E     | 114 | VAL  | 4.3  |
| 5   | E     | 134 | ILE  | 4.2  |
| 9   | V     | 77  | ARG  | 4.2  |
| 2   | B     | 230 | ALA  | 4.2  |
| 5   | E     | 104 | ALA  | 4.1  |
| 6   | S     | 10  | GLY  | 4.1  |
| 5   | E     | 82  | PRO  | 4.1  |
| 9   | V     | 53  | GLU  | 4.1  |
| 5   | E     | 159 | PRO  | 4.1  |
| 5   | E     | 85  | LYS  | 4.1  |
| 3   | P     | 5   | ILE  | 4.1  |
| 5   | E     | 101 | ARG  | 4.1  |
| 5   | E     | 108 | GLN  | 4.0  |
| 3   | P     | 380 | TYR  | 4.0  |
| 5   | E     | 184 | THR  | 4.0  |
| 7   | G     | 81  | GLN  | 4.0  |
| 5   | E     | 185 | TYR  | 4.0  |
| 4   | Q     | 142 | VAL  | 4.0  |
| 5   | E     | 136 | VAL  | 3.9  |
| 9   | I     | 71  | ASN  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 9   | HIS  | 3.9  |
| 5   | E     | 145 | VAL  | 3.9  |
| 5   | E     | 102 | THR  | 3.9  |
| 9   | V     | 52  | ARG  | 3.9  |
| 10  | J     | 61  | ALA  | 3.9  |
| 1   | A     | 432 | LEU  | 3.8  |
| 9   | I     | 64  | LEU  | 3.8  |
| 1   | N     | 38  | GLY  | 3.8  |
| 5   | E     | 87  | VAL  | 3.8  |
| 5   | R     | 196 | GLY  | 3.8  |
| 5   | E     | 150 | SER  | 3.8  |
| 5   | R     | 165 | TYR  | 3.8  |
| 5   | E     | 170 | ARG  | 3.8  |
| 7   | T     | 4   | PHE  | 3.8  |
| 5   | E     | 140 | THR  | 3.7  |
| 5   | R     | 147 | ILE  | 3.7  |
| 5   | E     | 110 | ALA  | 3.7  |
| 5   | E     | 194 | VAL  | 3.7  |
| 5   | E     | 153 | PHE  | 3.7  |
| 5   | E     | 138 | VAL  | 3.7  |
| 2   | O     | 371 | SER  | 3.7  |
| 3   | C     | 8   | SER  | 3.7  |
| 2   | B     | 224 | LEU  | 3.6  |
| 2   | O     | 296 | TYR  | 3.6  |
| 1   | N     | 190 | PHE  | 3.6  |
| 5   | E     | 192 | LEU  | 3.6  |
| 3   | C     | 7   | LYS  | 3.6  |
| 5   | E     | 128 | LYS  | 3.6  |
| 4   | D     | 1   | GLY  | 3.6  |
| 5   | E     | 111 | GLU  | 3.6  |
| 9   | V     | 55  | MET  | 3.6  |
| 9   | I     | 60  | ALA  | 3.5  |
| 5   | R     | 167 | ALA  | 3.5  |
| 3   | C     | 10  | PRO  | 3.5  |
| 1   | A     | 219 | VAL  | 3.5  |
| 7   | T     | 3   | HIS  | 3.5  |
| 9   | V     | 62  | ARG  | 3.5  |
| 2   | B     | 229 | GLY  | 3.5  |
| 8   | U     | 37  | LEU  | 3.5  |
| 5   | R     | 178 | TYR  | 3.5  |
| 2   | O     | 232 | THR  | 3.5  |
| 5   | E     | 107 | ASN  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 113 | ASP  | 3.5  |
| 3   | C     | 156 | TYR  | 3.4  |
| 5   | E     | 171 | ILE  | 3.4  |
| 5   | E     | 193 | VAL  | 3.4  |
| 5   | E     | 122 | HIS  | 3.4  |
| 5   | R     | 106 | ILE  | 3.4  |
| 5   | R     | 104 | ALA  | 3.4  |
| 5   | E     | 149 | ASN  | 3.4  |
| 1   | N     | 185 | TYR  | 3.4  |
| 5   | R     | 133 | VAL  | 3.4  |
| 5   | E     | 174 | GLY  | 3.3  |
| 8   | U     | 61  | PHE  | 3.3  |
| 9   | I     | 76  | VAL  | 3.3  |
| 3   | C     | 380 | TYR  | 3.3  |
| 1   | N     | 432 | LEU  | 3.3  |
| 9   | I     | 52  | ARG  | 3.3  |
| 1   | A     | 10  | ASN  | 3.3  |
| 5   | E     | 172 | ARG  | 3.3  |
| 5   | R     | 156 | TYR  | 3.3  |
| 9   | I     | 70  | LEU  | 3.3  |
| 2   | O     | 383 | GLY  | 3.3  |
| 4   | Q     | 1   | GLY  | 3.3  |
| 5   | R     | 110 | ALA  | 3.3  |
| 5   | E     | 89  | PHE  | 3.3  |
| 5   | E     | 123 | ASP  | 3.3  |
| 1   | N     | 443 | TRP  | 3.3  |
| 5   | R     | 157 | TYR  | 3.3  |
| 7   | T     | 6   | ASN  | 3.3  |
| 5   | E     | 119 | ASP  | 3.3  |
| 5   | E     | 99  | ARG  | 3.2  |
| 3   | C     | 1   | MET  | 3.2  |
| 1   | A     | 443 | TRP  | 3.2  |
| 2   | B     | 30  | PRO  | 3.2  |
| 7   | T     | 74  | PRO  | 3.2  |
| 2   | B     | 208 | GLY  | 3.2  |
| 9   | I     | 56  | SER  | 3.2  |
| 7   | T     | 79  | ASN  | 3.2  |
| 1   | A     | 28  | GLU  | 3.2  |
| 9   | V     | 48  | PRO  | 3.2  |
| 10  | W     | 61  | ALA  | 3.2  |
| 2   | B     | 216 | LEU  | 3.1  |
| 2   | O     | 238 | THR  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 162 | GLY  | 3.1  |
| 5   | R     | 115 | SER  | 3.1  |
| 5   | E     | 165 | TYR  | 3.1  |
| 1   | A     | 226 | ASP  | 3.1  |
| 8   | U     | 39  | LEU  | 3.1  |
| 7   | G     | 3   | HIS  | 3.1  |
| 9   | V     | 76  | VAL  | 3.1  |
| 8   | U     | 78  | LYS  | 3.1  |
| 5   | R     | 117 | LEU  | 3.1  |
| 2   | O     | 156 | GLN  | 3.1  |
| 5   | E     | 154 | GLY  | 3.1  |
| 2   | B     | 35  | ILE  | 3.1  |
| 7   | T     | 8   | ALA  | 3.1  |
| 9   | V     | 64  | LEU  | 3.1  |
| 9   | I     | 48  | PRO  | 3.1  |
| 5   | R     | 126 | ARG  | 3.1  |
| 2   | O     | 18  | CYS  | 3.1  |
| 5   | E     | 163 | SER  | 3.1  |
| 5   | E     | 96  | LEU  | 3.0  |
| 3   | P     | 4   | ASN  | 3.0  |
| 2   | B     | 292 | THR  | 3.0  |
| 2   | B     | 34  | ILE  | 3.0  |
| 3   | C     | 14  | MET  | 3.0  |
| 4   | Q     | 5   | LEU  | 3.0  |
| 8   | U     | 13  | LEU  | 3.0  |
| 5   | E     | 186 | GLN  | 3.0  |
| 3   | P     | 7   | LYS  | 3.0  |
| 5   | E     | 127 | VAL  | 3.0  |
| 1   | N     | 120 | CYS  | 3.0  |
| 5   | E     | 116 | LYS  | 3.0  |
| 5   | E     | 129 | LYS  | 3.0  |
| 2   | B     | 388 | LEU  | 3.0  |
| 4   | Q     | 241 | LYS  | 3.0  |
| 5   | R     | 116 | LYS  | 3.0  |
| 1   | N     | 223 | TYR  | 3.0  |
| 7   | T     | 24  | ARG  | 3.0  |
| 5   | R     | 148 | ALA  | 3.0  |
| 2   | O     | 405 | VAL  | 3.0  |
| 5   | E     | 100 | HIS  | 2.9  |
| 5   | R     | 128 | LYS  | 2.9  |
| 8   | U     | 68  | CYS  | 2.9  |
| 5   | E     | 152 | ASP  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | R     | 171 | ILE  | 2.9  |
| 2   | O     | 307 | PHE  | 2.9  |
| 3   | C     | 3   | PRO  | 2.9  |
| 5   | E     | 84  | GLY  | 2.9  |
| 9   | V     | 57  | GLY  | 2.9  |
| 2   | B     | 24  | LEU  | 2.9  |
| 4   | Q     | 3   | LEU  | 2.9  |
| 8   | U     | 36  | ARG  | 2.9  |
| 5   | E     | 88  | ALA  | 2.9  |
| 8   | U     | 74  | PHE  | 2.9  |
| 2   | O     | 110 | GLU  | 2.9  |
| 5   | E     | 103 | GLN  | 2.9  |
| 1   | N     | 179 | ARG  | 2.9  |
| 3   | P     | 6   | ARG  | 2.9  |
| 3   | C     | 16  | ASN  | 2.9  |
| 5   | E     | 179 | ASN  | 2.9  |
| 2   | B     | 232 | THR  | 2.9  |
| 1   | N     | 129 | LYS  | 2.9  |
| 8   | U     | 76  | LYS  | 2.9  |
| 2   | O     | 291 | VAL  | 2.9  |
| 5   | R     | 105 | GLU  | 2.8  |
| 9   | V     | 71  | ASN  | 2.8  |
| 5   | E     | 196 | GLY  | 2.8  |
| 2   | B     | 21  | ALA  | 2.8  |
| 1   | N     | 39  | VAL  | 2.8  |
| 2   | B     | 312 | PHE  | 2.8  |
| 5   | E     | 146 | PRO  | 2.8  |
| 1   | A     | 31  | SER  | 2.8  |
| 1   | N     | 104 | LYS  | 2.8  |
| 5   | R     | 85  | LYS  | 2.8  |
| 5   | E     | 190 | ASP  | 2.8  |
| 2   | O     | 386 | ALA  | 2.8  |
| 2   | B     | 223 | PHE  | 2.8  |
| 5   | R     | 101 | ARG  | 2.8  |
| 8   | U     | 26  | GLN  | 2.8  |
| 2   | O     | 384 | SER  | 2.8  |
| 2   | O     | 295 | LEU  | 2.8  |
| 2   | O     | 344 | LEU  | 2.8  |
| 3   | C     | 11  | LEU  | 2.8  |
| 2   | O     | 353 | THR  | 2.8  |
| 2   | B     | 41  | PHE  | 2.8  |
| 7   | T     | 78  | GLU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 6   | ARG  | 2.8  |
| 5   | E     | 115 | SER  | 2.8  |
| 2   | B     | 33  | LEU  | 2.8  |
| 7   | T     | 76  | ASP  | 2.8  |
| 7   | T     | 80  | ASP  | 2.8  |
| 10  | W     | 45  | HIS  | 2.8  |
| 2   | O     | 335 | GLU  | 2.8  |
| 9   | I     | 72  | ALA  | 2.8  |
| 3   | P     | 3   | PRO  | 2.7  |
| 8   | U     | 54  | CYS  | 2.7  |
| 9   | I     | 59  | SER  | 2.7  |
| 1   | N     | 160 | GLY  | 2.7  |
| 1   | N     | 380 | GLY  | 2.7  |
| 3   | P     | 14  | MET  | 2.7  |
| 6   | S     | 13  | MET  | 2.7  |
| 7   | G     | 80  | ASP  | 2.7  |
| 1   | A     | 86  | PHE  | 2.7  |
| 5   | R     | 153 | PHE  | 2.7  |
| 2   | O     | 19  | PRO  | 2.7  |
| 8   | U     | 30  | CYS  | 2.7  |
| 4   | Q     | 164 | ILE  | 2.7  |
| 9   | V     | 54  | SER  | 2.7  |
| 1   | A     | 2   | ALA  | 2.7  |
| 1   | N     | 26  | ALA  | 2.7  |
| 5   | E     | 176 | ALA  | 2.7  |
| 5   | R     | 118 | ARG  | 2.7  |
| 1   | N     | 122 | LEU  | 2.7  |
| 5   | E     | 191 | ASP  | 2.7  |
| 7   | G     | 4   | PHE  | 2.7  |
| 5   | E     | 94  | LYS  | 2.7  |
| 2   | O     | 26  | ILE  | 2.7  |
| 7   | T     | 5   | GLY  | 2.7  |
| 1   | N     | 34  | THR  | 2.7  |
| 3   | P     | 156 | TYR  | 2.6  |
| 10  | J     | 63  | GLU  | 2.6  |
| 2   | O     | 230 | ALA  | 2.6  |
| 4   | Q     | 143 | VAL  | 2.6  |
| 5   | R     | 112 | VAL  | 2.6  |
| 9   | V     | 72  | ALA  | 2.6  |
| 2   | O     | 249 | GLY  | 2.6  |
| 5   | R     | 187 | PHE  | 2.6  |
| 7   | T     | 75  | ALA  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 250 | HIS  | 2.6  |
| 2   | B     | 390 | GLY  | 2.6  |
| 2   | B     | 197 | ASN  | 2.6  |
| 5   | R     | 82  | PRO  | 2.6  |
| 5   | R     | 175 | PRO  | 2.6  |
| 2   | O     | 209 | ILE  | 2.6  |
| 5   | R     | 172 | ARG  | 2.6  |
| 5   | R     | 84  | GLY  | 2.6  |
| 1   | N     | 25  | VAL  | 2.6  |
| 1   | N     | 219 | VAL  | 2.6  |
| 2   | B     | 119 | VAL  | 2.6  |
| 2   | O     | 352 | VAL  | 2.6  |
| 3   | P     | 151 | PHE  | 2.6  |
| 5   | E     | 132 | TRP  | 2.5  |
| 3   | P     | 11  | LEU  | 2.5  |
| 2   | O     | 227 | ARG  | 2.5  |
| 9   | V     | 47  | ARG  | 2.5  |
| 2   | O     | 250 | HIS  | 2.5  |
| 5   | E     | 141 | HIS  | 2.5  |
| 9   | I     | 57  | GLY  | 2.5  |
| 6   | S     | 81  | VAL  | 2.5  |
| 2   | O     | 37  | SER  | 2.5  |
| 2   | B     | 36  | ALA  | 2.5  |
| 8   | U     | 24  | CYS  | 2.5  |
| 2   | O     | 289 | SER  | 2.5  |
| 5   | E     | 126 | ARG  | 2.5  |
| 9   | I     | 58  | ARG  | 2.5  |
| 2   | O     | 229 | GLY  | 2.5  |
| 2   | B     | 371 | SER  | 2.5  |
| 2   | O     | 430 | LEU  | 2.5  |
| 4   | D     | 2   | GLU  | 2.5  |
| 1   | N     | 22  | GLY  | 2.5  |
| 8   | U     | 16  | PRO  | 2.5  |
| 2   | O     | 279 | LEU  | 2.4  |
| 1   | N     | 217 | SER  | 2.4  |
| 2   | B     | 228 | SER  | 2.4  |
| 5   | R     | 164 | HIS  | 2.4  |
| 5   | R     | 190 | ASP  | 2.4  |
| 7   | G     | 32  | ASP  | 2.4  |
| 2   | O     | 20  | GLY  | 2.4  |
| 1   | N     | 69  | LYS  | 2.4  |
| 5   | E     | 77  | LYS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | R     | 89  | PHE  | 2.4  |
| 3   | C     | 345 | GLU  | 2.4  |
| 5   | E     | 137 | GLY  | 2.4  |
| 5   | E     | 148 | ALA  | 2.4  |
| 5   | R     | 134 | ILE  | 2.4  |
| 2   | O     | 193 | HIS  | 2.4  |
| 1   | N     | 72  | CYS  | 2.4  |
| 5   | E     | 105 | GLU  | 2.4  |
| 7   | G     | 5   | GLY  | 2.4  |
| 5   | R     | 103 | GLN  | 2.4  |
| 1   | N     | 386 | TYR  | 2.4  |
| 2   | B     | 281 | ALA  | 2.4  |
| 9   | I     | 62  | ARG  | 2.4  |
| 1   | N     | 127 | ILE  | 2.4  |
| 2   | B     | 225 | ASN  | 2.4  |
| 9   | I     | 55  | MET  | 2.4  |
| 2   | B     | 32  | GLY  | 2.4  |
| 2   | O     | 223 | PHE  | 2.4  |
| 1   | N     | 392 | LEU  | 2.3  |
| 2   | B     | 29  | LEU  | 2.3  |
| 5   | R     | 192 | LEU  | 2.3  |
| 7   | T     | 7   | LEU  | 2.3  |
| 7   | T     | 63  | THR  | 2.3  |
| 5   | E     | 83  | GLU  | 2.3  |
| 1   | N     | 187 | ASP  | 2.3  |
| 5   | R     | 169 | GLY  | 2.3  |
| 1   | N     | 37  | VAL  | 2.3  |
| 1   | N     | 117 | VAL  | 2.3  |
| 1   | N     | 64  | PHE  | 2.3  |
| 2   | O     | 312 | PHE  | 2.3  |
| 3   | P     | 15  | ILE  | 2.3  |
| 3   | P     | 224 | TYR  | 2.3  |
| 4   | Q     | 57  | THR  | 2.3  |
| 5   | E     | 161 | HIS  | 2.3  |
| 2   | B     | 317 | SER  | 2.3  |
| 5   | E     | 151 | GLY  | 2.3  |
| 2   | O     | 388 | LEU  | 2.3  |
| 5   | E     | 164 | HIS  | 2.3  |
| 1   | N     | 195 | MET  | 2.3  |
| 2   | B     | 206 | LEU  | 2.3  |
| 1   | N     | 121 | ALA  | 2.3  |
| 2   | B     | 26  | ILE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 386 | ALA  | 2.3  |
| 2   | O     | 36  | ALA  | 2.3  |
| 6   | S     | 21  | TYR  | 2.3  |
| 5   | R     | 31  | ASP  | 2.3  |
| 8   | U     | 69  | VAL  | 2.3  |
| 2   | B     | 220 | ALA  | 2.2  |
| 8   | U     | 33  | ALA  | 2.2  |
| 6   | S     | 84  | GLU  | 2.2  |
| 4   | D     | 172 | ASP  | 2.2  |
| 7   | T     | 43  | SER  | 2.2  |
| 1   | A     | 392 | LEU  | 2.2  |
| 1   | N     | 170 | THR  | 2.2  |
| 2   | O     | 368 | TYR  | 2.2  |
| 5   | R     | 86  | ASN  | 2.2  |
| 1   | N     | 218 | GLY  | 2.2  |
| 2   | O     | 308 | ASP  | 2.2  |
| 8   | U     | 29  | LYS  | 2.2  |
| 1   | A     | 203 | ILE  | 2.2  |
| 2   | O     | 402 | ILE  | 2.2  |
| 2   | B     | 171 | ALA  | 2.2  |
| 1   | N     | 111 | GLU  | 2.2  |
| 2   | O     | 306 | PRO  | 2.2  |
| 1   | N     | 23  | LEU  | 2.2  |
| 2   | B     | 344 | LEU  | 2.2  |
| 4   | D     | 241 | LYS  | 2.2  |
| 8   | U     | 73  | LEU  | 2.2  |
| 1   | A     | 366 | VAL  | 2.2  |
| 5   | R     | 111 | GLU  | 2.2  |
| 2   | B     | 304 | THR  | 2.2  |
| 4   | Q     | 144 | ARG  | 2.2  |
| 4   | Q     | 238 | ARG  | 2.2  |
| 5   | E     | 86  | ASN  | 2.2  |
| 6   | F     | 110 | LYS  | 2.2  |
| 2   | B     | 124 | LEU  | 2.2  |
| 7   | T     | 32  | ASP  | 2.2  |
| 5   | R     | 150 | SER  | 2.2  |
| 2   | B     | 402 | ILE  | 2.2  |
| 1   | N     | 216 | PHE  | 2.2  |
| 2   | O     | 281 | ALA  | 2.1  |
| 4   | D     | 76  | GLU  | 2.1  |
| 8   | U     | 34  | ARG  | 2.1  |
| 9   | V     | 51  | CYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 155 | PRO  | 2.1  |
| 2   | O     | 104 | LYS  | 2.1  |
| 4   | Q     | 31  | GLN  | 2.1  |
| 1   | N     | 182 | LEU  | 2.1  |
| 2   | B     | 38  | LEU  | 2.1  |
| 5   | E     | 78  | LEU  | 2.1  |
| 1   | A     | 228 | VAL  | 2.1  |
| 1   | N     | 86  | PHE  | 2.1  |
| 3   | P     | 244 | ALA  | 2.1  |
| 1   | N     | 28  | GLU  | 2.1  |
| 5   | R     | 16  | GLU  | 2.1  |
| 7   | T     | 38  | TRP  | 2.1  |
| 2   | O     | 292 | THR  | 2.1  |
| 5   | R     | 108 | GLN  | 2.1  |
| 2   | O     | 112 | LEU  | 2.1  |
| 8   | U     | 77  | LEU  | 2.1  |
| 3   | P     | 371 | GLY  | 2.1  |
| 5   | R     | 81  | ILE  | 2.1  |
| 8   | U     | 63  | HIS  | 2.1  |
| 8   | U     | 31  | VAL  | 2.1  |
| 2   | B     | 289 | SER  | 2.1  |
| 9   | I     | 75  | SER  | 2.1  |
| 2   | O     | 394 | ALA  | 2.1  |
| 10  | J     | 64  | GLU  | 2.1  |
| 1   | N     | 119 | ASN  | 2.1  |
| 2   | B     | 57  | TYR  | 2.1  |
| 5   | E     | 76  | ILE  | 2.1  |
| 3   | C     | 151 | PHE  | 2.1  |
| 2   | B     | 396 | SER  | 2.1  |
| 2   | O     | 102 | ARG  | 2.1  |
| 5   | R     | 102 | THR  | 2.1  |
| 2   | B     | 306 | PRO  | 2.1  |
| 1   | N     | 189 | HIS  | 2.1  |
| 5   | E     | 93  | GLY  | 2.1  |
| 2   | B     | 211 | VAL  | 2.1  |
| 2   | O     | 398 | VAL  | 2.1  |
| 1   | A     | 433 | ASP  | 2.0  |
| 1   | N     | 282 | ARG  | 2.0  |
| 5   | R     | 113 | ASP  | 2.0  |
| 1   | N     | 81  | SER  | 2.0  |
| 5   | E     | 90  | LYS  | 2.0  |
| 5   | E     | 95  | PRO  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 405 | VAL  | 2.0  |
| 2   | O     | 264 | VAL  | 2.0  |
| 5   | E     | 195 | VAL  | 2.0  |
| 2   | O     | 311 | ALA  | 2.0  |
| 2   | B     | 393 | THR  | 2.0  |
| 1   | N     | 42  | GLY  | 2.0  |
| 2   | O     | 35  | ILE  | 2.0  |
| 3   | P     | 154 | ILE  | 2.0  |
| 9   | I     | 68  | ILE  | 2.0  |
| 2   | B     | 291 | VAL  | 2.0  |
| 8   | U     | 43  | 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 |
|-----|------|-------|------|--------|------|------|----------------------------|-------|
| 18  | BOG  | Q     | 3091 | 13/20  | 0.29 | 0.35 | 183,186,187,187            | 0     |
| 11  | PEE  | A     | 2008 | 21/51  | 0.38 | 0.33 | 129,133,134,135            | 0     |
| 18  | BOG  | P     | 2010 | 12/20  | 0.54 | 0.29 | 135,137,138,138            | 0     |
| 18  | BOG  | D     | 2091 | 13/20  | 0.59 | 0.42 | 200,201,201,201            | 0     |
| 15  | CDL  | Q     | 3003 | 42/100 | 0.74 | 0.28 | 109,121,139,139            | 0     |
| 11  | PEE  | N     | 3008 | 5/51   | 0.75 | 0.16 | 110,111,112,112            | 0     |
| 11  | PEE  | P     | 3007 | 49/51  | 0.76 | 0.27 | 53,79,93,94                | 0     |
| 15  | CDL  | D     | 2003 | 42/100 | 0.78 | 0.24 | 82,92,106,108              | 0     |
| 15  | CDL  | P     | 3004 | 40/100 | 0.79 | 0.20 | 96,102,111,111             | 0     |
| 11  | PEE  | C     | 2007 | 49/51  | 0.80 | 0.24 | 43,58,70,73                | 0     |
| 11  | PEE  | R     | 3005 | 50/51  | 0.80 | 0.29 | 80,98,108,110              | 0     |
| 11  | PEE  | E     | 2005 | 50/51  | 0.84 | 0.24 | 68,89,95,97                | 0     |

*Continued on next page...*

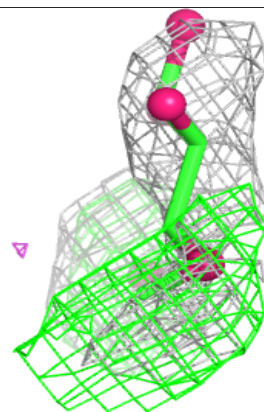
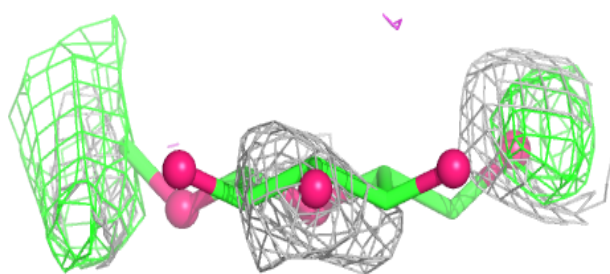
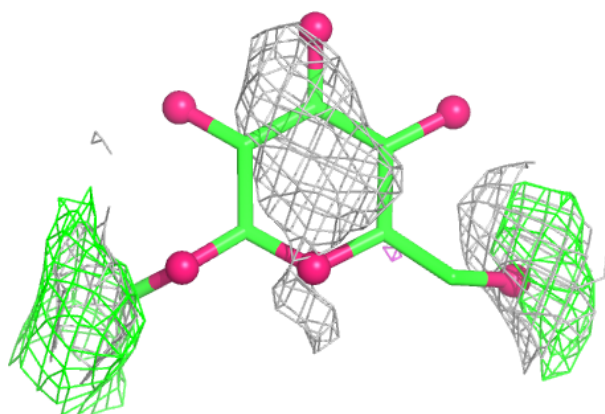
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms  | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|--------|------|------|-----------------------------|-------|
| 14  | UQ   | P     | 3002 | 19/63  | 0.84 | 0.36 | 119,124,125,126             | 0     |
| 16  | GOL  | P     | 3011 | 6/6    | 0.86 | 0.25 | 73,75,76,77                 | 0     |
| 14  | UQ   | C     | 2002 | 19/63  | 0.86 | 0.27 | 88,90,90,91                 | 0     |
| 13  | JZV  | P     | 3001 | 29/29  | 0.86 | 0.20 | 59,66,104,106               | 0     |
| 15  | CDL  | C     | 2004 | 40/100 | 0.86 | 0.17 | 66,80,91,93                 | 0     |
| 18  | BOG  | Q     | 3009 | 20/20  | 0.89 | 0.15 | 62,75,77,78                 | 0     |
| 19  | FES  | E     | 501  | 4/4    | 0.89 | 0.10 | 144,144,145,145             | 0     |
| 18  | BOG  | D     | 2009 | 20/20  | 0.90 | 0.12 | 53,59,62,64                 | 0     |
| 16  | GOL  | C     | 2011 | 6/6    | 0.91 | 0.21 | 67,70,72,72                 | 0     |
| 13  | JZV  | C     | 2001 | 29/29  | 0.91 | 0.14 | 38,46,86,87                 | 0     |
| 17  | HEC  | Q     | 501  | 43/43  | 0.97 | 0.10 | 52,56,64,65                 | 0     |
| 17  | HEC  | D     | 501  | 43/43  | 0.98 | 0.06 | 21,29,34,35                 | 0     |
| 12  | HEM  | P     | 501  | 43/43  | 0.98 | 0.08 | 33,40,48,54                 | 0     |
| 12  | HEM  | P     | 502  | 43/43  | 0.98 | 0.08 | 29,41,54,59                 | 0     |
| 12  | HEM  | C     | 501  | 43/43  | 0.98 | 0.07 | 23,30,37,42                 | 0     |
| 19  | FES  | R     | 501  | 4/4    | 0.98 | 0.05 | 74,76,77,78                 | 0     |
| 12  | HEM  | C     | 502  | 43/43  | 0.99 | 0.07 | 24,27,35,41                 | 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.

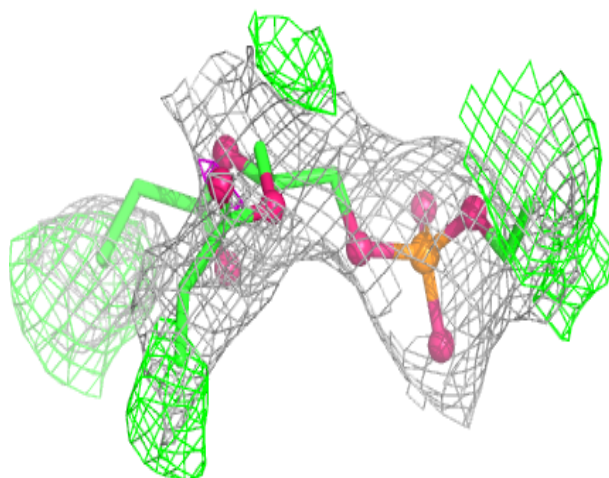
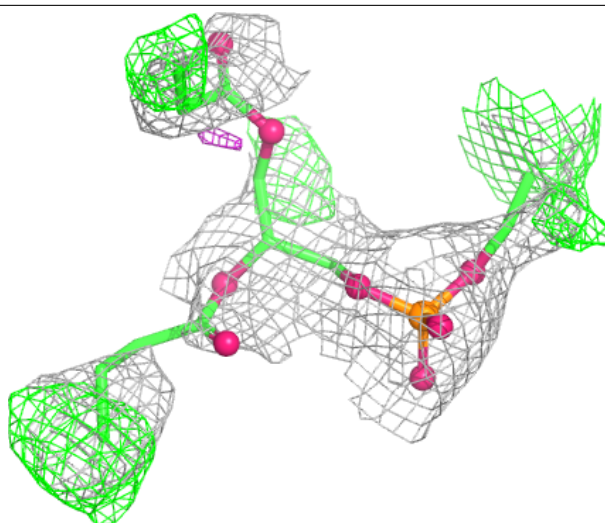
**Electron density around BOG Q 3091:**

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



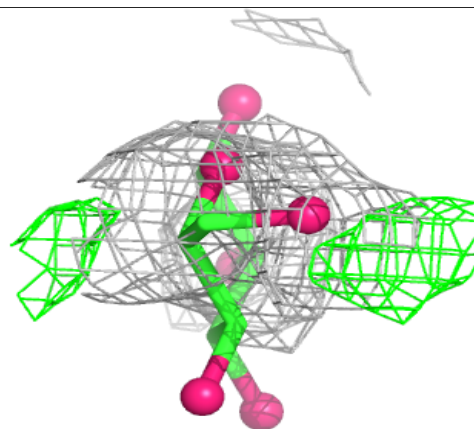
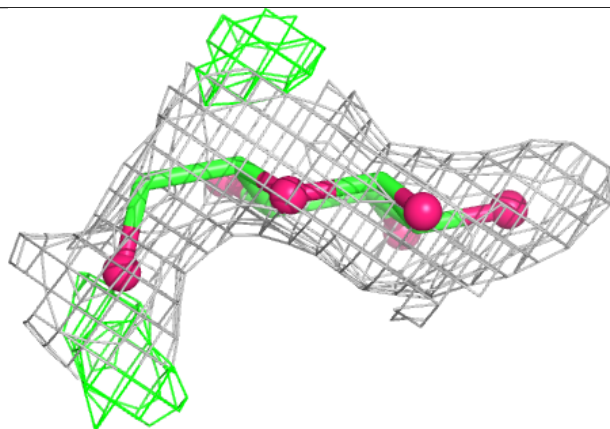
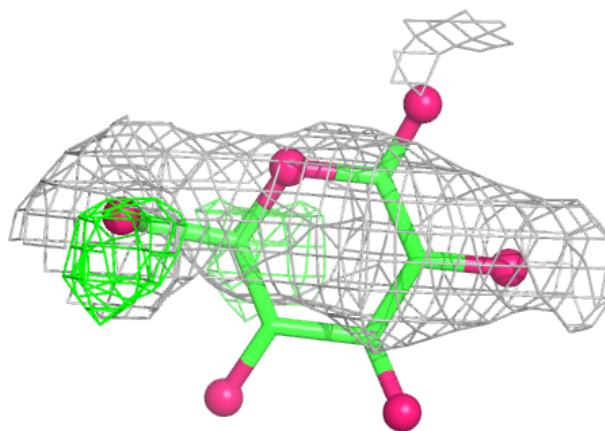
**Electron density around PEE A 2008:**

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



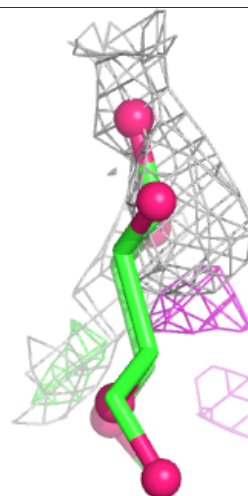
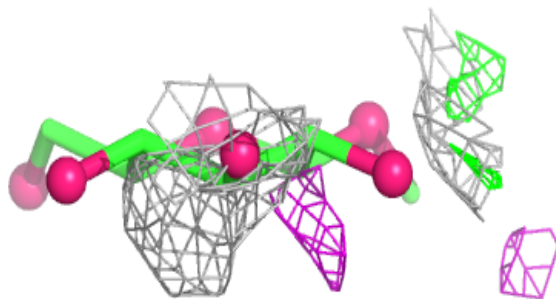
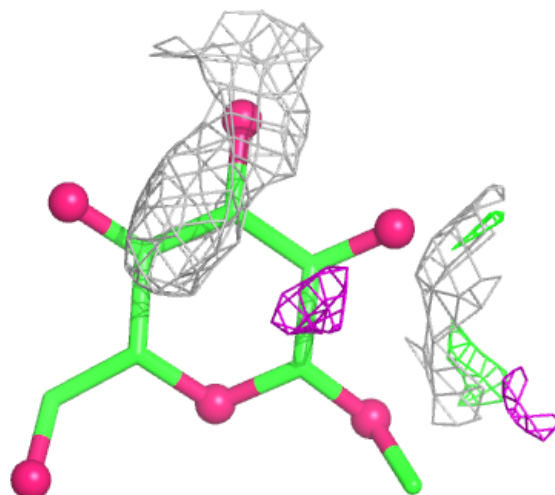
**Electron density around BOG P 2010:**

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



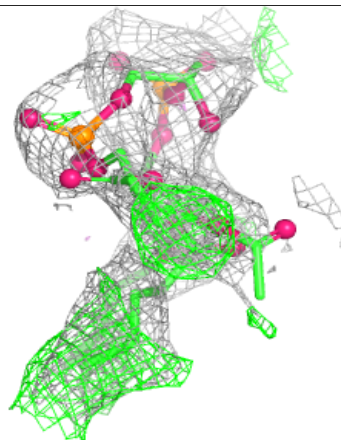
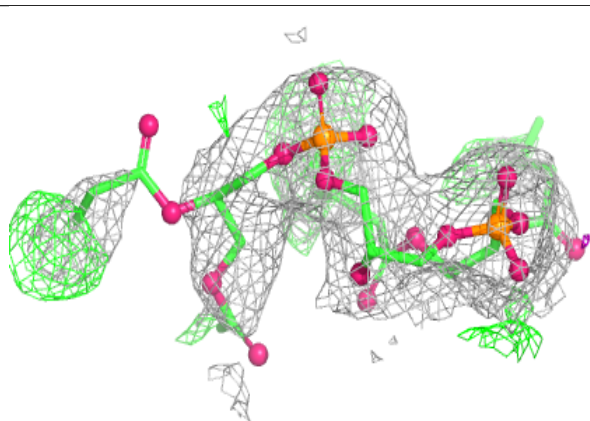
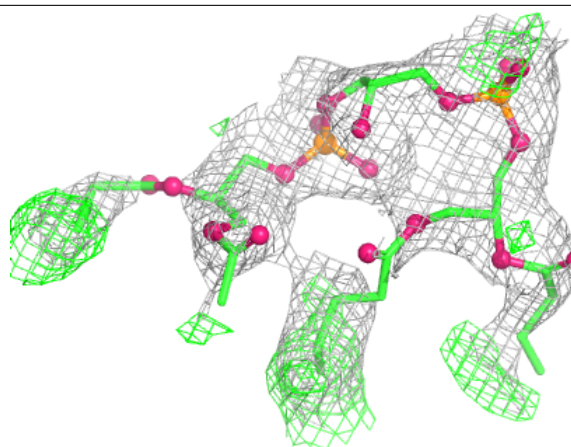
**Electron density around BOG D 2091:**

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



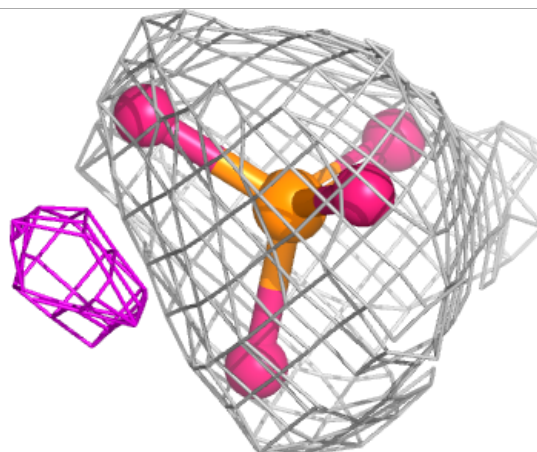
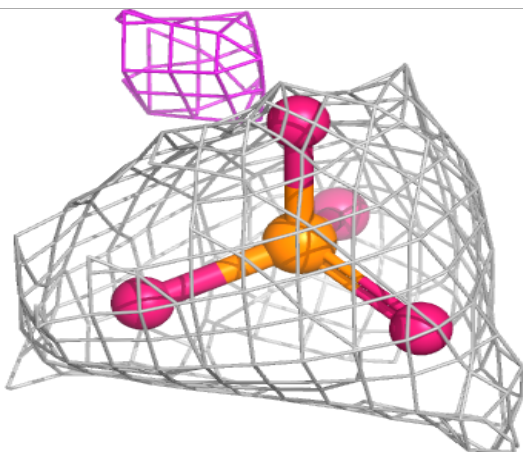
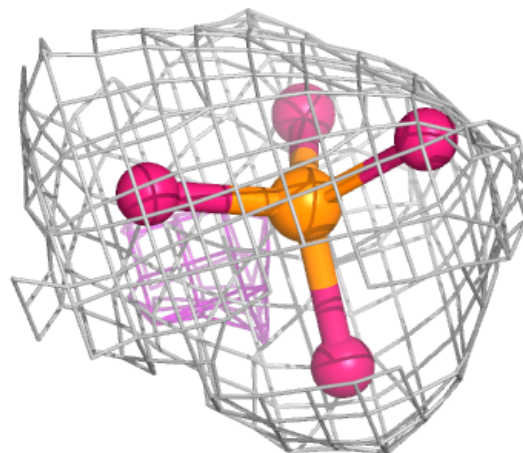
**Electron density around CDL Q 3003:**

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



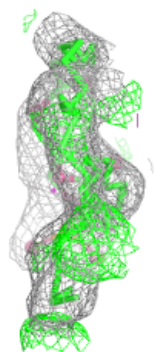
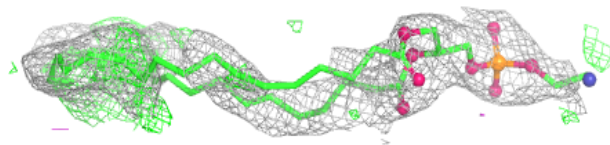
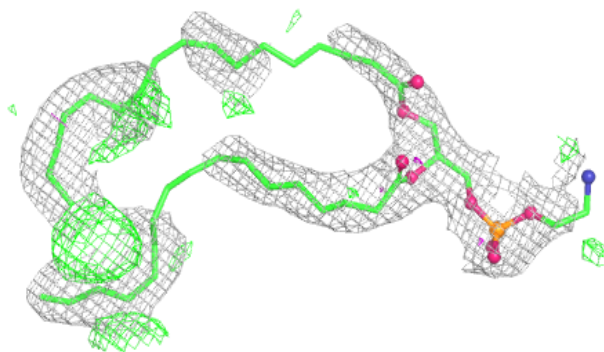
**Electron density around PEE N 3008:**

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



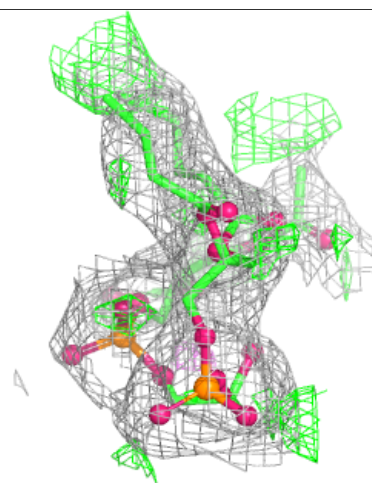
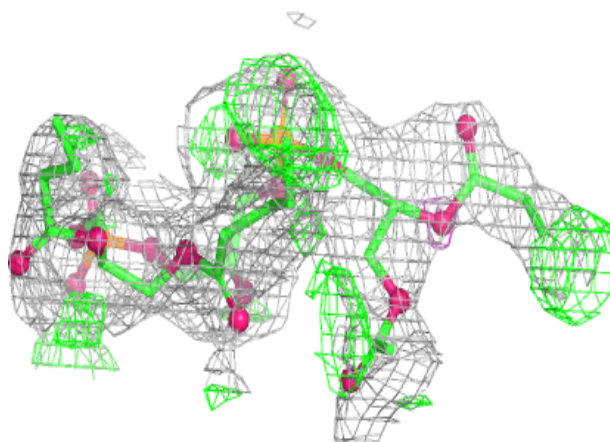
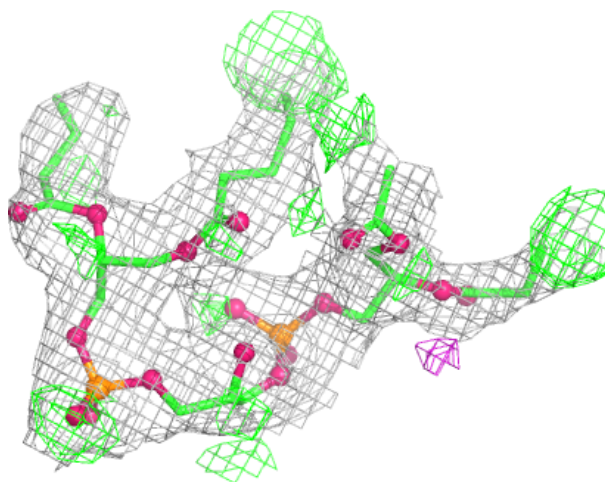
**Electron density around PEE P 3007:**

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



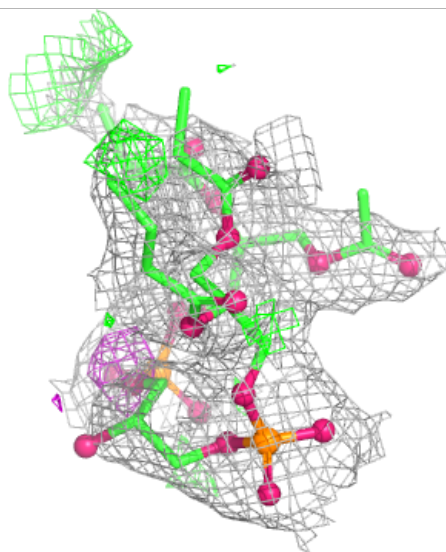
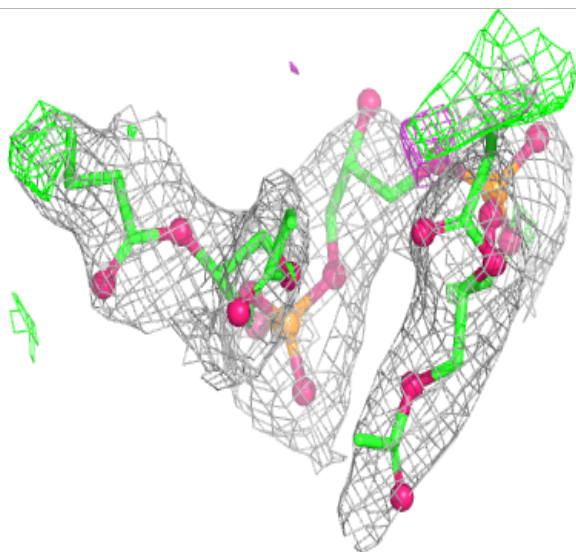
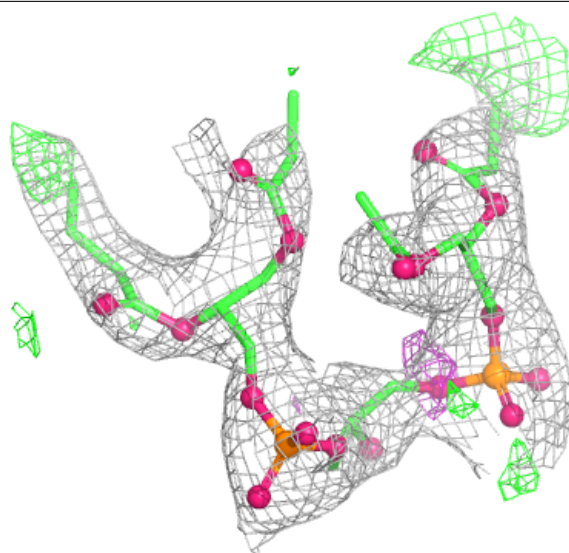
**Electron density around CDL D 2003:**

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



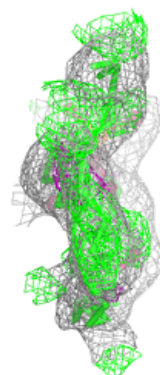
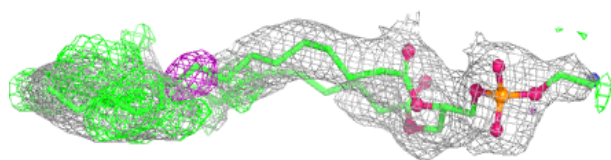
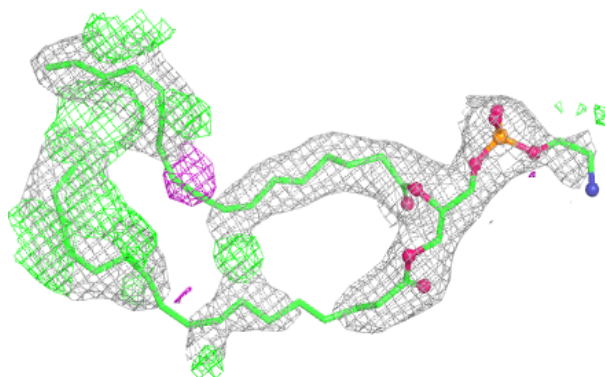
**Electron density around CDL P 3004:**

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

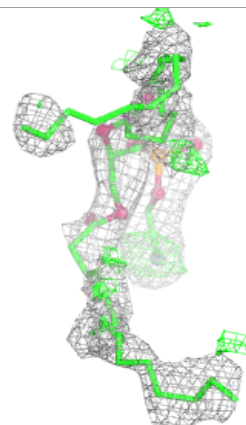
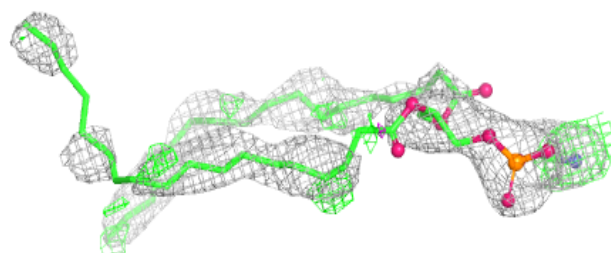
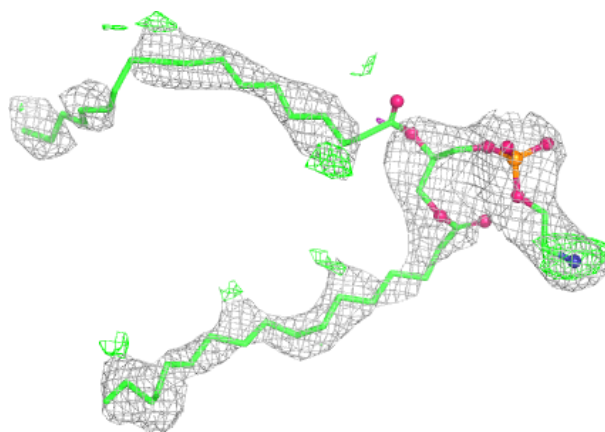


**Electron density around PEE C 2007:**

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

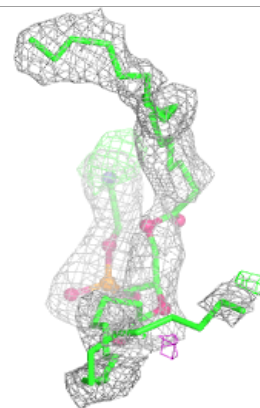
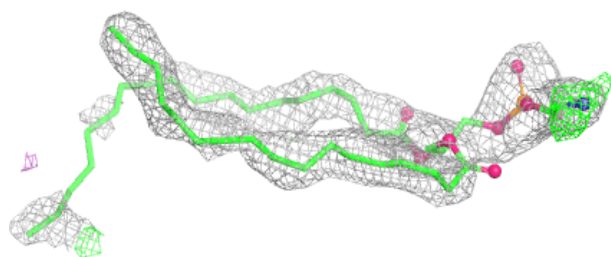
**Electron density around PEE R 3005:**

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

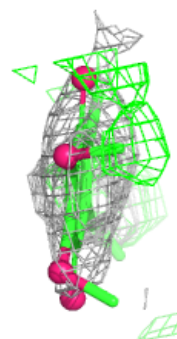
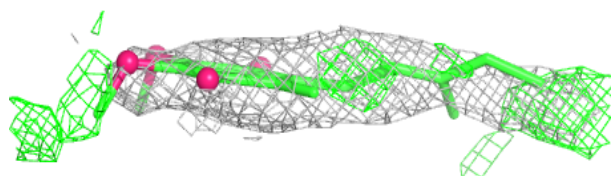
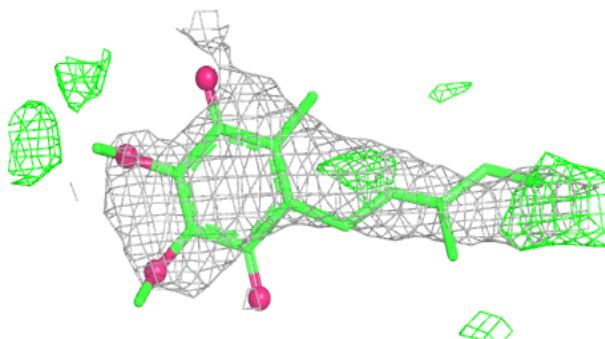


**Electron density around PEE E 2005:**

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and green (positive)

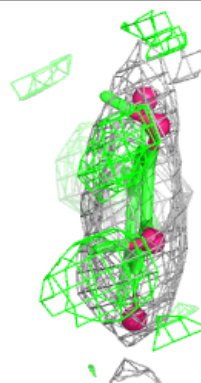
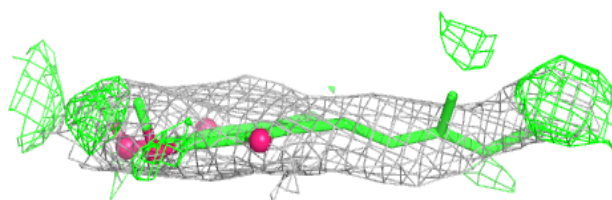
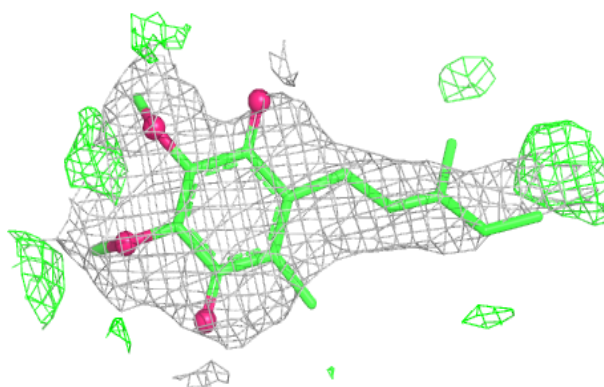
**Electron density around UQ P 3002:**

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and green (positive)

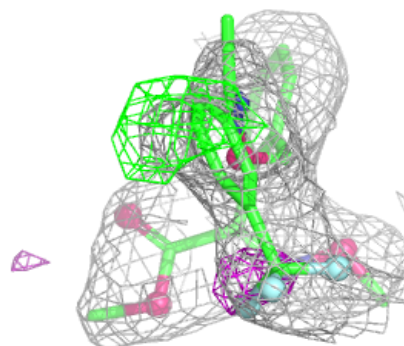
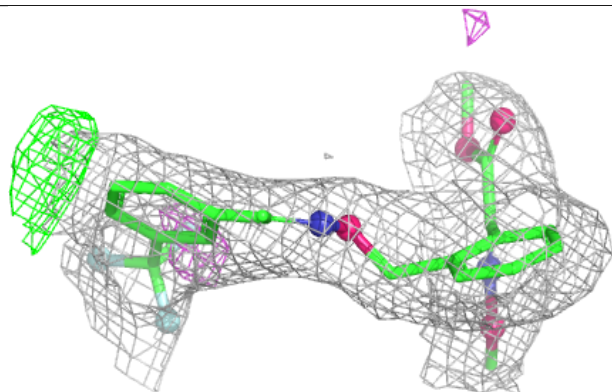
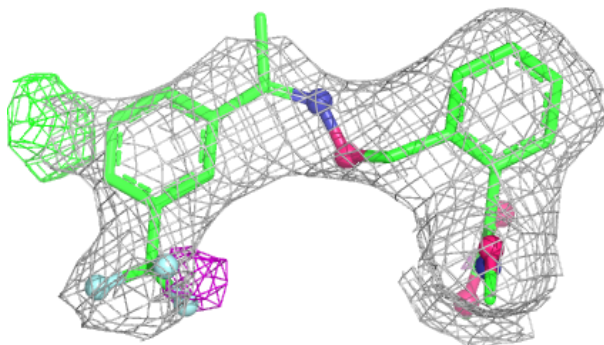


**Electron density around UQ C 2002:**

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and green (positive)

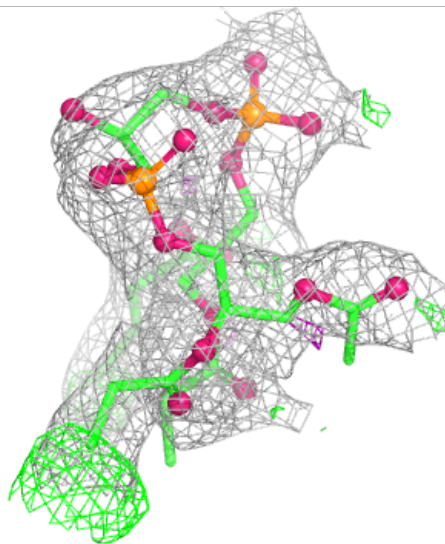
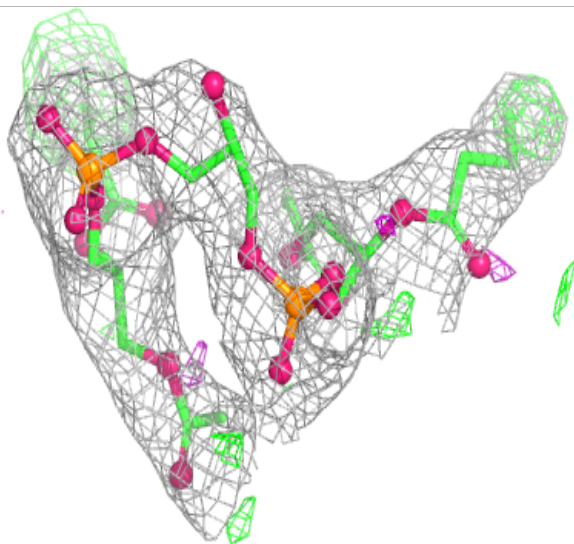
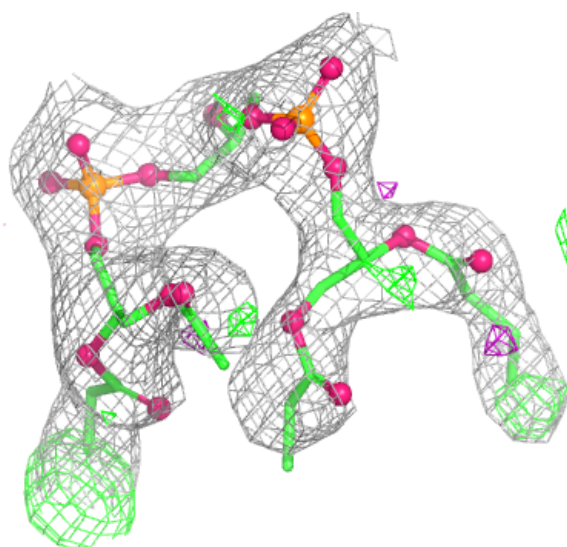
**Electron density around JZV P 3001:**

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



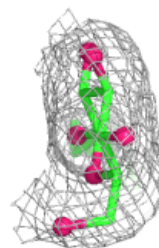
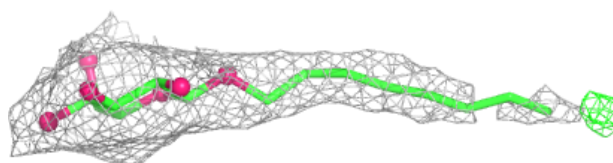
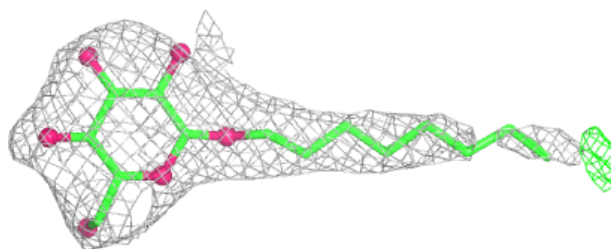
**Electron density around CDL C 2004:**

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

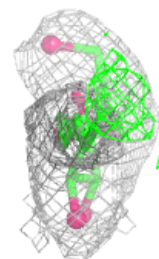


**Electron density around BOG Q 3009:**

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and green (positive)

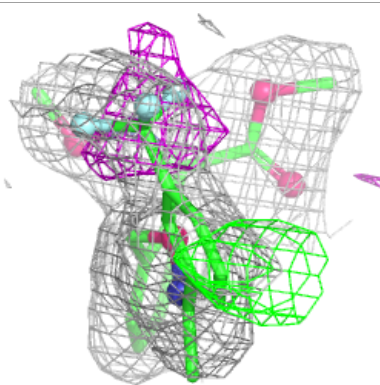
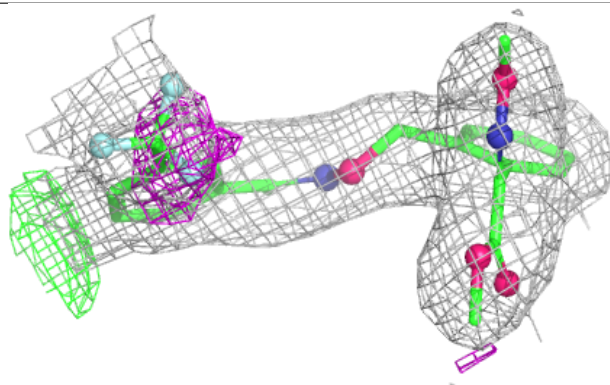
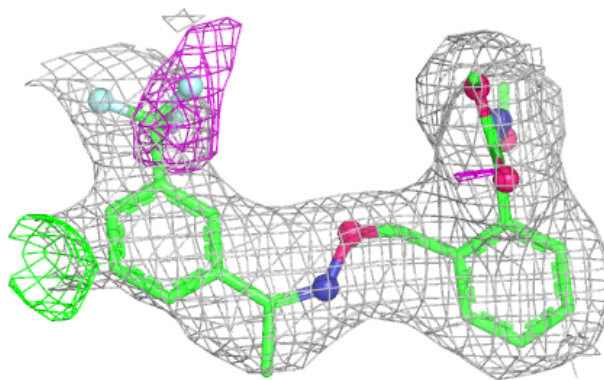
**Electron density around BOG D 2009:**

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and green (positive)

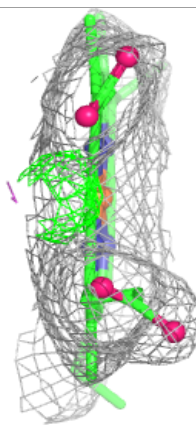
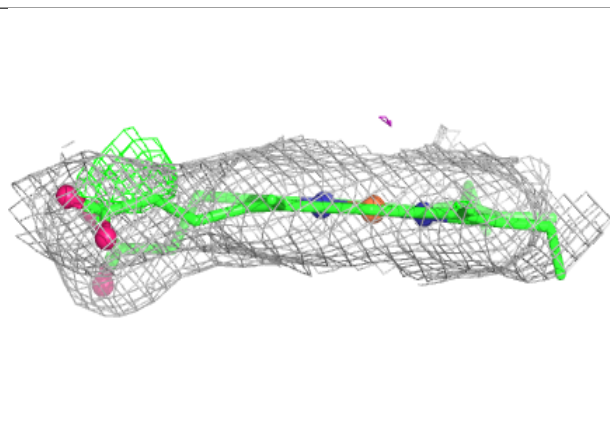
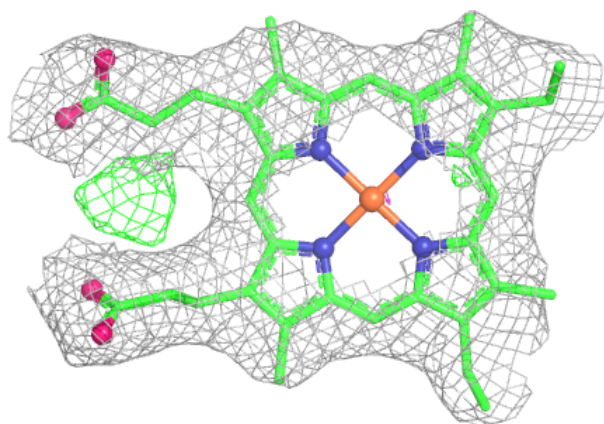


**Electron density around JZV C 2001:**

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

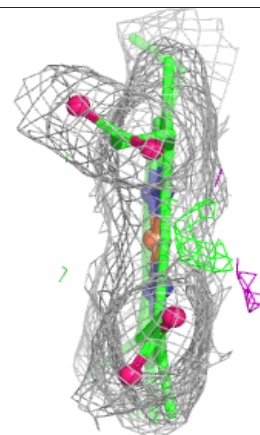
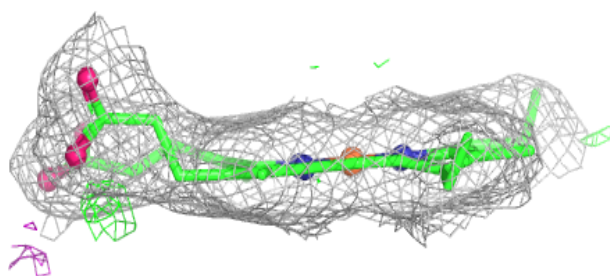
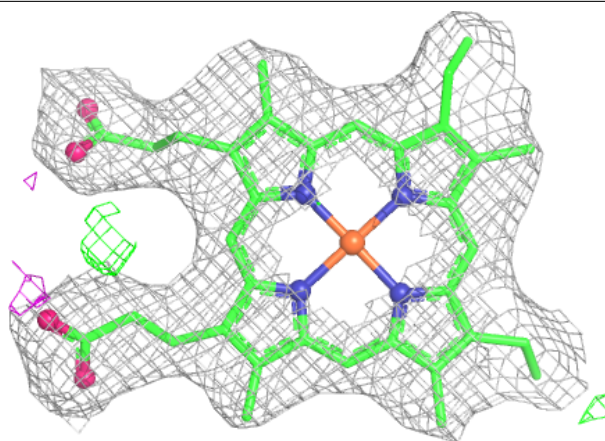
**Electron density around HEC Q 501:**

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and green (positive)



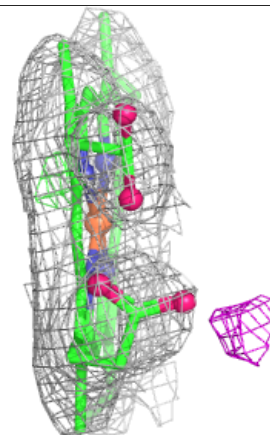
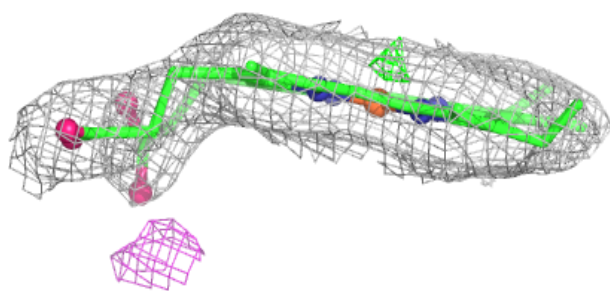
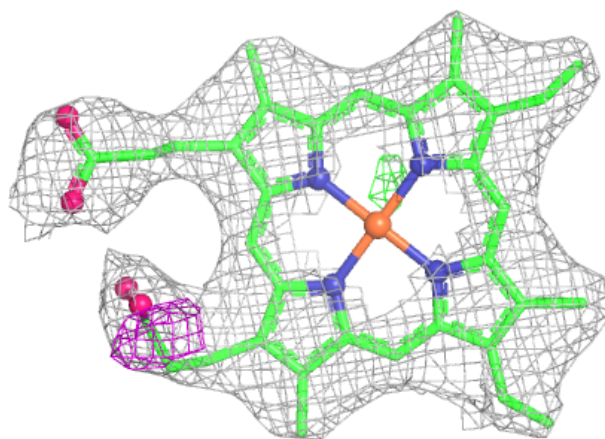
**Electron density around HEC D 501:**

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



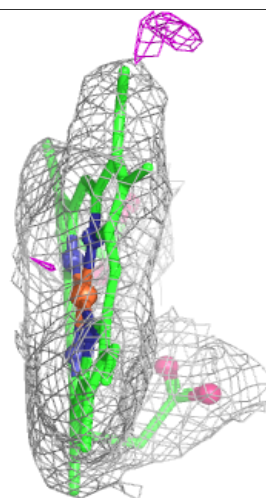
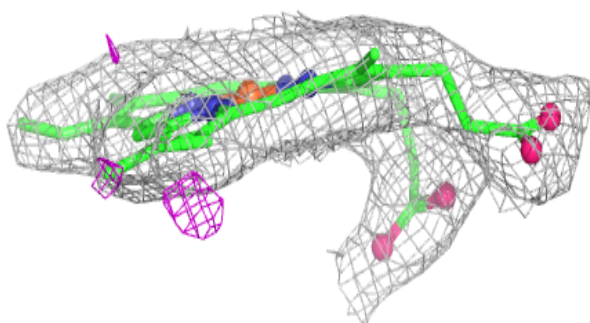
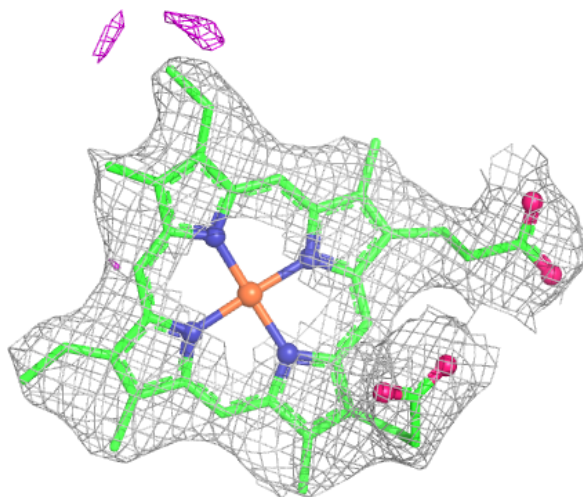
**Electron density around HEM P 501:**

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



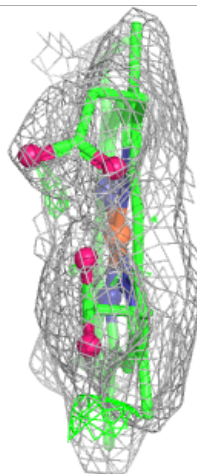
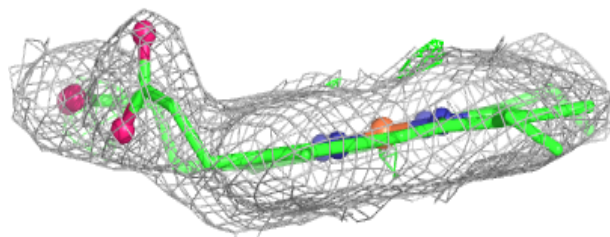
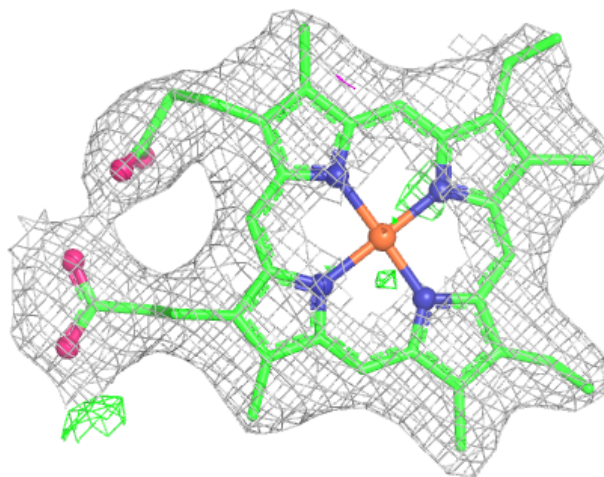
**Electron density around HEM P 502:**

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



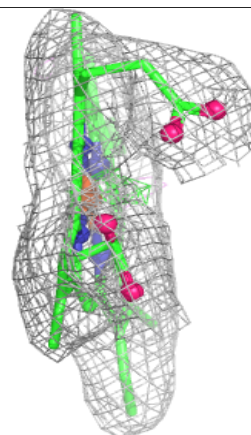
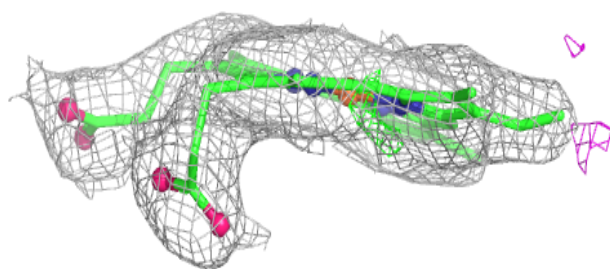
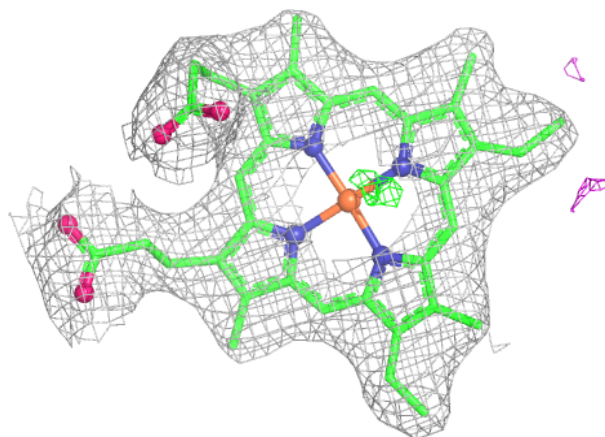
**Electron density around HEM C 501:**

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



**Electron density around HEM C 502:**

$2mF_o-DF_c$  (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.