



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 PM UTC

PDB ID : 1JQY / pdb\_00001jqy  
Title : HEAT-LABILE ENTEROTOXIN B-PENTAMER WITH LIGAND BMSC-0010  
Authors : Merritt, E.A.; Hol, W.G.J.  
Deposited on : 2001-08-09  
Resolution : 2.14 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:

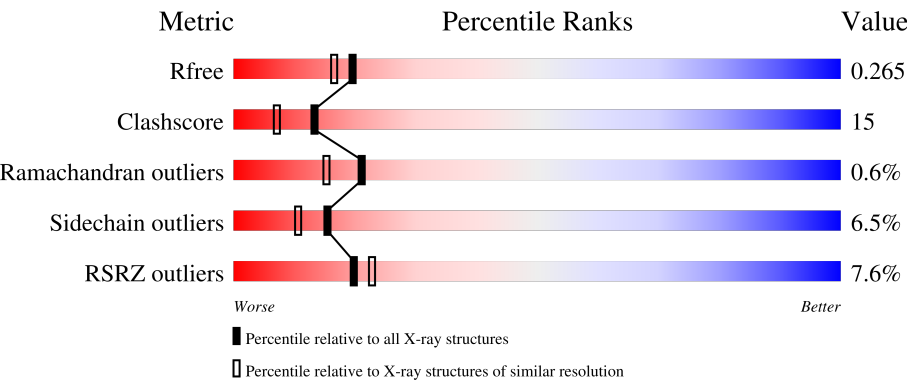
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 2.14 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 <sub>free</sub>     | 180053                      | 3689 (2.16-2.12)                                      |
| Clashscore            | 190562                      | 3812 (2.16-2.12)                                      |
| Ramachandran outliers | 187476                      | 3773 (2.16-2.12)                                      |
| Sidechain outliers    | 187428                      | 3772 (2.16-2.12)                                      |
| RSRZ outliers         | 180081                      | 3691 (2.16-2.12)                                      |

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   | D     | 103    | <div><div>%</div><div>61%32%. .</div></div>  |
| 1   | E     | 103    | <div><div>%</div><div>70%24%5% .</div></div> |
| 1   | F     | 103    | <div><div></div><div>65%28%6% .</div></div>  |
| 1   | G     | 103    | <div><div>3%</div><div>63%29%8%</div></div>  |
| 1   | H     | 103    | <div><div>%</div><div>61%32%5% .</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | L     | 103    |                  |
| 1   | M     | 103    |                  |
| 1   | N     | 103    |                  |
| 1   | O     | 103    |                  |
| 1   | P     | 103    |                  |
| 1   | V     | 103    |                  |
| 1   | W     | 103    |                  |
| 1   | X     | 103    |                  |
| 1   | Y     | 103    |                  |
| 1   | Z     | 103    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | A32  | V     | 104 | X         | -        | -       | -                |

## 2 Entry composition

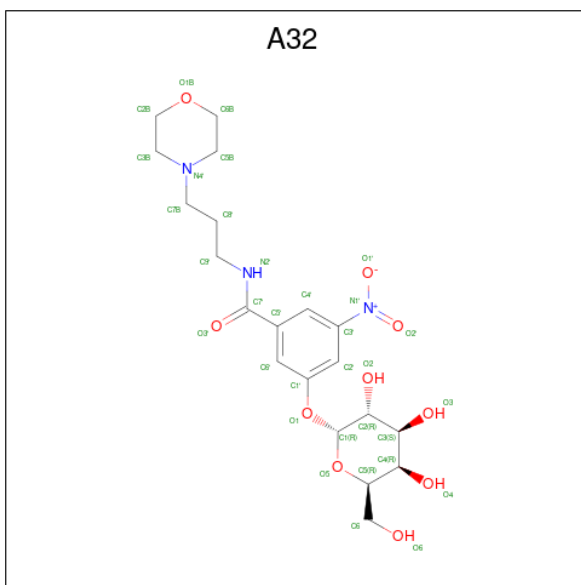
There are 3 unique types of molecules in this entry. The entry contains 13904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEAT-LABILE ENTEROTOXIN B CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | D     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | E     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | F     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | G     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | H     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | L     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | M     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | N     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | O     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | P     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | V     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | W     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | X     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | Y     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |
| 1   | Z     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 516 | 139 | 163 | 6 |         |         |       |

- Molecule 2 is (3-NITRO-5-(3-MORPHOLIN-4-YL-PROPYLAMINOCARBONYL)PHENYL)-GALACTOPYRANOSIDE (CCD ID: A32) (formula: C<sub>20</sub>H<sub>29</sub>N<sub>3</sub>O<sub>10</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 2   | D     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | E     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | F     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | G     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | H     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | L     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | M     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | O     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | P     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | V     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | W     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | X     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | Y     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |
| 2   | Z     | 1        | Total<br>33 | C<br>20 | N<br>3 | O<br>10 | 0       | 0       |

- Molecule 3 is water.

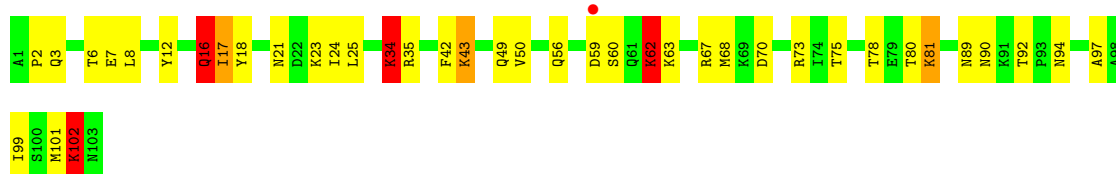
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | D     | 89       | Total<br>89  | O<br>89  | 0       | 0       |
| 3   | E     | 87       | Total<br>87  | O<br>87  | 0       | 0       |
| 3   | F     | 113      | Total<br>113 | O<br>113 | 0       | 0       |
| 3   | G     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 3   | H     | 100      | Total<br>100 | O<br>100 | 0       | 0       |
| 3   | L     | 51       | Total<br>51  | O<br>51  | 0       | 0       |
| 3   | M     | 49       | Total<br>49  | O<br>49  | 0       | 0       |
| 3   | N     | 65       | Total<br>65  | O<br>65  | 0       | 0       |
| 3   | O     | 75       | Total<br>75  | O<br>75  | 0       | 0       |
| 3   | P     | 80       | Total<br>80  | O<br>80  | 0       | 0       |
| 3   | V     | 41       | Total<br>41  | O<br>41  | 0       | 0       |
| 3   | W     | 49       | Total<br>49  | O<br>49  | 0       | 0       |
| 3   | X     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 3   | Y     | 63       | Total<br>63  | O<br>63  | 0       | 0       |
| 3   | Z     | 61       | Total<br>61  | O<br>61  | 0       | 0       |

### 3 Residue-property plots

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

- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain D: 



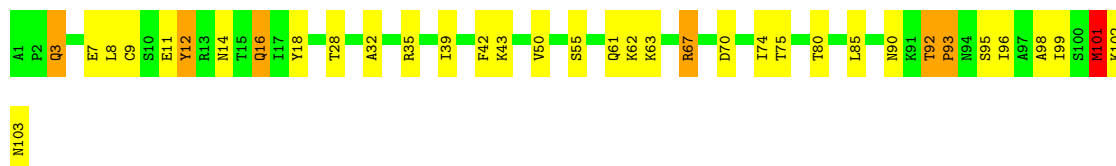
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain E: 



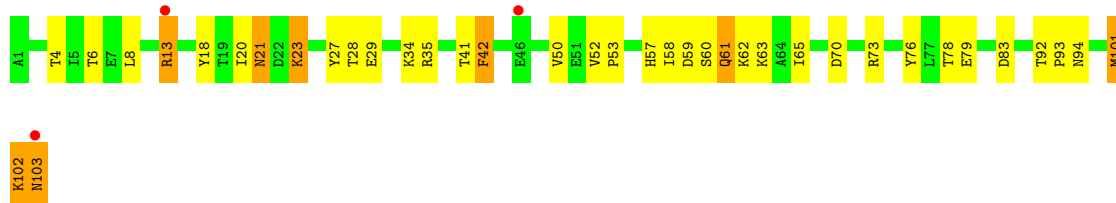
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain F: 

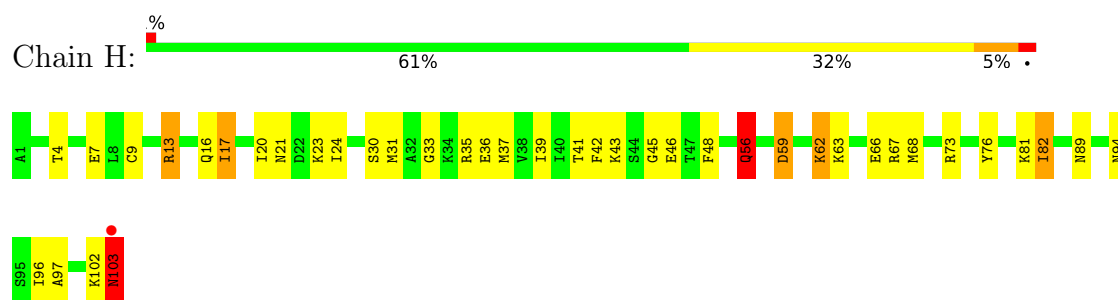


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

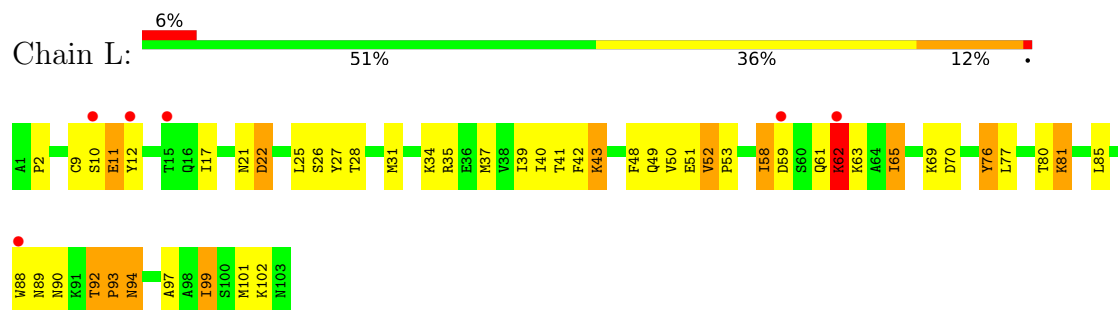
Chain G: 



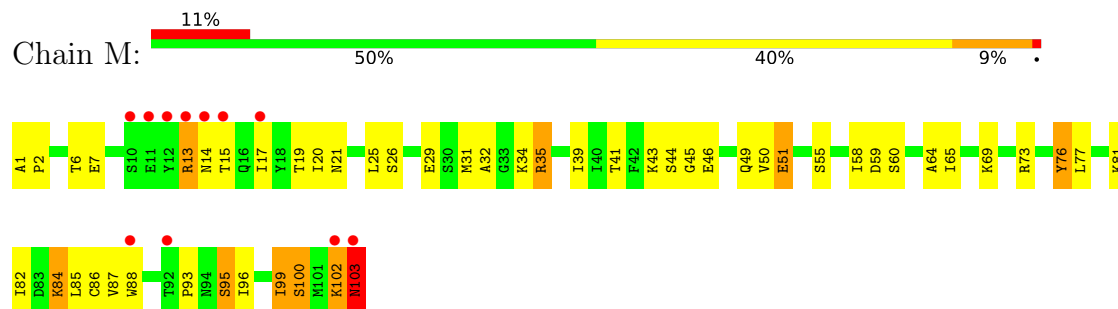
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



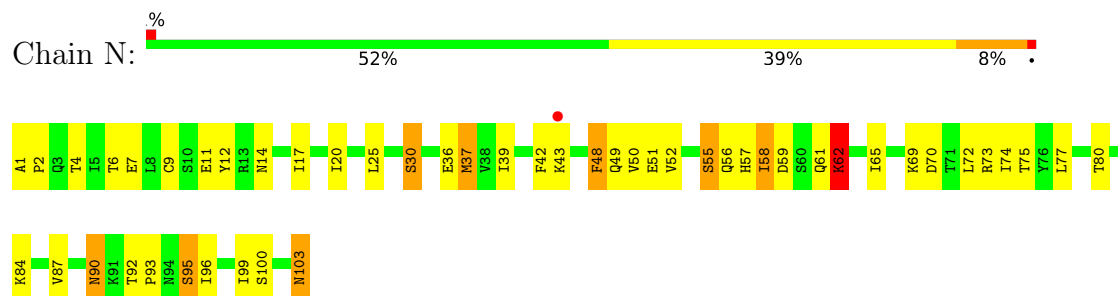
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



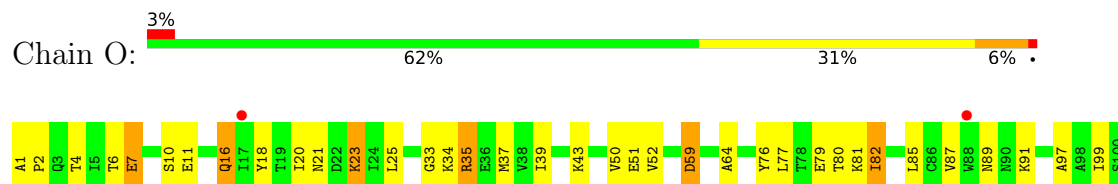
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



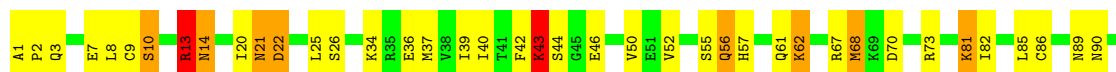
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN





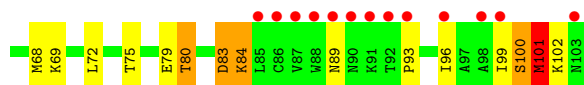
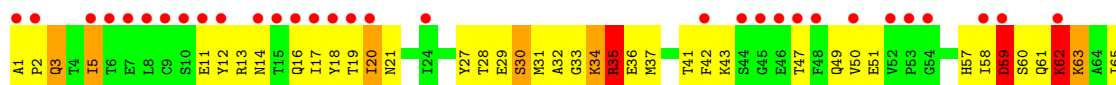
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain P: 57% 31% 10% .



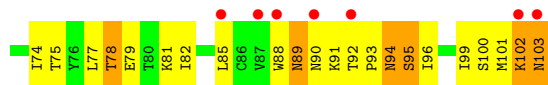
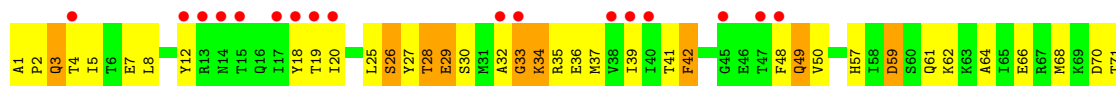
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain V: 43% 47% 40% 10% .



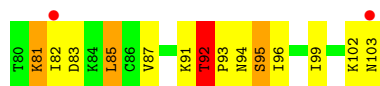
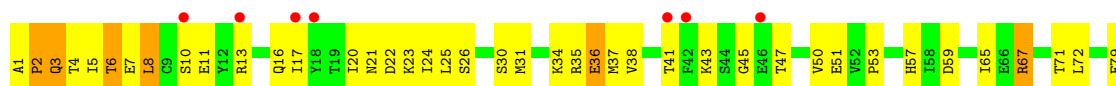
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain W: 23% 42% 44% 15% .



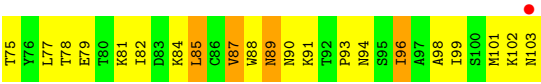
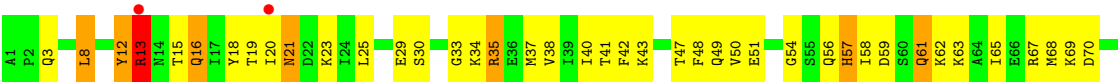
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain X: 9% 47% 44% 9% .

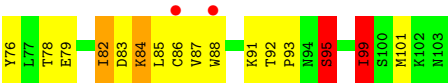
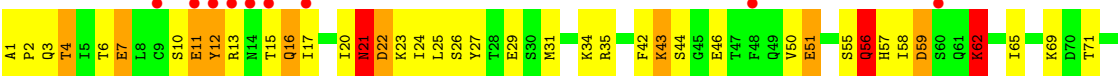


• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain Y: 3% 40% 49% 11% .



● Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 64.99Å 166.01Å 74.42Å<br>90.00° 92.13° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 25.00 – 2.14<br>25.00 – 2.14                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (25.00-2.14)<br>97.2 (25.00-2.14)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.05                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.46 (at 2.15Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.211 , 0.284<br>0.200 , 0.265                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4235 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 23.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.186                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 59.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.038 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 13904                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: A32

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   | D     | 1.10         | 0/835   | 2.19        | 31/1124 (2.8%)   |
| 1   | E     | 1.09         | 0/835   | 2.13        | 23/1124 (2.0%)   |
| 1   | F     | 1.11         | 0/835   | 2.17        | 35/1124 (3.1%)   |
| 1   | G     | 1.04         | 0/835   | 2.29        | 44/1124 (3.9%)   |
| 1   | H     | 1.06         | 0/835   | 2.35        | 52/1124 (4.6%)   |
| 1   | L     | 0.84         | 0/835   | 2.02        | 27/1124 (2.4%)   |
| 1   | M     | 0.80         | 0/835   | 2.13        | 28/1124 (2.5%)   |
| 1   | N     | 1.00         | 0/835   | 2.23        | 47/1124 (4.2%)   |
| 1   | O     | 0.88         | 0/835   | 1.99        | 22/1124 (2.0%)   |
| 1   | P     | 1.03         | 0/835   | 2.33        | 36/1124 (3.2%)   |
| 1   | V     | 0.68         | 0/835   | 1.84        | 20/1124 (1.8%)   |
| 1   | W     | 0.77         | 0/835   | 2.12        | 37/1124 (3.3%)   |
| 1   | X     | 0.96         | 0/835   | 2.33        | 47/1124 (4.2%)   |
| 1   | Y     | 0.94         | 0/835   | 2.16        | 35/1124 (3.1%)   |
| 1   | Z     | 0.88         | 0/835   | 2.11        | 33/1124 (2.9%)   |
| All | All   | 0.95         | 0/12525 | 2.16        | 517/16860 (3.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | N     | 0                   | 1                   |

There are no bond length outliers.

All (517) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | P     | 13  | ARG  | CD-NE-CZ | 21.03 | 153.84      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | E     | 103 | ASN  | CA-CB-CG   | 16.98  | 129.58      | 112.60   |
| 1   | F     | 35  | ARG  | CD-NE-CZ   | 15.91  | 146.68      | 124.40   |
| 1   | D     | 43  | LYS  | CA-CB-CG   | 14.11  | 142.32      | 114.10   |
| 1   | H     | 102 | LYS  | CA-C-O     | 13.75  | 137.46      | 120.54   |
| 1   | M     | 103 | ASN  | CA-CB-CG   | 13.08  | 125.68      | 112.60   |
| 1   | H     | 13  | ARG  | CD-NE-CZ   | 12.80  | 142.32      | 124.40   |
| 1   | P     | 13  | ARG  | CG-CD-NE   | 12.17  | 138.77      | 112.00   |
| 1   | V     | 59  | ASP  | CA-CB-CG   | 11.71  | 124.31      | 112.60   |
| 1   | M     | 21  | ASN  | CA-CB-CG   | 11.17  | 123.77      | 112.60   |
| 1   | G     | 103 | ASN  | CA-CB-CG   | 11.06  | 123.67      | 112.60   |
| 1   | P     | 73  | ARG  | NE-CZ-NH1  | 10.96  | 132.46      | 121.50   |
| 1   | P     | 67  | ARG  | CD-NE-CZ   | 10.91  | 139.67      | 124.40   |
| 1   | N     | 96  | ILE  | CA-C-N     | 10.71  | 140.99      | 122.79   |
| 1   | N     | 96  | ILE  | C-N-CA     | 10.71  | 140.99      | 122.79   |
| 1   | D     | 16  | GLN  | OE1-CD-NE2 | -10.31 | 112.29      | 122.60   |
| 1   | P     | 73  | ARG  | NE-CZ-NH2  | -9.99  | 110.21      | 119.20   |
| 1   | W     | 68  | MET  | CA-C-O     | -9.89  | 109.94      | 120.42   |
| 1   | D     | 59  | ASP  | CA-CB-CG   | 9.67   | 122.27      | 112.60   |
| 1   | W     | 48  | PHE  | CA-CB-CG   | -9.46  | 104.34      | 113.80   |
| 1   | N     | 58  | ILE  | CA-C-N     | 9.11   | 134.49      | 120.82   |
| 1   | N     | 58  | ILE  | C-N-CA     | 9.11   | 134.49      | 120.82   |
| 1   | E     | 81  | LYS  | CA-CB-CG   | 9.04   | 132.17      | 114.10   |
| 1   | Z     | 22  | ASP  | CA-C-O     | -9.02  | 111.63      | 121.28   |
| 1   | O     | 6   | THR  | CA-C-O     | -8.97  | 111.30      | 120.90   |
| 1   | X     | 6   | THR  | CA-C-O     | -8.86  | 111.16      | 120.55   |
| 1   | P     | 68  | MET  | CA-C-O     | 8.82   | 129.90      | 120.55   |
| 1   | N     | 72  | LEU  | CA-C-O     | -8.80  | 111.58      | 120.82   |
| 1   | X     | 57  | HIS  | CA-CB-CG   | -8.71  | 105.09      | 113.80   |
| 1   | P     | 73  | ARG  | CD-NE-CZ   | 8.62   | 136.47      | 124.40   |
| 1   | W     | 50  | VAL  | N-CA-C     | -8.53  | 92.91       | 107.24   |
| 1   | P     | 7   | GLU  | CA-CB-CG   | 8.50   | 131.10      | 114.10   |
| 1   | L     | 59  | ASP  | CA-CB-CG   | 8.45   | 121.05      | 112.60   |
| 1   | M     | 35  | ARG  | CD-NE-CZ   | 8.40   | 136.16      | 124.40   |
| 1   | G     | 102 | LYS  | CA-CB-CG   | 8.36   | 130.83      | 114.10   |
| 1   | M     | 50  | VAL  | N-CA-CB    | 8.30   | 121.92      | 111.46   |
| 1   | P     | 90  | ASN  | OD1-CG-ND2 | -8.26  | 114.34      | 122.60   |
| 1   | N     | 58  | ILE  | O-C-N      | -8.24  | 114.05      | 122.54   |
| 1   | Z     | 35  | ARG  | NE-CZ-NH2  | -8.20  | 111.82      | 119.20   |
| 1   | V     | 83  | ASP  | CA-CB-CG   | -8.17  | 104.43      | 112.60   |
| 1   | H     | 45  | GLY  | N-CA-C     | 8.13   | 124.36      | 114.69   |
| 1   | V     | 62  | LYS  | CA-C-O     | -8.08  | 112.26      | 120.90   |
| 1   | X     | 22  | ASP  | CA-CB-CG   | 8.00   | 120.60      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 102 | LYS  | CA-C-N     | 7.97  | 136.05      | 121.70   |
| 1   | H     | 102 | LYS  | C-N-CA     | 7.97  | 136.05      | 121.70   |
| 1   | H     | 33  | GLY  | O-C-N      | -7.92 | 112.41      | 122.70   |
| 1   | F     | 43  | LYS  | CA-C-N     | 7.91  | 133.93      | 120.72   |
| 1   | F     | 43  | LYS  | C-N-CA     | 7.91  | 133.93      | 120.72   |
| 1   | N     | 95  | SER  | CA-C-N     | -7.76 | 110.12      | 120.91   |
| 1   | N     | 95  | SER  | C-N-CA     | -7.76 | 110.12      | 120.91   |
| 1   | D     | 92  | THR  | CB-CA-C    | -7.75 | 96.75       | 109.15   |
| 1   | G     | 94  | ASN  | OD1-CG-ND2 | 7.69  | 130.29      | 122.60   |
| 1   | G     | 65  | ILE  | CA-C-O     | -7.68 | 112.97      | 120.95   |
| 1   | F     | 61  | GLN  | OE1-CD-NE2 | 7.63  | 130.23      | 122.60   |
| 1   | Z     | 12  | TYR  | N-CA-C     | 7.58  | 121.79      | 109.59   |
| 1   | F     | 18  | TYR  | CA-C-O     | -7.56 | 112.19      | 120.36   |
| 1   | G     | 61  | GLN  | OE1-CD-NE2 | 7.52  | 130.12      | 122.60   |
| 1   | Y     | 8   | LEU  | CA-C-O     | -7.50 | 112.94      | 120.82   |
| 1   | L     | 94  | ASN  | CA-CB-CG   | 7.48  | 120.08      | 112.60   |
| 1   | F     | 9   | CYS  | CA-C-O     | -7.45 | 111.68      | 120.10   |
| 1   | Y     | 75  | THR  | CA-C-O     | 7.44  | 128.43      | 120.55   |
| 1   | Z     | 71  | THR  | CA-CB-OG1  | -7.43 | 98.46       | 109.60   |
| 1   | X     | 16  | GLN  | CB-CG-CD   | 7.42  | 125.20      | 112.60   |
| 1   | Y     | 50  | VAL  | N-CA-C     | -7.37 | 97.82       | 108.36   |
| 1   | V     | 29  | GLU  | CA-C-N     | -7.33 | 111.94      | 122.94   |
| 1   | V     | 29  | GLU  | C-N-CA     | -7.33 | 111.94      | 122.94   |
| 1   | W     | 75  | THR  | O-C-N      | -7.33 | 113.68      | 122.11   |
| 1   | Y     | 56  | GLN  | OE1-CD-NE2 | -7.33 | 115.27      | 122.60   |
| 1   | G     | 28  | THR  | CA-C-O     | -7.32 | 112.80      | 120.70   |
| 1   | E     | 35  | ARG  | NE-CZ-NH2  | -7.28 | 112.65      | 119.20   |
| 1   | X     | 95  | SER  | CA-C-N     | -7.28 | 110.95      | 120.63   |
| 1   | X     | 95  | SER  | C-N-CA     | -7.28 | 110.95      | 120.63   |
| 1   | N     | 100 | SER  | CA-C-N     | 7.27  | 134.54      | 122.33   |
| 1   | N     | 100 | SER  | C-N-CA     | 7.27  | 134.54      | 122.33   |
| 1   | D     | 67  | ARG  | NE-CZ-NH2  | -7.26 | 112.66      | 119.20   |
| 1   | N     | 90  | ASN  | CA-C-O     | 7.23  | 128.17      | 119.78   |
| 1   | Z     | 12  | TYR  | CA-C-O     | 7.23  | 128.37      | 120.71   |
| 1   | N     | 77  | LEU  | CA-C-O     | -7.22 | 110.49      | 119.38   |
| 1   | V     | 37  | MET  | N-CA-C     | 7.20  | 118.10      | 108.38   |
| 1   | W     | 3   | GLN  | CA-CB-CG   | 7.19  | 128.48      | 114.10   |
| 1   | D     | 73  | ARG  | CA-C-O     | -7.19 | 113.30      | 120.70   |
| 1   | N     | 70  | ASP  | CA-CB-CG   | 7.19  | 119.79      | 112.60   |
| 1   | G     | 42  | PHE  | CA-CB-CG   | -7.18 | 106.62      | 113.80   |
| 1   | Y     | 57  | HIS  | CA-CB-CG   | -7.16 | 106.64      | 113.80   |
| 1   | W     | 62  | LYS  | CA-C-O     | -7.14 | 113.32      | 120.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | P     | 62  | LYS  | N-CA-CB    | 7.12  | 120.34      | 110.01   |
| 1   | F     | 35  | ARG  | NH1-CZ-NH2 | -7.11 | 110.06      | 119.30   |
| 1   | G     | 50  | VAL  | N-CA-CB    | 7.09  | 120.61      | 111.67   |
| 1   | Y     | 62  | LYS  | CA-C-O     | -7.05 | 113.41      | 120.82   |
| 1   | H     | 68  | MET  | N-CA-CB    | 7.05  | 120.23      | 110.01   |
| 1   | Y     | 50  | VAL  | N-CA-CB    | 7.05  | 119.45      | 110.99   |
| 1   | O     | 11  | GLU  | CA-CB-CG   | 7.03  | 128.15      | 114.10   |
| 1   | Z     | 99  | ILE  | CA-C-O     | 7.01  | 128.57      | 121.63   |
| 1   | H     | 23  | LYS  | CA-C-O     | -6.99 | 114.67      | 122.01   |
| 1   | G     | 83  | ASP  | CA-C-O     | -6.99 | 113.55      | 120.89   |
| 1   | M     | 59  | ASP  | N-CA-C     | 6.99  | 119.49      | 111.11   |
| 1   | X     | 92  | THR  | CA-CB-OG1  | 6.98  | 120.07      | 109.60   |
| 1   | N     | 51  | GLU  | N-CA-C     | 6.96  | 119.82      | 110.35   |
| 1   | P     | 99  | ILE  | O-C-N      | -6.96 | 115.55      | 123.00   |
| 1   | Y     | 67  | ARG  | CA-C-O     | -6.96 | 113.05      | 120.42   |
| 1   | Y     | 96  | ILE  | CA-C-O     | 6.95  | 128.67      | 121.23   |
| 1   | X     | 72  | LEU  | CA-C-N     | 6.93  | 129.45      | 120.44   |
| 1   | X     | 72  | LEU  | C-N-CA     | 6.93  | 129.45      | 120.44   |
| 1   | Z     | 21  | ASN  | CA-CB-CG   | -6.91 | 105.69      | 112.60   |
| 1   | G     | 94  | ASN  | CB-CG-ND2  | -6.85 | 106.12      | 116.40   |
| 1   | X     | 92  | THR  | CA-C-O     | 6.83  | 129.52      | 120.16   |
| 1   | O     | 59  | ASP  | CA-CB-CG   | -6.82 | 105.78      | 112.60   |
| 1   | O     | 37  | MET  | N-CA-C     | 6.82  | 119.12      | 108.96   |
| 1   | H     | 68  | MET  | O-C-N      | 6.80  | 129.08      | 122.07   |
| 1   | X     | 16  | GLN  | OE1-CD-NE2 | -6.80 | 115.80      | 122.60   |
| 1   | Z     | 56  | GLN  | N-CA-C     | 6.77  | 119.23      | 111.11   |
| 1   | D     | 56  | GLN  | OE1-CD-NE2 | -6.77 | 115.83      | 122.60   |
| 1   | M     | 60  | SER  | CA-C-N     | 6.76  | 132.01      | 120.72   |
| 1   | M     | 60  | SER  | C-N-CA     | 6.76  | 132.01      | 120.72   |
| 1   | D     | 94  | ASN  | CA-CB-CG   | 6.76  | 119.36      | 112.60   |
| 1   | H     | 73  | ARG  | NE-CZ-NH2  | -6.75 | 113.12      | 119.20   |
| 1   | H     | 16  | GLN  | CG-CD-NE2  | 6.73  | 126.50      | 116.40   |
| 1   | N     | 55  | SER  | CA-C-O     | -6.73 | 113.70      | 120.90   |
| 1   | L     | 97  | ALA  | N-CA-C     | -6.71 | 105.09      | 113.55   |
| 1   | L     | 42  | PHE  | CA-CB-CG   | -6.70 | 107.10      | 113.80   |
| 1   | O     | 7   | GLU  | CA-CB-CG   | 6.70  | 127.50      | 114.10   |
| 1   | F     | 50  | VAL  | N-CA-C     | -6.70 | 98.21       | 107.99   |
| 1   | N     | 103 | ASN  | CA-CB-CG   | 6.68  | 119.28      | 112.60   |
| 1   | G     | 41  | THR  | CA-C-N     | 6.68  | 133.30      | 122.81   |
| 1   | G     | 41  | THR  | C-N-CA     | 6.68  | 133.30      | 122.81   |
| 1   | V     | 18  | TYR  | CA-CB-CG   | 6.67  | 125.92      | 113.90   |
| 1   | M     | 35  | ARG  | NE-CZ-NH2  | -6.67 | 113.20      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 10  | SER  | CB-CA-C    | 6.67  | 122.78      | 110.11   |
| 1   | H     | 17  | ILE  | CA-C-O     | -6.67 | 113.33      | 120.59   |
| 1   | M     | 73  | ARG  | CD-NE-CZ   | 6.66  | 133.72      | 124.40   |
| 1   | X     | 65  | ILE  | CA-C-O     | -6.63 | 114.14      | 121.17   |
| 1   | G     | 21  | ASN  | O-C-N      | -6.63 | 114.91      | 122.86   |
| 1   | Y     | 59  | ASP  | CA-CB-CG   | 6.63  | 119.23      | 112.60   |
| 1   | E     | 63  | LYS  | CA-CB-CG   | -6.62 | 100.86      | 114.10   |
| 1   | Y     | 63  | LYS  | N-CA-CB    | 6.60  | 121.34      | 110.39   |
| 1   | M     | 58  | ILE  | CA-C-O     | -6.54 | 116.51      | 121.68   |
| 1   | H     | 89  | ASN  | CB-CG-ND2  | 6.54  | 126.21      | 116.40   |
| 1   | O     | 52  | VAL  | O-C-N      | -6.53 | 113.89      | 121.07   |
| 1   | N     | 4   | THR  | CA-C-O     | -6.53 | 114.03      | 121.40   |
| 1   | Z     | 62  | LYS  | O-C-N      | 6.52  | 128.78      | 122.07   |
| 1   | P     | 22  | ASP  | CA-CB-CG   | 6.52  | 119.12      | 112.60   |
| 1   | D     | 78  | THR  | CA-CB-OG1  | -6.51 | 99.83       | 109.60   |
| 1   | Y     | 61  | GLN  | OE1-CD-NE2 | -6.51 | 116.09      | 122.60   |
| 1   | X     | 2   | PRO  | CA-C-N     | 6.51  | 133.74      | 122.09   |
| 1   | X     | 2   | PRO  | C-N-CA     | 6.51  | 133.74      | 122.09   |
| 1   | N     | 55  | SER  | CA-C-N     | 6.50  | 133.96      | 121.54   |
| 1   | N     | 55  | SER  | C-N-CA     | 6.50  | 133.96      | 121.54   |
| 1   | H     | 39  | ILE  | O-C-N      | -6.50 | 116.24      | 123.26   |
| 1   | L     | 49  | GLN  | CB-CG-CD   | 6.50  | 123.64      | 112.60   |
| 1   | H     | 35  | ARG  | NE-CZ-NH1  | -6.46 | 115.03      | 121.50   |
| 1   | Z     | 50  | VAL  | N-CA-C     | -6.46 | 99.12       | 108.36   |
| 1   | Z     | 51  | GLU  | N-CA-C     | 6.45  | 119.82      | 110.28   |
| 1   | W     | 18  | TYR  | CA-C-O     | -6.43 | 113.23      | 120.43   |
| 1   | F     | 62  | LYS  | CB-CG-CD   | 6.43  | 126.08      | 111.30   |
| 1   | L     | 52  | VAL  | CB-CA-C    | -6.43 | 104.58      | 110.88   |
| 1   | M     | 96  | ILE  | N-CA-CB    | 6.42  | 117.53      | 110.53   |
| 1   | O     | 11  | GLU  | CA-C-O     | 6.42  | 127.05      | 119.28   |
| 1   | W     | 49  | GLN  | CA-C-O     | 6.41  | 129.02      | 121.58   |
| 1   | Y     | 70  | ASP  | CA-C-O     | 6.41  | 127.55      | 120.82   |
| 1   | P     | 21  | ASN  | CA-CB-CG   | -6.40 | 106.20      | 112.60   |
| 1   | G     | 102 | LYS  | O-C-N      | -6.38 | 115.59      | 123.44   |
| 1   | H     | 63  | LYS  | CA-C-N     | 6.36  | 128.81      | 120.28   |
| 1   | H     | 63  | LYS  | C-N-CA     | 6.36  | 128.81      | 120.28   |
| 1   | F     | 92  | THR  | CB-CA-C    | -6.36 | 101.70      | 110.16   |
| 1   | P     | 52  | VAL  | CA-C-N     | 6.35  | 126.30      | 119.76   |
| 1   | P     | 52  | VAL  | C-N-CA     | 6.35  | 126.30      | 119.76   |
| 1   | W     | 95  | SER  | CA-C-O     | -6.35 | 113.32      | 120.43   |
| 1   | G     | 102 | LYS  | CA-C-N     | 6.33  | 133.09      | 121.70   |
| 1   | G     | 102 | LYS  | C-N-CA     | 6.33  | 133.09      | 121.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 51  | GLU  | N-CA-C     | 6.31  | 118.94      | 110.35   |
| 1   | H     | 89  | ASN  | OD1-CG-ND2 | -6.31 | 116.29      | 122.60   |
| 1   | F     | 67  | ARG  | NE-CZ-NH2  | -6.30 | 113.53      | 119.20   |
| 1   | L     | 27  | TYR  | O-C-N      | 6.29  | 130.57      | 123.27   |
| 1   | X     | 59  | ASP  | N-CA-C     | 6.29  | 119.80      | 111.75   |
| 1   | F     | 70  | ASP  | N-CA-CB    | 6.29  | 119.13      | 110.01   |
| 1   | D     | 92  | THR  | O-C-N      | 6.28  | 127.88      | 121.72   |
| 1   | Y     | 87  | VAL  | N-CA-C     | 6.28  | 117.81      | 108.46   |
| 1   | M     | 99  | ILE  | CA-C-O     | -6.27 | 114.64      | 121.28   |
| 1   | H     | 33  | GLY  | CA-C-O     | 6.26  | 131.46      | 120.57   |
| 1   | O     | 103 | ASN  | CA-CB-CG   | 6.25  | 118.84      | 112.60   |
| 1   | X     | 87  | VAL  | N-CA-C     | 6.24  | 117.69      | 108.45   |
| 1   | X     | 67  | ARG  | NE-CZ-NH2  | -6.22 | 113.60      | 119.20   |
| 1   | D     | 42  | PHE  | CA-CB-CG   | -6.22 | 107.58      | 113.80   |
| 1   | Y     | 98  | ALA  | CA-C-N     | -6.21 | 113.39      | 122.58   |
| 1   | Y     | 98  | ALA  | C-N-CA     | -6.21 | 113.39      | 122.58   |
| 1   | G     | 34  | LYS  | O-C-N      | -6.19 | 115.26      | 121.88   |
| 1   | F     | 101 | MET  | CA-C-O     | -6.18 | 113.18      | 120.60   |
| 1   | G     | 35  | ARG  | CD-NE-CZ   | 6.17  | 133.04      | 124.40   |
| 1   | X     | 94  | ASN  | CA-CB-CG   | 6.17  | 118.77      | 112.60   |
| 1   | G     | 13  | ARG  | CD-NE-CZ   | 6.16  | 133.03      | 124.40   |
| 1   | X     | 2   | PRO  | CA-C-O     | 6.16  | 128.32      | 121.36   |
| 1   | G     | 4   | THR  | CA-C-O     | -6.16 | 114.61      | 121.51   |
| 1   | E     | 86  | CYS  | CA-C-O     | -6.15 | 114.14      | 120.54   |
| 1   | Y     | 12  | TYR  | CA-C-O     | 6.15  | 127.22      | 120.71   |
| 1   | X     | 4   | THR  | N-CA-CB    | 6.13  | 121.18      | 111.43   |
| 1   | H     | 56  | GLN  | OE1-CD-NE2 | -6.11 | 116.49      | 122.60   |
| 1   | M     | 35  | ARG  | NE-CZ-NH1  | 6.11  | 127.61      | 121.50   |
| 1   | L     | 62  | LYS  | CA-CB-CG   | 6.11  | 126.31      | 114.10   |
| 1   | E     | 89  | ASN  | CA-C-O     | 6.10  | 127.04      | 119.78   |
| 1   | H     | 48  | PHE  | CA-CB-CG   | -6.09 | 107.71      | 113.80   |
| 1   | N     | 11  | GLU  | CA-C-N     | 6.09  | 132.37      | 122.81   |
| 1   | N     | 11  | GLU  | C-N-CA     | 6.09  | 132.37      | 122.81   |
| 1   | M     | 39  | ILE  | CA-C-O     | -6.08 | 114.13      | 120.27   |
| 1   | F     | 61  | GLN  | CB-CG-CD   | -6.06 | 102.30      | 112.60   |
| 1   | N     | 96  | ILE  | O-C-N      | -6.06 | 116.01      | 122.61   |
| 1   | H     | 102 | LYS  | O-C-N      | -6.02 | 116.36      | 123.41   |
| 1   | M     | 76  | TYR  | O-C-N      | -6.02 | 115.87      | 122.07   |
| 1   | F     | 50  | VAL  | N-CA-CB    | 6.02  | 118.25      | 111.21   |
| 1   | Y     | 21  | ASN  | CA-CB-CG   | -6.02 | 106.58      | 112.60   |
| 1   | D     | 81  | LYS  | CA-C-O     | -6.01 | 113.89      | 120.81   |
| 1   | W     | 26  | SER  | CA-C-O     | -6.01 | 113.86      | 120.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | X     | 23  | LYS  | O-C-N      | -6.01 | 115.59      | 122.68   |
| 1   | Y     | 13  | ARG  | CD-NE-CZ   | 6.00  | 132.81      | 124.40   |
| 1   | O     | 87  | VAL  | N-CA-C     | 6.00  | 117.40      | 108.46   |
| 1   | L     | 50  | VAL  | N-CA-CB    | 5.99  | 119.22      | 111.67   |
| 1   | W     | 94  | ASN  | CB-CA-C    | 5.99  | 119.66      | 109.72   |
| 1   | N     | 49  | GLN  | CA-C-O     | 5.98  | 128.16      | 121.40   |
| 1   | P     | 62  | LYS  | CA-CB-CG   | 5.98  | 126.05      | 114.10   |
| 1   | E     | 7   | GLU  | CA-C-O     | 5.97  | 126.88      | 120.55   |
| 1   | H     | 48  | PHE  | O-C-N      | 5.97  | 131.10      | 123.11   |
| 1   | P     | 14  | ASN  | CA-CB-CG   | 5.96  | 118.56      | 112.60   |
| 1   | N     | 99  | ILE  | O-C-N      | -5.96 | 116.21      | 123.00   |
| 1   | P     | 21  | ASN  | CB-CG-OD1  | -5.95 | 108.89      | 120.80   |
| 1   | Z     | 71  | THR  | N-CA-C     | 5.94  | 117.76      | 111.28   |
| 1   | Z     | 42  | PHE  | CA-C-N     | 5.94  | 128.83      | 120.28   |
| 1   | Z     | 42  | PHE  | C-N-CA     | 5.94  | 128.83      | 120.28   |
| 1   | D     | 6   | THR  | O-C-N      | -5.93 | 115.96      | 122.07   |
| 1   | H     | 24  | ILE  | CA-CB-CG2  | 5.91  | 120.54      | 110.50   |
| 1   | D     | 56  | GLN  | N-CA-CB    | 5.90  | 119.42      | 110.28   |
| 1   | L     | 70  | ASP  | CA-C-O     | 5.89  | 127.01      | 120.82   |
| 1   | Z     | 95  | SER  | O-C-N      | 5.89  | 130.08      | 123.19   |
| 1   | P     | 70  | ASP  | CA-CB-CG   | 5.88  | 118.48      | 112.60   |
| 1   | E     | 28  | THR  | CA-CB-CG2  | 5.88  | 120.49      | 110.50   |
| 1   | W     | 3   | GLN  | N-CA-C     | -5.88 | 105.95      | 114.12   |
| 1   | P     | 36  | GLU  | CA-C-O     | -5.88 | 114.78      | 121.66   |
| 1   | H     | 46  | GLU  | CA-C-N     | 5.88  | 131.05      | 122.77   |
| 1   | H     | 46  | GLU  | C-N-CA     | 5.88  | 131.05      | 122.77   |
| 1   | N     | 7   | GLU  | CA-C-N     | 5.87  | 128.46      | 120.54   |
| 1   | N     | 7   | GLU  | C-N-CA     | 5.87  | 128.46      | 120.54   |
| 1   | E     | 89  | ASN  | OD1-CG-ND2 | 5.86  | 128.46      | 122.60   |
| 1   | L     | 58  | ILE  | CA-C-N     | 5.85  | 129.60      | 120.82   |
| 1   | L     | 58  | ILE  | C-N-CA     | 5.85  | 129.60      | 120.82   |
| 1   | H     | 4   | THR  | CA-C-O     | -5.85 | 114.96      | 121.51   |
| 1   | X     | 13  | ARG  | CA-CB-CG   | 5.85  | 125.80      | 114.10   |
| 1   | G     | 76  | TYR  | N-CA-C     | -5.85 | 104.83      | 111.14   |
| 1   | X     | 7   | GLU  | CA-CB-CG   | 5.83  | 125.77      | 114.10   |
| 1   | Z     | 84  | LYS  | CA-CB-CG   | 5.83  | 125.77      | 114.10   |
| 1   | N     | 58  | ILE  | CA-C-O     | 5.83  | 128.60      | 122.13   |
| 1   | L     | 48  | PHE  | CA-CB-CG   | -5.82 | 107.98      | 113.80   |
| 1   | X     | 23  | LYS  | CA-C-O     | 5.82  | 128.61      | 122.03   |
| 1   | E     | 76  | TYR  | CA-C-O     | -5.82 | 114.68      | 120.90   |
| 1   | Y     | 54  | GLY  | O-C-N      | -5.81 | 119.47      | 123.95   |
| 1   | O     | 39  | ILE  | O-C-N      | -5.80 | 117.00      | 123.26   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | N     | 48  | PHE  | CA-CB-CG  | 5.79  | 119.59      | 113.80   |
| 1   | O     | 35  | ARG  | CA-CB-CG  | 5.78  | 125.67      | 114.10   |
| 1   | F     | 12  | TYR  | CA-C-O    | -5.77 | 114.59      | 121.11   |
| 1   | H     | 7   | GLU  | N-CA-CB   | 5.76  | 118.58      | 110.12   |
| 1   | P     | 50  | VAL  | N-CA-C    | -5.75 | 98.94       | 107.51   |
| 1   | P     | 57  | HIS  | N-CA-C    | 5.75  | 118.99      | 110.48   |
| 1   | D     | 50  | VAL  | N-CA-CB   | 5.74  | 118.90      | 111.67   |
| 1   | G     | 27  | TYR  | CA-C-O    | -5.74 | 114.17      | 120.36   |
| 1   | Z     | 22  | ASP  | O-C-N     | 5.74  | 129.03      | 123.29   |
| 1   | X     | 91  | LYS  | CA-C-O    | -5.72 | 114.93      | 121.40   |
| 1   | H     | 94  | ASN  | CA-CB-CG  | 5.72  | 118.32      | 112.60   |
| 1   | O     | 64  | ALA  | CA-C-O    | 5.71  | 126.52      | 119.79   |
| 1   | X     | 96  | ILE  | N-CA-C    | 5.71  | 117.07      | 109.37   |
| 1   | W     | 71  | THR  | CA-CB-OG1 | -5.69 | 101.06      | 109.60   |
| 1   | X     | 8   | LEU  | CA-C-O    | 5.69  | 126.56      | 120.70   |
| 1   | W     | 59  | ASP  | CA-C-O    | -5.69 | 114.81      | 120.90   |
| 1   | H     | 66  | GLU  | CA-C-O    | -5.68 | 114.52      | 120.55   |
| 1   | W     | 75  | THR  | CA-C-N    | 5.68  | 128.94      | 120.31   |
| 1   | W     | 75  | THR  | C-N-CA    | 5.68  | 128.94      | 120.31   |
| 1   | X     | 59  | ASP  | CA-C-N    | 5.68  | 130.20      | 120.72   |
| 1   | X     | 59  | ASP  | C-N-CA    | 5.68  | 130.20      | 120.72   |
| 1   | L     | 77  | LEU  | CA-C-O    | -5.68 | 114.53      | 120.55   |
| 1   | V     | 79  | GLU  | N-CA-C    | -5.67 | 103.62      | 111.28   |
| 1   | X     | 50  | VAL  | N-CA-CB   | 5.67  | 118.61      | 111.46   |
| 1   | L     | 65  | ILE  | N-CA-C    | -5.67 | 104.98      | 110.42   |
| 1   | H     | 17  | ILE  | O-C-N     | 5.67  | 130.45      | 122.97   |
| 1   | M     | 84  | LYS  | N-CA-C    | 5.66  | 118.44      | 109.50   |
| 1   | G     | 102 | LYS  | CB-CA-C   | 5.65  | 119.41      | 109.80   |
| 1   | W     | 103 | ASN  | CA-CB-CG  | 5.65  | 118.25      | 112.60   |
| 1   | D     | 73  | ARG  | NE-CZ-NH1 | 5.65  | 127.15      | 121.50   |
| 1   | E     | 94  | ASN  | CA-C-O    | -5.64 | 115.35      | 121.44   |
| 1   | W     | 89  | ASN  | CA-C-O    | -5.64 | 113.72      | 120.10   |
| 1   | H     | 42  | PHE  | CA-CB-CG  | -5.63 | 108.17      | 113.80   |
| 1   | F     | 101 | MET  | CA-C-N    | -5.63 | 113.00      | 122.29   |
| 1   | F     | 101 | MET  | C-N-CA    | -5.63 | 113.00      | 122.29   |
| 1   | Y     | 67  | ARG  | NE-CZ-NH1 | 5.63  | 127.13      | 121.50   |
| 1   | N     | 62  | LYS  | CB-CA-C   | -5.63 | 101.44      | 110.79   |
| 1   | M     | 45  | GLY  | CA-C-O    | 5.63  | 125.44      | 119.03   |
| 1   | W     | 59  | ASP  | CA-C-N    | 5.62  | 129.59      | 120.60   |
| 1   | W     | 59  | ASP  | C-N-CA    | 5.62  | 129.59      | 120.60   |
| 1   | W     | 70  | ASP  | N-CA-CB   | 5.62  | 118.11      | 109.91   |
| 1   | F     | 96  | ILE  | CA-C-O    | 5.61  | 127.44      | 121.04   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | X     | 92  | THR  | CA-CB-CG2  | -5.61 | 100.96      | 110.50   |
| 1   | W     | 66  | GLU  | N-CA-C     | -5.61 | 105.25      | 111.36   |
| 1   | Y     | 63  | LYS  | CA-C-O     | -5.61 | 112.48      | 119.38   |
| 1   | E     | 20  | ILE  | N-CA-C     | 5.60  | 116.66      | 111.45   |
| 1   | F     | 7   | GLU  | N-CA-CB    | -5.60 | 101.89      | 110.01   |
| 1   | G     | 34  | LYS  | CA-CB-CG   | -5.60 | 102.90      | 114.10   |
| 1   | E     | 55  | SER  | CB-CA-C    | -5.58 | 101.19      | 110.68   |
| 1   | P     | 25  | LEU  | CA-C-N     | -5.58 | 111.97      | 121.85   |
| 1   | P     | 25  | LEU  | C-N-CA     | -5.58 | 111.97      | 121.85   |
| 1   | E     | 14  | ASN  | CA-CB-CG   | 5.57  | 118.17      | 112.60   |
| 1   | Y     | 94  | ASN  | N-CA-CB    | 5.56  | 118.23      | 109.83   |
| 1   | H     | 68  | MET  | CA-C-N     | -5.56 | 112.83      | 120.28   |
| 1   | H     | 68  | MET  | C-N-CA     | -5.56 | 112.83      | 120.28   |
| 1   | N     | 6   | THR  | CA-C-N     | 5.56  | 127.67      | 120.44   |
| 1   | N     | 6   | THR  | C-N-CA     | 5.56  | 127.67      | 120.44   |
| 1   | D     | 68  | MET  | CA-C-O     | -5.56 | 114.53      | 120.42   |
| 1   | Z     | 58  | ILE  | CA-C-N     | 5.55  | 128.75      | 120.31   |
| 1   | Z     | 58  | ILE  | C-N-CA     | 5.55  | 128.75      | 120.31   |
| 1   | D     | 18  | TYR  | N-CA-CB    | 5.54  | 119.25      | 110.55   |
| 1   | N     | 17  | ILE  | CB-CA-C    | -5.54 | 104.59      | 111.08   |
| 1   | N     | 37  | MET  | N-CA-C     | 5.54  | 116.38      | 108.74   |
| 1   | G     | 18  | TYR  | N-CA-CB    | 5.53  | 119.28      | 110.65   |
| 1   | Y     | 63  | LYS  | CB-CA-C    | -5.53 | 98.76       | 110.31   |
| 1   | Z     | 11  | GLU  | CA-C-N     | 5.53  | 130.94      | 122.93   |
| 1   | Z     | 11  | GLU  | C-N-CA     | 5.53  | 130.94      | 122.93   |
| 1   | H     | 89  | ASN  | CA-C-O     | 5.52  | 126.35      | 119.78   |
| 1   | Z     | 86  | CYS  | CA-CB-SG   | -5.52 | 101.71      | 114.40   |
| 1   | H     | 59  | ASP  | CA-C-O     | -5.51 | 114.68      | 120.63   |
| 1   | M     | 64  | ALA  | CA-C-O     | -5.51 | 113.63      | 119.97   |
| 1   | E     | 69  | LYS  | CG-CD-CE   | 5.51  | 123.97      | 111.30   |
| 1   | V     | 20  | ILE  | CB-CA-C    | -5.51 | 105.21      | 111.55   |
| 1   | M     | 29  | GLU  | CA-C-N     | -5.49 | 113.83      | 122.73   |
| 1   | M     | 29  | GLU  | C-N-CA     | -5.49 | 113.83      | 122.73   |
| 1   | X     | 3   | GLN  | N-CA-C     | -5.49 | 106.71      | 113.41   |
| 1   | O     | 7   | GLU  | N-CA-CB    | 5.49  | 117.92      | 109.91   |
| 1   | D     | 50  | VAL  | N-CA-C     | -5.49 | 99.25       | 107.37   |
| 1   | X     | 85  | LEU  | N-CA-CB    | 5.48  | 120.02      | 110.81   |
| 1   | N     | 73  | ARG  | NH1-CZ-NH2 | 5.47  | 126.41      | 119.30   |
| 1   | W     | 59  | ASP  | CA-CB-CG   | 5.46  | 118.06      | 112.60   |
| 1   | D     | 70  | ASP  | CB-CA-C    | -5.46 | 101.72      | 110.79   |
| 1   | L     | 41  | THR  | N-CA-CB    | 5.46  | 121.06      | 111.55   |
| 1   | E     | 35  | ARG  | CD-NE-CZ   | 5.45  | 132.03      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 76  | TYR  | CA-C-O     | 5.45  | 126.54      | 120.82   |
| 1   | N     | 61  | GLN  | CB-CG-CD   | -5.44 | 103.34      | 112.60   |
| 1   | W     | 95  | SER  | N-CA-C     | 5.44  | 117.61      | 108.96   |
| 1   | E     | 74  | ILE  | O-C-N      | -5.43 | 116.23      | 121.83   |
| 1   | H     | 16  | GLN  | OE1-CD-NE2 | -5.43 | 117.17      | 122.60   |
| 1   | O     | 77  | LEU  | CA-C-O     | -5.42 | 113.97      | 120.10   |
| 1   | N     | 74  | ILE  | CA-C-N     | 5.42  | 127.54      | 120.28   |
| 1   | N     | 74  | ILE  | C-N-CA     | 5.42  | 127.54      | 120.28   |
| 1   | G     | 52  | VAL  | O-C-N      | 5.41  | 127.02      | 121.07   |
| 1   | V     | 35  | ARG  | CG-CD-NE   | 5.41  | 123.91      | 112.00   |
| 1   | N     | 56  | GLN  | OE1-CD-NE2 | -5.41 | 117.19      | 122.60   |
| 1   | O     | 25  | LEU  | CA-C-N     | -5.41 | 114.18      | 122.62   |
| 1   | O     | 25  | LEU  | C-N-CA     | -5.41 | 114.18      | 122.62   |
| 1   | M     | 77  | LEU  | CA-C-O     | -5.41 | 114.82      | 120.55   |
| 1   | M     | 100 | SER  | O-C-N      | -5.41 | 116.63      | 123.17   |
| 1   | O     | 79  | GLU  | CA-C-O     | -5.40 | 114.85      | 121.28   |
| 1   | H     | 20  | ILE  | N-CA-CB    | -5.40 | 101.55      | 110.56   |
| 1   | X     | 36  | GLU  | CA-C-O     | 5.39  | 127.22      | 121.02   |
| 1   | P     | 26  | SER  | CA-C-N     | 5.39  | 130.59      | 122.99   |
| 1   | P     | 26  | SER  | C-N-CA     | 5.39  | 130.59      | 122.99   |
| 1   | N     | 14  | ASN  | CA-C-N     | -5.39 | 113.44      | 122.92   |
| 1   | N     | 14  | ASN  | C-N-CA     | -5.39 | 113.44      | 122.92   |
| 1   | G     | 41  | THR  | CA-C-O     | 5.39  | 127.74      | 121.44   |
| 1   | H     | 37  | MET  | N-CA-C     | 5.38  | 117.25      | 109.07   |
| 1   | X     | 50  | VAL  | N-CA-C     | -5.38 | 100.00      | 107.80   |
| 1   | X     | 8   | LEU  | O-C-N      | -5.37 | 116.29      | 122.09   |
| 1   | H     | 68  | MET  | CA-C-O     | -5.37 | 115.18      | 120.82   |
| 1   | P     | 100 | SER  | CA-C-N     | 5.37  | 131.35      | 122.33   |
| 1   | P     | 100 | SER  | C-N-CA     | 5.37  | 131.35      | 122.33   |
| 1   | N     | 75  | THR  | N-CA-C     | -5.36 | 105.44      | 111.28   |
| 1   | X     | 53  | PRO  | CA-C-N     | 5.35  | 131.90      | 121.41   |
| 1   | X     | 53  | PRO  | C-N-CA     | 5.35  | 131.90      | 121.41   |
| 1   | G     | 63  | LYS  | CA-C-N     | 5.35  | 127.45      | 120.28   |
| 1   | G     | 63  | LYS  | C-N-CA     | 5.35  | 127.45      | 120.28   |
| 1   | H     | 96  | ILE  | N-CA-C     | 5.35  | 115.99      | 109.30   |
| 1   | Z     | 99  | ILE  | CA-C-N     | 5.35  | 131.57      | 122.37   |
| 1   | Z     | 99  | ILE  | C-N-CA     | 5.35  | 131.57      | 122.37   |
| 1   | V     | 72  | LEU  | CA-C-O     | -5.35 | 115.20      | 120.82   |
| 1   | Y     | 57  | HIS  | O-C-N      | 5.35  | 129.31      | 123.27   |
| 1   | W     | 42  | PHE  | CA-C-N     | 5.34  | 127.75      | 120.54   |
| 1   | W     | 42  | PHE  | C-N-CA     | 5.34  | 127.75      | 120.54   |
| 1   | D     | 17  | ILE  | CA-C-O     | -5.33 | 114.24      | 121.02   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 97  | ALA  | N-CA-C     | -5.33 | 107.32      | 113.88   |
| 1   | F     | 16  | GLN  | N-CA-CB    | -5.33 | 102.06      | 111.39   |
| 1   | N     | 84  | LYS  | O-C-N      | -5.33 | 116.22      | 123.10   |
| 1   | V     | 35  | ARG  | NE-CZ-NH2  | 5.33  | 124.00      | 119.20   |
| 1   | D     | 90  | ASN  | N-CA-C     | -5.33 | 105.23      | 112.26   |
| 1   | P     | 43  | LYS  | CA-C-N     | 5.33  | 131.73      | 121.18   |
| 1   | P     | 43  | LYS  | C-N-CA     | 5.33  | 131.73      | 121.18   |
| 1   | D     | 62  | LYS  | CA-C-O     | -5.32 | 115.23      | 120.82   |
| 1   | F     | 18  | TYR  | O-C-N      | 5.32  | 129.64      | 123.30   |
| 1   | Z     | 26  | SER  | CA-C-N     | -5.32 | 115.50      | 123.00   |
| 1   | Z     | 26  | SER  | C-N-CA     | -5.32 | 115.50      | 123.00   |
| 1   | X     | 102 | LYS  | CA-C-O     | 5.32  | 127.23      | 121.06   |
| 1   | F     | 35  | ARG  | CG-CD-NE   | 5.32  | 123.69      | 112.00   |
| 1   | Z     | 4   | THR  | N-CA-CB    | 5.32  | 121.42      | 111.53   |
| 1   | G     | 53  | PRO  | CA-C-O     | -5.31 | 115.36      | 121.36   |
| 1   | L     | 52  | VAL  | CA-C-O     | -5.31 | 115.09      | 119.76   |
| 1   | X     | 71  | THR  | CA-C-O     | -5.31 | 115.25      | 120.82   |
| 1   | G     | 50  | VAL  | CA-C-O     | -5.30 | 114.46      | 120.66   |
| 1   | D     | 102 | LYS  | O-C-N      | 5.29  | 129.73      | 123.27   |
| 1   | Y     | 68  | MET  | CA-C-N     | -5.29 | 112.66      | 120.28   |
| 1   | Y     | 68  | MET  | C-N-CA     | -5.29 | 112.66      | 120.28   |
| 1   | Z     | 24  | ILE  | CB-CA-C    | -5.29 | 102.97      | 111.59   |
| 1   | H     | 82  | ILE  | CA-C-O     | -5.29 | 114.91      | 120.57   |
| 1   | D     | 35  | ARG  | NE-CZ-NH2  | -5.28 | 114.45      | 119.20   |
| 1   | V     | 31  | MET  | CA-C-N     | -5.28 | 114.75      | 122.19   |
| 1   | V     | 31  | MET  | C-N-CA     | -5.28 | 114.75      | 122.19   |
| 1   | W     | 26  | SER  | N-CA-CB    | -5.28 | 101.81      | 110.68   |
| 1   | X     | 45  | GLY  | N-CA-C     | -5.28 | 107.73      | 114.85   |
| 1   | V     | 3   | GLN  | CA-C-O     | 5.27  | 124.75      | 118.69   |
| 1   | X     | 95  | SER  | N-CA-C     | 5.27  | 117.11      | 108.52   |
| 1   | G     | 76  | TYR  | N-CA-CB    | 5.27  | 117.71      | 110.07   |
| 1   | L     | 51  | GLU  | N-CA-C     | 5.27  | 117.33      | 110.43   |
| 1   | W     | 78  | THR  | CA-CB-OG1  | -5.27 | 101.70      | 109.60   |
| 1   | H     | 48  | PHE  | CA-C-O     | -5.27 | 115.30      | 121.46   |
| 1   | N     | 50  | VAL  | CB-CA-C    | -5.27 | 103.27      | 110.96   |
| 1   | P     | 50  | VAL  | N-CA-CB    | 5.26  | 117.98      | 111.41   |
| 1   | Y     | 21  | ASN  | CA-C-O     | 5.25  | 127.50      | 120.98   |
| 1   | D     | 24  | ILE  | O-C-N      | -5.25 | 116.95      | 122.67   |
| 1   | H     | 48  | PHE  | N-CA-CB    | 5.25  | 119.70      | 111.20   |
| 1   | X     | 7   | GLU  | N-CA-CB    | 5.25  | 118.31      | 110.22   |
| 1   | G     | 78  | THR  | CA-C-O     | -5.25 | 113.42      | 119.56   |
| 1   | F     | 67  | ARG  | NH1-CZ-NH2 | 5.25  | 126.12      | 119.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 34  | LYS  | CG-CD-CE | 5.25  | 123.36      | 111.30   |
| 1   | W     | 74  | ILE  | N-CA-CB  | 5.24  | 116.68      | 110.55   |
| 1   | N     | 80  | THR  | O-C-N    | 5.24  | 129.04      | 122.86   |
| 1   | F     | 85  | LEU  | CA-C-O   | -5.23 | 115.05      | 120.70   |
| 1   | Y     | 75  | THR  | O-C-N    | -5.23 | 116.58      | 122.12   |
| 1   | G     | 70  | ASP  | N-CA-C   | -5.22 | 105.49      | 111.07   |
| 1   | Z     | 50  | VAL  | N-CA-CB  | 5.22  | 117.25      | 110.99   |
| 1   | P     | 40  | ILE  | CA-C-N   | -5.22 | 114.40      | 122.59   |
| 1   | P     | 40  | ILE  | C-N-CA   | -5.22 | 114.40      | 122.59   |
| 1   | W     | 68  | MET  | N-CA-CB  | 5.21  | 117.88      | 110.16   |
| 1   | Y     | 63  | LYS  | CA-CB-CG | 5.21  | 124.53      | 114.10   |
| 1   | P     | 10  | SER  | CA-CB-OG | -5.21 | 100.69      | 111.10   |
| 1   | G     | 18  | TYR  | N-CA-C   | -5.21 | 99.93       | 108.41   |
| 1   | H     | 97  | ALA  | N-CA-C   | -5.21 | 107.48      | 113.88   |
| 1   | L     | 50  | VAL  | N-CA-C   | -5.21 | 99.67       | 107.37   |
| 1   | M     | 50  | VAL  | N-CA-C   | -5.20 | 100.26      | 107.80   |
| 1   | Z     | 99  | ILE  | O-C-N    | -5.20 | 117.14      | 123.02   |
| 1   | F     | 14  | ASN  | CA-C-N   | -5.19 | 113.74      | 123.03   |
| 1   | F     | 14  | ASN  | C-N-CA   | -5.19 | 113.74      | 123.03   |
| 1   | F     | 98  | ALA  | CA-C-O   | -5.19 | 115.68      | 121.23   |
| 1   | V     | 41  | THR  | N-CA-CB  | 5.19  | 120.58      | 111.55   |
| 1   | F     | 93  | PRO  | CB-CA-C  | -5.19 | 99.03       | 112.00   |
| 1   | N     | 11  | GLU  | O-C-N    | -5.19 | 114.86      | 122.43   |
| 1   | L     | 42  | PHE  | CA-C-O   | -5.18 | 115.57      | 121.68   |
| 1   | O     | 52  | VAL  | N-CA-CB  | -5.18 | 105.26      | 110.08   |
| 1   | H     | 67  | ARG  | CA-C-O   | 5.18  | 126.04      | 120.55   |
| 1   | Y     | 77  | LEU  | CA-C-O   | -5.18 | 114.25      | 120.10   |
| 1   | H     | 89  | ASN  | O-C-N    | -5.18 | 115.98      | 122.35   |
| 1   | E     | 99  | ILE  | CA-C-O   | -5.17 | 115.80      | 121.28   |
| 1   | V     | 101 | MET  | CA-CB-CG | 5.17  | 124.44      | 114.10   |
| 1   | M     | 86  | CYS  | N-CA-CB  | 5.17  | 119.05      | 110.47   |
| 1   | G     | 101 | MET  | CA-C-O   | -5.17 | 114.40      | 120.60   |
| 1   | X     | 81  | LYS  | CA-CB-CG | 5.17  | 124.43      | 114.10   |
| 1   | G     | 65  | ILE  | O-C-N    | 5.16  | 126.88      | 121.87   |
| 1   | Y     | 85  | LEU  | N-CA-CB  | 5.16  | 119.73      | 110.80   |
| 1   | L     | 22  | ASP  | N-CA-CB  | -5.16 | 103.72      | 111.56   |
| 1   | F     | 42  | PHE  | CA-CB-CG | -5.16 | 108.64      | 113.80   |
| 1   | H     | 16  | GLN  | CA-C-O   | 5.16  | 126.56      | 120.89   |
| 1   | E     | 14  | ASN  | CA-C-N   | -5.15 | 113.64      | 123.32   |
| 1   | E     | 14  | ASN  | C-N-CA   | -5.15 | 113.64      | 123.32   |
| 1   | E     | 57  | HIS  | CA-CB-CG | -5.15 | 108.65      | 113.80   |
| 1   | X     | 79  | GLU  | CB-CA-C  | -5.15 | 104.42      | 111.73   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 11  | GLU  | N-CA-C     | -5.14 | 106.41      | 113.30   |
| 1   | L     | 43  | LYS  | CA-CB-CG   | 5.14  | 124.38      | 114.10   |
| 1   | G     | 6   | THR  | CA-C-N     | -5.14 | 112.50      | 120.31   |
| 1   | G     | 6   | THR  | C-N-CA     | -5.14 | 112.50      | 120.31   |
| 1   | O     | 76  | TYR  | CA-C-O     | -5.14 | 115.42      | 120.82   |
| 1   | G     | 21  | ASN  | N-CA-CB    | -5.13 | 103.91      | 111.71   |
| 1   | D     | 49  | GLN  | CA-C-O     | 5.13  | 127.46      | 121.46   |
| 1   | Z     | 78  | THR  | CA-C-N     | 5.13  | 129.40      | 122.07   |
| 1   | Z     | 78  | THR  | C-N-CA     | 5.13  | 129.40      | 122.07   |
| 1   | W     | 50  | VAL  | CB-CA-C    | 5.13  | 116.83      | 110.73   |
| 1   | H     | 41  | THR  | CA-C-O     | -5.12 | 115.11      | 121.11   |
| 1   | P     | 100 | SER  | O-C-N      | -5.12 | 116.94      | 123.24   |
| 1   | F     | 16  | GLN  | O-C-N      | 5.12  | 129.21      | 123.48   |
| 1   | X     | 85  | LEU  | CB-CA-C    | -5.12 | 100.69      | 109.65   |
| 1   | V     | 35  | ARG  | CD-NE-CZ   | 5.12  | 131.56      | 124.40   |
| 1   | X     | 47  | THR  | CA-C-O     | 5.12  | 125.89      | 120.36   |
| 1   | V     | 30  | SER  | CA-CB-OG   | -5.12 | 100.87      | 111.10   |
| 1   | Y     | 35  | ARG  | CD-NE-CZ   | 5.12  | 131.56      | 124.40   |
| 1   | F     | 55  | SER  | CA-C-O     | 5.11  | 125.64      | 119.31   |
| 1   | M     | 19  | THR  | CB-CA-C    | 5.10  | 118.74      | 110.22   |
| 1   | G     | 70  | ASP  | CA-CB-CG   | 5.10  | 117.70      | 112.60   |
| 1   | Y     | 43  | LYS  | CA-C-N     | 5.10  | 127.42      | 120.54   |
| 1   | Y     | 43  | LYS  | C-N-CA     | 5.10  | 127.42      | 120.54   |
| 1   | E     | 66  | GLU  | CA-C-O     | -5.09 | 115.16      | 120.55   |
| 1   | W     | 29  | GLU  | CA-C-N     | -5.08 | 114.50      | 122.73   |
| 1   | W     | 29  | GLU  | C-N-CA     | -5.08 | 114.50      | 122.73   |
| 1   | V     | 50  | VAL  | N-CA-CB    | 5.07  | 118.07      | 111.83   |
| 1   | L     | 25  | LEU  | N-CA-C     | -5.07 | 104.74      | 112.04   |
| 1   | G     | 73  | ARG  | NE-CZ-NH1  | 5.07  | 126.57      | 121.50   |
| 1   | G     | 73  | ARG  | NE-CZ-NH2  | -5.06 | 114.64      | 119.20   |
| 1   | L     | 76  | TYR  | CA-CB-CG   | -5.06 | 104.80      | 113.90   |
| 1   | E     | 44  | SER  | CB-CA-C    | -5.05 | 99.75       | 110.31   |
| 1   | F     | 90  | ASN  | N-CA-C     | -5.05 | 106.96      | 112.72   |
| 1   | F     | 95  | SER  | N-CA-CB    | -5.05 | 102.20      | 110.43   |
| 1   | H     | 103 | ASN  | OD1-CG-ND2 | -5.05 | 117.55      | 122.60   |
| 1   | D     | 60  | SER  | N-CA-CB    | -5.05 | 101.56      | 110.39   |
| 1   | N     | 30  | SER  | CA-C-N     | -5.05 | 115.14      | 122.86   |
| 1   | N     | 30  | SER  | C-N-CA     | -5.05 | 115.14      | 122.86   |
| 1   | P     | 89  | ASN  | CA-CB-CG   | 5.04  | 117.64      | 112.60   |
| 1   | W     | 50  | VAL  | CA-C-O     | -5.04 | 115.37      | 120.31   |
| 1   | H     | 13  | ARG  | CG-CD-NE   | 5.04  | 123.08      | 112.00   |
| 1   | H     | 59  | ASP  | N-CA-C     | 5.04  | 117.43      | 111.33   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 93  | PRO  | CA-C-N    | 5.04  | 127.92      | 120.82   |
| 1   | L     | 93  | PRO  | C-N-CA    | 5.04  | 127.92      | 120.82   |
| 1   | O     | 50  | VAL  | N-CA-CB   | 5.03  | 117.80      | 111.46   |
| 1   | F     | 35  | ARG  | NE-CZ-NH1 | 5.03  | 126.53      | 121.50   |
| 1   | W     | 94  | ASN  | CA-C-N    | 5.02  | 129.08      | 122.30   |
| 1   | W     | 94  | ASN  | C-N-CA    | 5.02  | 129.08      | 122.30   |
| 1   | D     | 78  | THR  | O-C-N     | -5.01 | 115.45      | 122.37   |
| 1   | M     | 59  | ASP  | CB-CA-C   | -5.01 | 102.78      | 110.81   |
| 1   | Z     | 34  | LYS  | O-C-N     | -5.01 | 115.92      | 122.59   |
| 1   | G     | 23  | LYS  | N-CA-C    | -5.01 | 102.36      | 110.32   |
| 1   | O     | 50  | VAL  | CA-C-O    | -5.00 | 115.17      | 120.53   |
| 1   | W     | 71  | THR  | CA-CB-CG2 | 5.00  | 119.00      | 110.50   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | N     | 52  | VAL  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 824   | 0        | 841      | 20      | 0            |
| 1   | E     | 824   | 0        | 841      | 20      | 0            |
| 1   | F     | 824   | 0        | 841      | 20      | 0            |
| 1   | G     | 824   | 0        | 841      | 18      | 0            |
| 1   | H     | 824   | 0        | 841      | 15      | 0            |
| 1   | L     | 824   | 0        | 841      | 29      | 0            |
| 1   | M     | 824   | 0        | 841      | 27      | 0            |
| 1   | N     | 824   | 0        | 841      | 27      | 0            |
| 1   | O     | 824   | 0        | 841      | 19      | 0            |
| 1   | P     | 824   | 0        | 841      | 27      | 0            |
| 1   | V     | 824   | 0        | 841      | 60      | 0            |
| 1   | W     | 824   | 0        | 841      | 41      | 0            |
| 1   | X     | 824   | 0        | 841      | 24      | 0            |
| 1   | Y     | 824   | 0        | 841      | 45      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Z     | 824   | 0        | 841      | 42      | 0            |
| 2   | D     | 33    | 0        | 28       | 9       | 0            |
| 2   | E     | 33    | 0        | 29       | 2       | 0            |
| 2   | F     | 33    | 0        | 29       | 5       | 0            |
| 2   | G     | 33    | 0        | 29       | 2       | 0            |
| 2   | H     | 33    | 0        | 28       | 1       | 0            |
| 2   | L     | 33    | 0        | 28       | 3       | 0            |
| 2   | M     | 33    | 0        | 28       | 2       | 0            |
| 2   | O     | 33    | 0        | 28       | 8       | 0            |
| 2   | P     | 33    | 0        | 29       | 0       | 0            |
| 2   | V     | 33    | 0        | 28       | 6       | 0            |
| 2   | W     | 33    | 0        | 28       | 4       | 0            |
| 2   | X     | 33    | 0        | 29       | 1       | 0            |
| 2   | Y     | 33    | 0        | 28       | 5       | 0            |
| 2   | Z     | 33    | 0        | 28       | 9       | 0            |
| 3   | D     | 89    | 0        | 0        | 1       | 0            |
| 3   | E     | 87    | 0        | 0        | 4       | 0            |
| 3   | F     | 113   | 0        | 0        | 3       | 0            |
| 3   | G     | 78    | 0        | 0        | 1       | 0            |
| 3   | H     | 100   | 0        | 0        | 3       | 0            |
| 3   | L     | 51    | 0        | 0        | 1       | 0            |
| 3   | M     | 49    | 0        | 0        | 1       | 0            |
| 3   | N     | 65    | 0        | 0        | 4       | 0            |
| 3   | O     | 75    | 0        | 0        | 1       | 0            |
| 3   | P     | 80    | 0        | 0        | 1       | 0            |
| 3   | V     | 41    | 0        | 0        | 1       | 0            |
| 3   | W     | 49    | 0        | 0        | 3       | 0            |
| 3   | X     | 81    | 0        | 0        | 1       | 0            |
| 3   | Y     | 63    | 0        | 0        | 1       | 0            |
| 3   | Z     | 61    | 0        | 0        | 2       | 0            |
| All | All   | 13904 | 0        | 13012    | 383     | 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 15.

All (383) 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) |
|------------------|----------------|--------------------------|-------------------|
| 2:O:104:A32:H5'1 | 1:P:34:LYS:HB2 | 1.33                     | 1.06              |
| 2:D:104:A32:H5'2 | 1:E:34:LYS:HB2 | 1.47                     | 0.97              |
| 1:N:57:HIS:HB3   | 1:N:62:LYS:HZ2 | 1.30                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:34:LYS:HB3   | 2:Z:104:A32:H2'2 | 1.52                     | 0.89              |
| 1:W:1:ALA:HB1    | 1:W:2:PRO:HD2    | 1.53                     | 0.89              |
| 1:V:47:THR:HG21  | 1:Z:3:GLN:HB3    | 1.55                     | 0.89              |
| 2:O:104:A32:H9'1 | 2:O:104:A32:H4'1 | 1.55                     | 0.89              |
| 1:H:56:GLN:HE21  | 1:H:56:GLN:H     | 1.20                     | 0.88              |
| 1:Y:58:ILE:HG21  | 2:Y:104:A32:H7'2 | 1.58                     | 0.85              |
| 1:D:80:THR:HG21  | 1:D:101:MET:HE3  | 1.59                     | 0.85              |
| 1:E:16:GLN:HE21  | 1:E:89:ASN:HD22  | 1.25                     | 0.84              |
| 1:V:1:ALA:HB1    | 1:V:2:PRO:HD2    | 1.58                     | 0.83              |
| 1:P:56:GLN:H     | 1:P:56:GLN:HE21  | 1.25                     | 0.82              |
| 1:Z:11:GLU:HB3   | 2:Z:104:A32:H5'1 | 1.63                     | 0.81              |
| 1:N:1:ALA:HB1    | 1:N:2:PRO:HD2    | 1.61                     | 0.81              |
| 1:W:37:MET:HE2   | 1:W:39:ILE:HG12  | 1.65                     | 0.79              |
| 1:Y:3:GLN:HG2    | 1:Z:93:PRO:HG3   | 1.64                     | 0.78              |
| 1:Z:56:GLN:H     | 1:Z:56:GLN:HE21  | 1.28                     | 0.78              |
| 1:Z:6:THR:HA     | 1:Z:17:ILE:HD11  | 1.66                     | 0.78              |
| 1:O:4:THR:OG1    | 1:O:7:GLU:HG2    | 1.85                     | 0.77              |
| 1:N:57:HIS:CB    | 1:N:62:LYS:HZ2   | 1.98                     | 0.76              |
| 1:M:103:ASN:HB2  | 3:M:133:HOH:O    | 1.85                     | 0.76              |
| 1:N:57:HIS:HB3   | 1:N:62:LYS:NZ    | 2.00                     | 0.76              |
| 1:N:103:ASN:HD22 | 1:O:23:LYS:HE2   | 1.51                     | 0.76              |
| 1:W:82:ILE:HG12  | 1:W:99:ILE:HD11  | 1.68                     | 0.76              |
| 1:V:3:GLN:HG2    | 1:W:93:PRO:HG3   | 1.69                     | 0.75              |
| 1:W:1:ALA:HB1    | 1:W:2:PRO:CD     | 2.16                     | 0.75              |
| 2:O:104:A32:H4'1 | 2:O:104:A32:C9'  | 2.18                     | 0.74              |
| 1:X:26:SER:HB3   | 1:X:41:THR:OG1   | 1.88                     | 0.73              |
| 1:N:62:LYS:HD2   | 3:N:142:HOH:O    | 1.88                     | 0.73              |
| 2:O:104:A32:H5'1 | 1:P:34:LYS:CB    | 2.15                     | 0.72              |
| 1:M:65:ILE:HG22  | 1:M:69:LYS:HE2   | 1.72                     | 0.72              |
| 2:O:104:A32:C5B  | 1:P:34:LYS:HB2   | 2.15                     | 0.72              |
| 1:O:16:GLN:HE21  | 1:O:89:ASN:HD22  | 1.37                     | 0.70              |
| 1:V:19:THR:HA    | 1:V:84:LYS:HG3   | 1.72                     | 0.70              |
| 1:F:99:ILE:HG12  | 1:F:101:MET:HE2  | 1.74                     | 0.70              |
| 1:P:20:ILE:HG13  | 1:P:85:LEU:HD12  | 1.74                     | 0.69              |
| 1:E:16:GLN:NE2   | 1:E:89:ASN:HD22  | 1.91                     | 0.69              |
| 1:Y:65:ILE:HG22  | 1:Y:69:LYS:HE2   | 1.75                     | 0.69              |
| 1:M:26:SER:HB3   | 1:M:41:THR:OG1   | 1.94                     | 0.68              |
| 1:V:1:ALA:HB1    | 1:V:2:PRO:CD     | 2.25                     | 0.67              |
| 1:V:2:PRO:HG3    | 1:V:11:GLU:OE2   | 1.94                     | 0.67              |
| 1:D:25:LEU:O     | 1:H:103:ASN:HB2  | 1.95                     | 0.66              |
| 1:X:92:THR:HG22  | 1:X:93:PRO:HA    | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:82:ILE:HG12  | 1:M:99:ILE:HD11  | 1.75                     | 0.66              |
| 1:N:9:CYS:HB3    | 3:N:159:HOH:O    | 1.94                     | 0.66              |
| 1:O:82:ILE:HG12  | 1:O:99:ILE:HD11  | 1.77                     | 0.66              |
| 1:V:34:LYS:CB    | 2:Z:104:A32:H2'2 | 2.26                     | 0.66              |
| 2:D:104:A32:H9'1 | 2:D:104:A32:H4'1 | 1.79                     | 0.65              |
| 1:X:92:THR:HA    | 1:X:93:PRO:C     | 2.22                     | 0.65              |
| 1:Y:48:PHE:CD2   | 1:Y:87:VAL:HG11  | 2.33                     | 0.64              |
| 2:D:104:A32:H5'2 | 1:E:34:LYS:CB    | 2.27                     | 0.64              |
| 1:V:27:TYR:CD1   | 1:Z:101:MET:HE2  | 2.33                     | 0.63              |
| 1:V:102:LYS:HE3  | 1:W:25:LEU:HD11  | 1.80                     | 0.63              |
| 1:L:9:CYS:HB2    | 1:L:17:ILE:HD11  | 1.81                     | 0.63              |
| 1:L:101:MET:HE2  | 1:M:76:TYR:CE2   | 2.33                     | 0.63              |
| 1:N:58:ILE:O     | 1:N:62:LYS:NZ    | 2.30                     | 0.63              |
| 2:L:104:A32:H6'1 | 3:L:154:HOH:O    | 1.96                     | 0.63              |
| 1:F:99:ILE:HG12  | 1:F:101:MET:CE   | 2.28                     | 0.62              |
| 2:O:104:A32:H9'1 | 2:O:104:A32:C4'  | 2.29                     | 0.62              |
| 1:Y:89:ASN:HD22  | 1:Y:89:ASN:C     | 2.05                     | 0.62              |
| 2:D:104:A32:N2'  | 1:E:33:GLY:HA3   | 2.14                     | 0.62              |
| 1:N:37:MET:HE2   | 1:N:39:ILE:HD11  | 1.81                     | 0.62              |
| 1:D:101:MET:HE2  | 1:E:76:TYR:CE2   | 2.35                     | 0.61              |
| 1:Z:59:ASP:O     | 1:Z:62:LYS:HG2   | 2.00                     | 0.61              |
| 1:V:65:ILE:HG22  | 1:V:69:LYS:HE2   | 1.83                     | 0.61              |
| 1:P:68:MET:HE1   | 1:P:99:ILE:HG22  | 1.83                     | 0.61              |
| 2:D:104:A32:C5B  | 1:E:34:LYS:HB2   | 2.27                     | 0.60              |
| 1:V:93:PRO:HG3   | 1:Z:3:GLN:HG2    | 1.83                     | 0.60              |
| 1:M:1:ALA:HB1    | 1:N:37:MET:HE1   | 1.84                     | 0.60              |
| 1:P:56:GLN:HE21  | 1:P:56:GLN:N     | 1.99                     | 0.60              |
| 1:Y:51:GLU:OE1   | 1:Y:91:LYS:HE2   | 2.02                     | 0.60              |
| 1:P:13:ARG:HG3   | 1:P:14:ASN:N     | 2.16                     | 0.60              |
| 1:Z:82:ILE:HD13  | 1:Z:99:ILE:HD12  | 1.83                     | 0.60              |
| 1:Z:88:TRP:CH2   | 2:Z:104:A32:H62  | 2.37                     | 0.60              |
| 1:V:101:MET:HE1  | 1:W:77:LEU:HD21  | 1.84                     | 0.59              |
| 1:W:37:MET:HE2   | 1:W:39:ILE:CG1   | 2.32                     | 0.59              |
| 1:Y:58:ILE:HD13  | 2:Y:104:A32:H7'2 | 1.84                     | 0.59              |
| 1:W:27:TYR:OH    | 1:W:29:GLU:OE1   | 2.18                     | 0.59              |
| 1:Y:48:PHE:CE2   | 1:Y:87:VAL:HG11  | 2.38                     | 0.59              |
| 1:M:2:PRO:HB3    | 1:M:7:GLU:HG2    | 1.84                     | 0.58              |
| 1:L:101:MET:HE2  | 1:M:76:TYR:HE2   | 1.67                     | 0.58              |
| 1:V:83:ASP:OD2   | 1:V:84:LYS:HD2   | 2.03                     | 0.58              |
| 1:V:12:TYR:CE2   | 2:V:104:A32:H6'2 | 2.39                     | 0.58              |
| 1:M:44:SER:OG    | 1:M:46:GLU:HG3   | 2.04                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:V:80:THR:HG21 | 1:V:101:MET:HE2  | 1.85                     | 0.58              |
| 1:X:1:ALA:HB1   | 1:X:2:PRO:HD2    | 1.86                     | 0.57              |
| 1:P:2:PRO:HG3   | 1:P:8:LEU:HD12   | 1.85                     | 0.57              |
| 1:Z:51:GLU:HG3  | 1:Z:95:SER:HB2   | 1.87                     | 0.57              |
| 1:Z:85:LEU:HD23 | 1:Z:99:ILE:HG22  | 1.87                     | 0.57              |
| 1:Y:13:ARG:O    | 1:Y:15:THR:HG23  | 2.04                     | 0.57              |
| 1:V:35:ARG:NH1  | 2:Z:104:A32:O1B  | 2.38                     | 0.57              |
| 1:Z:65:ILE:HG22 | 1:Z:69:LYS:HE2   | 1.86                     | 0.57              |
| 1:G:61:GLN:HG2  | 1:H:31:MET:O     | 2.05                     | 0.56              |
| 1:Y:101:MET:HE2 | 1:Z:27:TYR:CD2   | 2.40                     | 0.56              |
| 1:Z:11:GLU:O    | 2:Z:104:A32:H7'2 | 2.06                     | 0.56              |
| 1:V:12:TYR:CZ   | 2:V:104:A32:H6'2 | 2.40                     | 0.56              |
| 1:M:102:LYS:NZ  | 1:N:25:LEU:HD11  | 2.20                     | 0.56              |
| 1:P:20:ILE:HG13 | 1:P:85:LEU:CD1   | 2.35                     | 0.56              |
| 1:V:60:SER:O    | 1:W:36:GLU:HG2   | 2.06                     | 0.55              |
| 1:L:11:GLU:O    | 2:L:104:A32:H7'1 | 2.06                     | 0.55              |
| 1:X:8:LEU:HD11  | 1:Y:30:SER:HB2   | 1.88                     | 0.55              |
| 1:X:11:GLU:OE2  | 1:Y:35:ARG:NH2   | 2.34                     | 0.55              |
| 1:Z:25:LEU:HD13 | 1:Z:43:LYS:HE3   | 1.87                     | 0.55              |
| 1:O:80:THR:HG21 | 1:O:101:MET:HE3  | 1.88                     | 0.55              |
| 1:M:13:ARG:O    | 1:M:15:THR:HG23  | 2.07                     | 0.55              |
| 1:Z:56:GLN:HG2  | 1:Z:57:HIS:N     | 2.20                     | 0.55              |
| 1:M:51:GLU:HG3  | 1:M:95:SER:OG    | 2.06                     | 0.54              |
| 1:O:20:ILE:HG13 | 1:O:85:LEU:HD12  | 1.88                     | 0.54              |
| 1:Z:17:ILE:HG21 | 1:Z:84:LYS:HD3   | 1.90                     | 0.54              |
| 1:L:76:TYR:OH   | 1:P:103:ASN:HB2  | 2.08                     | 0.54              |
| 1:V:17:ILE:HG23 | 1:V:84:LYS:HG2   | 1.89                     | 0.54              |
| 1:M:84:LYS:HB2  | 1:M:100:SER:OG   | 2.07                     | 0.54              |
| 1:O:1:ALA:HB1   | 1:O:2:PRO:HD2    | 1.89                     | 0.54              |
| 1:V:35:ARG:HB2  | 1:Z:12:TYR:OH    | 2.07                     | 0.54              |
| 1:W:88:TRP:HB2  | 1:W:95:SER:HB3   | 1.89                     | 0.54              |
| 1:D:34:LYS:HE2  | 3:D:139:HOH:O    | 2.08                     | 0.54              |
| 1:M:102:LYS:HZ3 | 1:N:25:LEU:HD11  | 1.72                     | 0.54              |
| 1:L:52:VAL:HG12 | 1:L:53:PRO:O     | 2.07                     | 0.53              |
| 1:W:78:THR:O    | 1:W:79:GLU:C     | 2.52                     | 0.53              |
| 1:L:62:LYS:HZ1  | 1:L:63:LYS:HE2   | 1.74                     | 0.53              |
| 1:F:3:GLN:NE2   | 1:G:92:THR:HG22  | 2.24                     | 0.53              |
| 1:L:58:ILE:HD13 | 1:M:34:LYS:HE2   | 1.90                     | 0.53              |
| 1:Y:61:GLN:O    | 1:Y:65:ILE:HG13  | 2.09                     | 0.53              |
| 1:H:56:GLN:HE21 | 1:H:56:GLN:N     | 2.00                     | 0.53              |
| 1:Y:102:LYS:O   | 1:Y:103:ASN:HB2  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:23:LYS:HE2   | 1:H:103:ASN:ND2  | 2.25                     | 0.52              |
| 1:D:80:THR:CG2   | 1:D:101:MET:HE3  | 2.34                     | 0.52              |
| 1:N:12:TYR:OH    | 1:O:35:ARG:HG2   | 2.10                     | 0.52              |
| 1:H:43:LYS:HG3   | 3:H:119:HOH:O    | 2.08                     | 0.52              |
| 1:F:75:THR:HG23  | 1:F:80:THR:HB    | 1.91                     | 0.52              |
| 1:L:2:PRO:HD3    | 1:M:35:ARG:CZ    | 2.40                     | 0.52              |
| 1:L:93:PRO:HG3   | 1:P:3:GLN:HG2    | 1.90                     | 0.52              |
| 1:V:13:ARG:O     | 1:V:14:ASN:HB2   | 2.09                     | 0.52              |
| 1:P:1:ALA:HB1    | 1:P:2:PRO:HD2    | 1.91                     | 0.52              |
| 1:W:32:ALA:O     | 1:W:33:GLY:C     | 2.52                     | 0.52              |
| 1:F:103:ASN:HD22 | 1:G:23:LYS:NZ    | 2.07                     | 0.52              |
| 1:N:1:ALA:HB1    | 1:N:2:PRO:CD     | 2.34                     | 0.52              |
| 1:V:100:SER:HB2  | 1:W:28:THR:OG1   | 2.10                     | 0.52              |
| 2:D:104:A32:H9'1 | 2:D:104:A32:C4'  | 2.40                     | 0.51              |
| 1:Y:65:ILE:HG12  | 1:Z:31:MET:CE    | 2.40                     | 0.51              |
| 1:E:12:TYR:CZ    | 1:F:32:ALA:HB1   | 2.45                     | 0.51              |
| 1:X:103:ASN:O    | 1:Y:25:LEU:HD12  | 2.09                     | 0.51              |
| 1:Y:89:ASN:HD22  | 1:Y:90:ASN:N     | 2.08                     | 0.51              |
| 2:F:104:A32:H6'1 | 3:F:216:HOH:O    | 2.10                     | 0.51              |
| 1:L:62:LYS:NZ    | 1:L:63:LYS:HG2   | 2.26                     | 0.51              |
| 1:W:100:SER:HB2  | 3:W:142:HOH:O    | 2.09                     | 0.51              |
| 1:X:6:THR:HA     | 1:X:17:ILE:HD11  | 1.92                     | 0.51              |
| 1:L:21:ASN:HD21  | 1:L:81:LYS:HZ1   | 1.58                     | 0.51              |
| 1:W:59:ASP:HB2   | 3:W:124:HOH:O    | 2.11                     | 0.51              |
| 2:W:104:A32:H2A1 | 1:X:34:LYS:HB2   | 1.93                     | 0.51              |
| 1:M:49:GLN:HB3   | 1:M:93:PRO:HG2   | 1.93                     | 0.50              |
| 1:N:43:LYS:HG2   | 3:N:147:HOH:O    | 2.12                     | 0.50              |
| 1:D:101:MET:HE2  | 1:E:76:TYR:HE2   | 1.76                     | 0.50              |
| 1:P:13:ARG:O     | 1:P:14:ASN:HB2   | 2.10                     | 0.50              |
| 1:Y:101:MET:HE3  | 1:Z:76:TYR:CE2   | 2.46                     | 0.50              |
| 1:Z:11:GLU:HB3   | 2:Z:104:A32:C5B  | 2.38                     | 0.50              |
| 1:Z:20:ILE:O     | 1:Z:21:ASN:C     | 2.54                     | 0.50              |
| 1:W:93:PRO:HA    | 3:W:140:HOH:O    | 2.11                     | 0.50              |
| 1:X:51:GLU:HG3   | 1:X:95:SER:OG    | 2.12                     | 0.50              |
| 1:D:2:PRO:HB3    | 1:D:7:GLU:HG2    | 1.93                     | 0.50              |
| 1:V:20:ILE:O     | 1:V:21:ASN:C     | 2.54                     | 0.50              |
| 1:X:8:LEU:HD11   | 1:Y:30:SER:CB    | 2.40                     | 0.50              |
| 1:Y:12:TYR:HB2   | 1:Y:15:THR:HG21  | 1.93                     | 0.49              |
| 1:Z:2:PRO:HB3    | 1:Z:7:GLU:HB2    | 1.92                     | 0.49              |
| 1:P:9:CYS:O      | 1:P:10:SER:C     | 2.55                     | 0.49              |
| 1:V:11:GLU:C     | 2:V:104:A32:H6A1 | 2.37                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:N:30:SER:O     | 1:N:36:GLU:HA   | 2.12                     | 0.49              |
| 1:W:7:GLU:O      | 1:W:8:LEU:C     | 2.55                     | 0.49              |
| 1:W:102:LYS:HA   | 1:X:25:LEU:O    | 2.12                     | 0.49              |
| 1:V:2:PRO:HD3    | 1:W:35:ARG:CZ   | 2.42                     | 0.49              |
| 1:L:9:CYS:CB     | 1:L:17:ILE:HD11 | 2.43                     | 0.49              |
| 1:G:20:ILE:O     | 1:G:21:ASN:C    | 2.55                     | 0.49              |
| 1:E:82:ILE:HG12  | 1:E:99:ILE:HD11 | 1.95                     | 0.49              |
| 1:L:35:ARG:HB3   | 1:P:8:LEU:HD11  | 1.94                     | 0.49              |
| 1:V:20:ILE:HG21  | 1:V:42:PHE:CE1  | 2.47                     | 0.49              |
| 1:V:30:SER:HB3   | 1:V:35:ARG:O    | 2.13                     | 0.49              |
| 1:Z:88:TRP:CZ3   | 2:Z:104:A32:H62 | 2.48                     | 0.48              |
| 2:F:104:A32:H4'1 | 3:F:217:HOH:O   | 2.12                     | 0.48              |
| 2:O:104:A32:C9'  | 2:O:104:A32:C4' | 2.86                     | 0.48              |
| 1:V:49:GLN:O     | 1:V:96:ILE:HG13 | 2.13                     | 0.48              |
| 1:Y:81:LYS:HB2   | 1:Y:81:LYS:NZ   | 2.28                     | 0.48              |
| 1:N:62:LYS:NZ    | 1:N:62:LYS:N    | 2.61                     | 0.48              |
| 1:X:30:SER:O     | 1:X:36:GLU:HA   | 2.14                     | 0.48              |
| 1:G:92:THR:HA    | 1:G:93:PRO:C    | 2.38                     | 0.48              |
| 1:H:81:LYS:HE2   | 3:H:141:HOH:O   | 2.13                     | 0.48              |
| 1:L:37:MET:HE1   | 1:P:1:ALA:HB1   | 1.94                     | 0.48              |
| 1:L:61:GLN:HG2   | 1:M:31:MET:O    | 2.14                     | 0.48              |
| 1:V:68:MET:HE2   | 1:W:29:GLU:OE2  | 2.14                     | 0.48              |
| 1:V:75:THR:HG23  | 1:V:80:THR:HB   | 1.96                     | 0.48              |
| 1:F:103:ASN:HD22 | 1:G:23:LYS:HZ3  | 1.62                     | 0.47              |
| 1:N:65:ILE:HG22  | 1:N:69:LYS:HE2  | 1.95                     | 0.47              |
| 1:E:44:SER:HB2   | 3:E:156:HOH:O   | 2.14                     | 0.47              |
| 1:G:8:LEU:C      | 1:G:8:LEU:HD23  | 2.39                     | 0.47              |
| 1:P:43:LYS:HB2   | 3:P:139:HOH:O   | 2.13                     | 0.47              |
| 1:V:16:GLN:HB2   | 1:V:89:ASN:ND2  | 2.29                     | 0.47              |
| 1:V:68:MET:HE1   | 1:V:99:ILE:HG22 | 1.96                     | 0.47              |
| 1:W:20:ILE:HD12  | 1:W:85:LEU:HG   | 1.95                     | 0.47              |
| 1:D:3:GLN:HG2    | 1:E:93:PRO:HD3  | 1.96                     | 0.47              |
| 1:X:21:ASN:OD1   | 1:X:81:LYS:HD2  | 2.14                     | 0.47              |
| 1:V:80:THR:HG21  | 1:V:101:MET:CE  | 2.43                     | 0.47              |
| 1:L:85:LEU:HD23  | 1:L:99:ILE:HG13 | 1.97                     | 0.47              |
| 1:X:103:ASN:ND2  | 1:Y:23:LYS:NZ   | 2.63                     | 0.47              |
| 1:F:103:ASN:HB3  | 1:G:23:LYS:HZ1  | 1.79                     | 0.47              |
| 1:D:62:LYS:HD2   | 1:D:62:LYS:O    | 2.15                     | 0.47              |
| 1:F:28:THR:HB    | 1:F:39:ILE:HB   | 1.97                     | 0.47              |
| 1:L:21:ASN:HD21  | 1:L:81:LYS:NZ   | 2.13                     | 0.47              |
| 1:P:56:GLN:H     | 1:P:56:GLN:NE2  | 2.03                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:93:PRO:HG3   | 1:Z:3:GLN:CG     | 2.43                     | 0.47              |
| 2:X:104:A32:H6'1 | 3:X:141:HOH:O    | 2.14                     | 0.47              |
| 1:Y:65:ILE:HG12  | 1:Z:31:MET:HE1   | 1.95                     | 0.47              |
| 1:Y:88:TRP:HZ2   | 3:Y:167:HOH:O    | 1.97                     | 0.47              |
| 1:V:61:GLN:NE2   | 1:W:33:GLY:H     | 2.12                     | 0.47              |
| 1:W:57:HIS:HA    | 1:W:61:GLN:OE1   | 2.15                     | 0.47              |
| 1:Y:89:ASN:C     | 1:Y:89:ASN:ND2   | 2.73                     | 0.47              |
| 1:Y:91:LYS:NZ    | 2:Y:104:A32:O3   | 2.41                     | 0.47              |
| 2:D:104:A32:H4'1 | 2:D:104:A32:C9'  | 2.45                     | 0.47              |
| 2:W:104:A32:H3'1 | 2:W:104:A32:H8'1 | 1.75                     | 0.47              |
| 1:L:80:THR:HG21  | 1:L:101:MET:HE3  | 1.97                     | 0.47              |
| 1:O:20:ILE:CG1   | 1:O:85:LEU:HD12  | 2.45                     | 0.47              |
| 1:N:37:MET:HE2   | 1:N:39:ILE:CD1   | 2.43                     | 0.46              |
| 1:W:91:LYS:O     | 1:W:94:ASN:ND2   | 2.47                     | 0.46              |
| 1:F:12:TYR:CE1   | 2:F:104:A32:H7'2 | 2.50                     | 0.46              |
| 1:F:92:THR:HA    | 1:F:93:PRO:C     | 2.40                     | 0.46              |
| 2:G:104:A32:H2'1 | 2:G:104:A32:H51  | 1.97                     | 0.46              |
| 1:O:33:GLY:O     | 1:O:34:LYS:HB2   | 2.16                     | 0.46              |
| 1:X:35:ARG:O     | 1:X:37:MET:HG2   | 2.15                     | 0.46              |
| 1:W:4:THR:O      | 1:W:5:ILE:C      | 2.58                     | 0.46              |
| 1:D:16:GLN:OE1   | 1:D:89:ASN:HB3   | 2.15                     | 0.46              |
| 1:Z:92:THR:HA    | 1:Z:93:PRO:C     | 2.40                     | 0.46              |
| 1:H:43:LYS:O     | 1:Z:13:ARG:HD3   | 2.15                     | 0.46              |
| 1:V:57:HIS:HA    | 1:V:61:GLN:OE1   | 2.16                     | 0.46              |
| 1:Y:18:TYR:O     | 1:Y:84:LYS:HA    | 2.16                     | 0.46              |
| 1:V:99:ILE:HG12  | 1:V:100:SER:H    | 1.79                     | 0.46              |
| 1:Y:88:TRP:CE2   | 2:Y:104:A32:H51  | 2.51                     | 0.46              |
| 1:L:89:ASN:HA    | 1:L:94:ASN:ND2   | 2.30                     | 0.46              |
| 1:O:16:GLN:HG2   | 1:O:18:TYR:CE1   | 2.51                     | 0.46              |
| 1:V:12:TYR:CZ    | 2:V:104:A32:H2A1 | 2.51                     | 0.46              |
| 1:Y:13:ARG:HH11  | 1:Y:13:ARG:HG3   | 1.80                     | 0.45              |
| 1:F:103:ASN:ND2  | 1:G:79:GLU:OE2   | 2.34                     | 0.45              |
| 1:Y:8:LEU:C      | 1:Y:8:LEU:HD23   | 2.41                     | 0.45              |
| 1:G:57:HIS:O     | 1:G:62:LYS:NZ    | 2.50                     | 0.45              |
| 1:M:88:TRP:HE3   | 1:M:95:SER:HB3   | 1.82                     | 0.45              |
| 1:H:9:CYS:HB2    | 1:H:17:ILE:HD11  | 1.98                     | 0.45              |
| 1:N:90:ASN:HB3   | 3:N:154:HOH:O    | 2.17                     | 0.45              |
| 1:V:75:THR:HG23  | 1:V:80:THR:CG2   | 2.46                     | 0.45              |
| 1:Z:10:SER:HB2   | 3:Z:146:HOH:O    | 2.16                     | 0.45              |
| 1:N:48:PHE:CD2   | 1:N:87:VAL:HG11  | 2.51                     | 0.45              |
| 1:W:64:ALA:HB1   | 1:X:31:MET:HA    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:23:LYS:HE3   | 3:Z:152:HOH:O    | 2.16                     | 0.45              |
| 1:Z:31:MET:HE3   | 1:Z:31:MET:HB2   | 1.62                     | 0.45              |
| 1:E:20:ILE:O     | 1:E:21:ASN:C     | 2.60                     | 0.45              |
| 1:E:44:SER:HA    | 3:E:146:HOH:O    | 2.17                     | 0.45              |
| 1:X:24:ILE:HD11  | 1:X:82:ILE:HD11  | 1.99                     | 0.45              |
| 1:X:8:LEU:CD1    | 1:Y:30:SER:HB2   | 2.46                     | 0.45              |
| 1:E:8:LEU:C      | 1:E:8:LEU:HD23   | 2.42                     | 0.45              |
| 1:N:20:ILE:HG21  | 1:N:42:PHE:CE1   | 2.52                     | 0.45              |
| 1:D:102:LYS:HE3  | 1:E:25:LEU:HD11  | 1.98                     | 0.45              |
| 1:O:97:ALA:HB1   | 3:O:158:HOH:O    | 2.17                     | 0.45              |
| 2:O:104:A32:H5'1 | 1:P:34:LYS:CG    | 2.47                     | 0.45              |
| 1:F:11:GLU:OE1   | 2:F:104:A32:H3'1 | 2.18                     | 0.44              |
| 1:F:99:ILE:CG1   | 1:F:101:MET:HE2  | 2.45                     | 0.44              |
| 1:W:20:ILE:HD13  | 1:W:42:PHE:CE2   | 2.51                     | 0.44              |
| 1:G:20:ILE:HG21  | 1:G:42:PHE:CE1   | 2.52                     | 0.44              |
| 1:V:17:ILE:CG2   | 1:V:84:LYS:HG2   | 2.47                     | 0.44              |
| 1:E:92:THR:HA    | 1:E:93:PRO:C     | 2.41                     | 0.44              |
| 1:L:21:ASN:O     | 1:L:22:ASP:HB2   | 2.17                     | 0.44              |
| 1:P:86:CYS:HB3   | 1:P:98:ALA:HB3   | 1.98                     | 0.44              |
| 1:W:33:GLY:O     | 1:W:34:LYS:HB2   | 2.18                     | 0.44              |
| 3:H:164:HOH:O    | 1:Z:13:ARG:HD2   | 2.18                     | 0.44              |
| 2:L:104:A32:H6A1 | 1:M:34:LYS:HD2   | 2.00                     | 0.44              |
| 2:M:104:A32:H2'1 | 2:M:104:A32:O5   | 2.16                     | 0.44              |
| 1:W:88:TRP:CH2   | 2:W:104:A32:H62  | 2.52                     | 0.44              |
| 1:Z:44:SER:OG    | 1:Z:46:GLU:OE1   | 2.36                     | 0.44              |
| 1:V:75:THR:HG23  | 1:V:80:THR:HG22  | 2.00                     | 0.44              |
| 1:Y:85:LEU:HD13  | 1:Y:96:ILE:HG12  | 2.00                     | 0.44              |
| 1:G:20:ILE:HD12  | 3:G:156:HOH:O    | 2.17                     | 0.44              |
| 1:L:65:ILE:HG22  | 1:L:69:LYS:HE2   | 1.99                     | 0.44              |
| 1:V:58:ILE:HD11  | 1:W:33:GLY:HA2   | 2.00                     | 0.44              |
| 1:X:1:ALA:HB1    | 1:Y:37:MET:HE1   | 2.00                     | 0.44              |
| 1:G:58:ILE:CD1   | 1:G:60:SER:OG    | 2.66                     | 0.43              |
| 1:W:8:LEU:C      | 1:W:8:LEU:HD23   | 2.42                     | 0.43              |
| 1:X:85:LEU:HD23  | 1:X:99:ILE:HG13  | 2.00                     | 0.43              |
| 1:Y:57:HIS:NE2   | 2:Y:104:A32:H61  | 2.33                     | 0.43              |
| 1:D:75:THR:HG23  | 1:D:80:THR:HB    | 2.00                     | 0.43              |
| 2:E:104:A32:H8'1 | 2:E:104:A32:H3'1 | 1.46                     | 0.43              |
| 1:O:2:PRO:CB     | 1:O:7:GLU:HG3    | 2.48                     | 0.43              |
| 1:V:19:THR:HG23  | 1:V:84:LYS:HE2   | 1.99                     | 0.43              |
| 1:V:35:ARG:HA    | 1:V:35:ARG:HD3   | 1.73                     | 0.43              |
| 1:Y:49:GLN:HB3   | 1:Y:93:PRO:HG2   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:91:LYS:NZ    | 2:Z:104:A32:O4   | 2.51                     | 0.43              |
| 2:F:104:A32:H5'1 | 2:F:104:A32:H8'1 | 1.50                     | 0.43              |
| 1:V:30:SER:O     | 1:V:36:GLU:HA    | 2.18                     | 0.43              |
| 1:V:58:ILE:O     | 1:V:59:ASP:C     | 2.60                     | 0.43              |
| 1:F:8:LEU:HD23   | 1:F:8:LEU:C      | 2.43                     | 0.43              |
| 1:M:85:LEU:HD23  | 1:M:99:ILE:HG13  | 2.00                     | 0.43              |
| 2:V:104:A32:H2'1 | 2:V:104:A32:H11  | 1.78                     | 0.43              |
| 1:W:26:SER:HB3   | 1:W:41:THR:OG1   | 2.18                     | 0.43              |
| 1:V:32:ALA:O     | 1:V:33:GLY:C     | 2.62                     | 0.43              |
| 1:V:35:ARG:HG2   | 1:V:35:ARG:HH11  | 1.84                     | 0.43              |
| 1:F:67:ARG:HG2   | 1:G:29:GLU:OE2   | 2.19                     | 0.43              |
| 1:G:59:ASP:HA    | 1:G:62:LYS:HG2   | 2.01                     | 0.43              |
| 1:G:101:MET:HE2  | 1:H:76:TYR:CE2   | 2.53                     | 0.43              |
| 1:X:20:ILE:O     | 1:X:21:ASN:C     | 2.61                     | 0.43              |
| 1:Y:21:ASN:OD1   | 1:Y:81:LYS:HD3   | 2.17                     | 0.43              |
| 1:P:20:ILE:HG21  | 1:P:42:PHE:CE2   | 2.54                     | 0.43              |
| 1:V:80:THR:CG2   | 1:V:101:MET:HE2  | 2.49                     | 0.43              |
| 1:Z:6:THR:HG23   | 1:Z:17:ILE:HD12  | 2.01                     | 0.43              |
| 2:E:104:A32:H6'1 | 3:E:191:HOH:O    | 2.19                     | 0.43              |
| 1:X:67:ARG:HG2   | 1:Y:29:GLU:OE2   | 2.19                     | 0.43              |
| 1:Y:78:THR:O     | 1:Y:79:GLU:HB2   | 2.19                     | 0.43              |
| 1:L:102:LYS:HE3  | 1:M:25:LEU:HD11  | 2.00                     | 0.42              |
| 1:P:37:MET:HE2   | 1:P:39:ILE:CG1   | 2.48                     | 0.42              |
| 1:V:62:LYS:HE3   | 1:V:63:LYS:HG2   | 2.01                     | 0.42              |
| 1:H:9:CYS:CB     | 1:H:17:ILE:HD11  | 2.49                     | 0.42              |
| 1:O:20:ILE:O     | 1:O:21:ASN:C     | 2.63                     | 0.42              |
| 1:M:6:THR:HG23   | 1:M:17:ILE:HG13  | 2.01                     | 0.42              |
| 1:V:58:ILE:HG13  | 1:V:61:GLN:HG3   | 2.02                     | 0.42              |
| 1:W:1:ALA:CB     | 1:W:2:PRO:CD     | 2.87                     | 0.42              |
| 1:Y:20:ILE:HG21  | 1:Y:42:PHE:CZ    | 2.54                     | 0.42              |
| 1:N:92:THR:HA    | 1:N:93:PRO:C     | 2.44                     | 0.42              |
| 1:O:102:LYS:O    | 1:O:103:ASN:C    | 2.62                     | 0.42              |
| 1:H:62:LYS:HA    | 1:H:62:LYS:HD2   | 1.77                     | 0.42              |
| 1:E:9:CYS:HB3    | 3:E:122:HOH:O    | 2.20                     | 0.42              |
| 1:F:63:LYS:HE3   | 3:F:209:HOH:O    | 2.19                     | 0.42              |
| 1:M:87:VAL:HA    | 1:M:95:SER:O     | 2.20                     | 0.42              |
| 1:P:22:ASP:HA    | 1:P:81:LYS:HG3   | 2.02                     | 0.42              |
| 1:Z:85:LEU:CD2   | 1:Z:99:ILE:HG22  | 2.49                     | 0.42              |
| 2:D:104:A32:H8'1 | 1:E:34:LYS:HE2   | 2.02                     | 0.42              |
| 1:F:102:LYS:HE3  | 1:F:102:LYS:HB2  | 1.82                     | 0.42              |
| 1:Y:99:ILE:HG22  | 1:Z:29:GLU:HB3   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:15:THR:O     | 1:Z:16:GLN:HB3   | 2.19                     | 0.42              |
| 1:P:21:ASN:HA    | 1:P:82:ILE:O     | 2.20                     | 0.42              |
| 1:W:30:SER:O     | 1:W:36:GLU:HA    | 2.20                     | 0.41              |
| 1:Y:15:THR:O     | 1:Y:16:GLN:HB3   | 2.19                     | 0.41              |
| 1:D:8:LEU:C      | 1:D:8:LEU:HD23   | 2.45                     | 0.41              |
| 2:G:104:A32:H8'1 | 2:G:104:A32:H5'1 | 1.51                     | 0.41              |
| 1:V:49:GLN:OE1   | 1:V:51:GLU:HA    | 2.19                     | 0.41              |
| 1:V:58:ILE:HD11  | 1:W:33:GLY:CA    | 2.49                     | 0.41              |
| 1:W:49:GLN:O     | 1:W:96:ILE:HG13  | 2.19                     | 0.41              |
| 1:O:16:GLN:NE2   | 1:O:89:ASN:HD22  | 2.11                     | 0.41              |
| 1:V:5:ILE:HG22   | 3:V:110:HOH:O    | 2.19                     | 0.41              |
| 1:V:93:PRO:HD3   | 1:Z:1:ALA:O      | 2.21                     | 0.41              |
| 1:Y:40:ILE:O     | 1:Y:40:ILE:HG13  | 2.20                     | 0.41              |
| 1:E:43:LYS:HE2   | 1:E:43:LYS:HB3   | 1.84                     | 0.41              |
| 1:Y:33:GLY:O     | 1:Y:34:LYS:HB2   | 2.20                     | 0.41              |
| 1:V:20:ILE:HG21  | 1:V:42:PHE:CD1   | 2.54                     | 0.41              |
| 1:W:89:ASN:O     | 1:W:91:LYS:N     | 2.52                     | 0.41              |
| 1:W:12:TYR:CE2   | 2:W:104:A32:H7'2 | 2.55                     | 0.41              |
| 1:W:37:MET:CE    | 1:W:39:ILE:HG12  | 2.42                     | 0.41              |
| 1:Y:41:THR:HG22  | 1:Y:47:THR:HG23  | 2.02                     | 0.41              |
| 1:Z:21:ASN:O     | 1:Z:22:ASP:HB2   | 2.20                     | 0.41              |
| 1:D:12:TYR:OH    | 2:D:104:A32:H6A1 | 2.20                     | 0.41              |
| 1:F:99:ILE:CD1   | 1:F:101:MET:HE2  | 2.51                     | 0.41              |
| 1:X:25:LEU:HD22  | 1:X:43:LYS:HA    | 2.01                     | 0.41              |
| 1:D:17:ILE:HD13  | 1:D:17:ILE:HA    | 1.89                     | 0.41              |
| 1:H:30:SER:O     | 1:H:36:GLU:HA    | 2.21                     | 0.41              |
| 1:N:57:HIS:O     | 1:N:62:LYS:HE3   | 2.21                     | 0.41              |
| 1:V:99:ILE:HG12  | 1:V:100:SER:N    | 2.36                     | 0.41              |
| 1:D:99:ILE:HD13  | 1:D:99:ILE:HG21  | 1.88                     | 0.41              |
| 1:L:31:MET:O     | 1:P:61:GLN:HG2   | 2.21                     | 0.41              |
| 1:L:92:THR:HA    | 1:L:93:PRO:HA    | 1.85                     | 0.41              |
| 1:D:23:LYS:CE    | 1:H:103:ASN:ND2  | 2.84                     | 0.41              |
| 1:D:34:LYS:HB2   | 2:H:104:A32:H7'2 | 2.03                     | 0.41              |
| 1:N:103:ASN:HD22 | 1:O:23:LYS:CE    | 2.28                     | 0.41              |
| 1:O:51:GLU:OE2   | 1:O:91:LYS:HE2   | 2.21                     | 0.41              |
| 1:Y:82:ILE:HG12  | 1:Y:99:ILE:HD11  | 2.03                     | 0.41              |
| 1:D:21:ASN:ND2   | 1:D:81:LYS:HD3   | 2.36                     | 0.40              |
| 1:F:103:ASN:ND2  | 1:G:23:LYS:NZ    | 2.69                     | 0.40              |
| 1:L:88:TRP:HB3   | 1:L:90:ASN:OD1   | 2.21                     | 0.40              |
| 1:M:20:ILE:CD1   | 1:M:85:LEU:HG    | 2.51                     | 0.40              |
| 1:M:88:TRP:CE2   | 2:M:104:A32:H51  | 2.55                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:25:LEU:CD2  | 1:N:43:LYS:HA    | 2.51                     | 0.40              |
| 1:V:58:ILE:HD13 | 1:W:34:LYS:HE2   | 2.01                     | 0.40              |
| 1:H:21:ASN:HA   | 1:H:82:ILE:O     | 2.21                     | 0.40              |
| 1:L:26:SER:O    | 1:L:40:ILE:HA    | 2.21                     | 0.40              |
| 1:Z:87:VAL:HB   | 1:Z:95:SER:O     | 2.21                     | 0.40              |
| 1:L:12:TYR:CZ   | 1:M:32:ALA:HB1   | 2.57                     | 0.40              |
| 1:L:28:THR:HB   | 1:L:39:ILE:HB    | 2.03                     | 0.40              |
| 1:N:58:ILE:CD1  | 1:O:34:LYS:HE3   | 2.52                     | 0.40              |
| 1:V:12:TYR:CD2  | 2:V:104:A32:H6'2 | 2.55                     | 0.40              |
| 1:G:58:ILE:H    | 1:G:58:ILE:HG13  | 1.75                     | 0.40              |
| 1:P:44:SER:OG   | 1:P:46:GLU:OE1   | 2.35                     | 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   | D     | 101/103 (98%) | 98 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 1   | E     | 101/103 (98%) | 99 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 1   | F     | 101/103 (98%) | 100 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 1   | G     | 101/103 (98%) | 98 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 1   | H     | 101/103 (98%) | 97 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 1   | L     | 101/103 (98%) | 97 (96%)  | 3 (3%)   | 1 (1%)   | 12          | 7   |
| 1   | M     | 101/103 (98%) | 97 (96%)  | 3 (3%)   | 1 (1%)   | 12          | 7   |
| 1   | N     | 101/103 (98%) | 96 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 1   | O     | 101/103 (98%) | 95 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 1   | P     | 101/103 (98%) | 98 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 1   | V     | 101/103 (98%) | 88 (87%)  | 12 (12%) | 1 (1%)   | 12          | 7   |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | W     | 101/103 (98%)   | 92 (91%)   | 7 (7%)  | 2 (2%)   | 6           | 1   |
| 1   | X     | 101/103 (98%)   | 95 (94%)   | 5 (5%)  | 1 (1%)   | 12          | 7   |
| 1   | Y     | 101/103 (98%)   | 98 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 1   | Z     | 101/103 (98%)   | 94 (93%)   | 4 (4%)  | 3 (3%)   | 3           | 0   |
| All | All   | 1515/1545 (98%) | 1442 (95%) | 64 (4%) | 9 (1%)   | 21          | 15  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 14  | ASN  |
| 1   | V     | 59  | ASP  |
| 1   | X     | 83  | ASP  |
| 1   | W     | 90  | ASN  |
| 1   | Z     | 16  | GLN  |
| 1   | L     | 10  | SER  |
| 1   | Z     | 21  | ASN  |
| 1   | Z     | 83  | ASP  |
| 1   | W     | 33  | GLY  |

### 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   | D     | 95/95 (100%) | 89 (94%)  | 6 (6%)   | 16          | 11 |
| 1   | E     | 95/95 (100%) | 93 (98%)  | 2 (2%)   | 47          | 51 |
| 1   | F     | 95/95 (100%) | 91 (96%)  | 4 (4%)   | 26          | 23 |
| 1   | G     | 95/95 (100%) | 92 (97%)  | 3 (3%)   | 34          | 35 |
| 1   | H     | 95/95 (100%) | 90 (95%)  | 5 (5%)   | 20          | 16 |
| 1   | L     | 95/95 (100%) | 89 (94%)  | 6 (6%)   | 16          | 11 |
| 1   | M     | 95/95 (100%) | 88 (93%)  | 7 (7%)   | 13          | 8  |
| 1   | N     | 95/95 (100%) | 91 (96%)  | 4 (4%)   | 26          | 23 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | O     | 95/95 (100%)     | 88 (93%)   | 7 (7%)   | 13          | 8  |
| 1   | P     | 95/95 (100%)     | 88 (93%)   | 7 (7%)   | 13          | 8  |
| 1   | V     | 95/95 (100%)     | 84 (88%)   | 11 (12%) | 5           | 2  |
| 1   | W     | 95/95 (100%)     | 86 (90%)   | 9 (10%)  | 8           | 4  |
| 1   | X     | 95/95 (100%)     | 90 (95%)   | 5 (5%)   | 20          | 16 |
| 1   | Y     | 95/95 (100%)     | 90 (95%)   | 5 (5%)   | 20          | 16 |
| 1   | Z     | 95/95 (100%)     | 84 (88%)   | 11 (12%) | 5           | 2  |
| All | All   | 1425/1425 (100%) | 1333 (94%) | 92 (6%)  | 15          | 10 |

All (92) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 16  | GLN  |
| 1   | D     | 34  | LYS  |
| 1   | D     | 43  | LYS  |
| 1   | D     | 62  | LYS  |
| 1   | D     | 63  | LYS  |
| 1   | D     | 102 | LYS  |
| 1   | E     | 44  | SER  |
| 1   | E     | 103 | ASN  |
| 1   | F     | 3   | GLN  |
| 1   | F     | 16  | GLN  |
| 1   | F     | 74  | ILE  |
| 1   | F     | 101 | MET  |
| 1   | G     | 13  | ARG  |
| 1   | G     | 102 | LYS  |
| 1   | G     | 103 | ASN  |
| 1   | H     | 13  | ARG  |
| 1   | H     | 56  | GLN  |
| 1   | H     | 59  | ASP  |
| 1   | H     | 62  | LYS  |
| 1   | H     | 103 | ASN  |
| 1   | L     | 34  | LYS  |
| 1   | L     | 43  | LYS  |
| 1   | L     | 62  | LYS  |
| 1   | L     | 81  | LYS  |
| 1   | L     | 92  | THR  |
| 1   | L     | 99  | ILE  |
| 1   | M     | 13  | ARG  |
| 1   | M     | 43  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 55  | SER  |
| 1   | M     | 81  | LYS  |
| 1   | M     | 95  | SER  |
| 1   | M     | 102 | LYS  |
| 1   | M     | 103 | ASN  |
| 1   | N     | 55  | SER  |
| 1   | N     | 59  | ASP  |
| 1   | N     | 62  | LYS  |
| 1   | N     | 95  | SER  |
| 1   | O     | 16  | GLN  |
| 1   | O     | 23  | LYS  |
| 1   | O     | 43  | LYS  |
| 1   | O     | 59  | ASP  |
| 1   | O     | 81  | LYS  |
| 1   | O     | 82  | ILE  |
| 1   | O     | 103 | ASN  |
| 1   | P     | 13  | ARG  |
| 1   | P     | 43  | LYS  |
| 1   | P     | 55  | SER  |
| 1   | P     | 56  | GLN  |
| 1   | P     | 62  | LYS  |
| 1   | P     | 81  | LYS  |
| 1   | P     | 103 | ASN  |
| 1   | V     | 5   | ILE  |
| 1   | V     | 28  | THR  |
| 1   | V     | 34  | LYS  |
| 1   | V     | 35  | ARG  |
| 1   | V     | 43  | LYS  |
| 1   | V     | 62  | LYS  |
| 1   | V     | 63  | LYS  |
| 1   | V     | 80  | THR  |
| 1   | V     | 84  | LYS  |
| 1   | V     | 100 | SER  |
| 1   | V     | 101 | MET  |
| 1   | W     | 3   | GLN  |
| 1   | W     | 19  | THR  |
| 1   | W     | 28  | THR  |
| 1   | W     | 34  | LYS  |
| 1   | W     | 81  | LYS  |
| 1   | W     | 92  | THR  |
| 1   | W     | 101 | MET  |
| 1   | W     | 102 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 103 | ASN  |
| 1   | X     | 3   | GLN  |
| 1   | X     | 5   | ILE  |
| 1   | X     | 10  | SER  |
| 1   | X     | 38  | VAL  |
| 1   | X     | 92  | THR  |
| 1   | Y     | 13  | ARG  |
| 1   | Y     | 16  | GLN  |
| 1   | Y     | 19  | THR  |
| 1   | Y     | 38  | VAL  |
| 1   | Y     | 89  | ASN  |
| 1   | Z     | 4   | THR  |
| 1   | Z     | 7   | GLU  |
| 1   | Z     | 43  | LYS  |
| 1   | Z     | 55  | SER  |
| 1   | Z     | 56  | GLN  |
| 1   | Z     | 59  | ASP  |
| 1   | Z     | 62  | LYS  |
| 1   | Z     | 79  | GLU  |
| 1   | Z     | 82  | ILE  |
| 1   | Z     | 95  | SER  |
| 1   | Z     | 99  | ILE  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 21  | ASN  |
| 1   | D     | 103 | ASN  |
| 1   | E     | 14  | ASN  |
| 1   | E     | 16  | GLN  |
| 1   | E     | 94  | ASN  |
| 1   | F     | 3   | GLN  |
| 1   | F     | 14  | ASN  |
| 1   | F     | 94  | ASN  |
| 1   | F     | 103 | ASN  |
| 1   | G     | 3   | GLN  |
| 1   | G     | 49  | GLN  |
| 1   | H     | 14  | ASN  |
| 1   | H     | 56  | GLN  |
| 1   | H     | 103 | ASN  |
| 1   | L     | 21  | ASN  |
| 1   | L     | 49  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 94  | ASN  |
| 1   | L     | 103 | ASN  |
| 1   | M     | 49  | GLN  |
| 1   | M     | 94  | ASN  |
| 1   | M     | 103 | ASN  |
| 1   | N     | 3   | GLN  |
| 1   | N     | 14  | ASN  |
| 1   | N     | 49  | GLN  |
| 1   | N     | 90  | ASN  |
| 1   | N     | 94  | ASN  |
| 1   | N     | 103 | ASN  |
| 1   | O     | 89  | ASN  |
| 1   | P     | 56  | GLN  |
| 1   | P     | 89  | ASN  |
| 1   | P     | 94  | ASN  |
| 1   | P     | 103 | ASN  |
| 1   | V     | 21  | ASN  |
| 1   | V     | 94  | ASN  |
| 1   | V     | 103 | ASN  |
| 1   | W     | 3   | GLN  |
| 1   | W     | 21  | ASN  |
| 1   | X     | 49  | GLN  |
| 1   | X     | 103 | ASN  |
| 1   | Y     | 3   | GLN  |
| 1   | Y     | 16  | GLN  |
| 1   | Y     | 89  | ASN  |
| 1   | Y     | 94  | ASN  |
| 1   | Z     | 3   | GLN  |
| 1   | Z     | 16  | GLN  |
| 1   | Z     | 56  | GLN  |
| 1   | Z     | 89  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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 |
| 2   | A32  | G     | 104 | -    | 35,35,35     | 1.59 | 6 (17%)  | 46,48,48    | 1.41 | 7 (15%)  |
| 2   | A32  | W     | 104 | -    | 35,35,35     | 1.81 | 11 (31%) | 46,48,48    | 2.53 | 13 (28%) |
| 2   | A32  | P     | 104 | -    | 35,35,35     | 1.76 | 8 (22%)  | 46,48,48    | 2.11 | 12 (26%) |
| 2   | A32  | O     | 104 | -    | 35,35,35     | 1.71 | 8 (22%)  | 46,48,48    | 2.10 | 9 (19%)  |
| 2   | A32  | Y     | 104 | -    | 35,35,35     | 1.80 | 7 (20%)  | 46,48,48    | 1.62 | 10 (21%) |
| 2   | A32  | Z     | 104 | -    | 35,35,35     | 1.82 | 11 (31%) | 46,48,48    | 2.06 | 15 (32%) |
| 2   | A32  | H     | 104 | -    | 35,35,35     | 2.06 | 13 (37%) | 46,48,48    | 3.32 | 17 (36%) |
| 2   | A32  | X     | 104 | -    | 35,35,35     | 1.69 | 10 (28%) | 46,48,48    | 2.70 | 11 (23%) |
| 2   | A32  | V     | 104 | -    | 35,35,35     | 1.78 | 6 (17%)  | 46,48,48    | 1.98 | 15 (32%) |
| 2   | A32  | M     | 104 | -    | 35,35,35     | 1.66 | 7 (20%)  | 46,48,48    | 1.97 | 13 (28%) |
| 2   | A32  | L     | 104 | -    | 35,35,35     | 1.73 | 10 (28%) | 46,48,48    | 1.88 | 14 (30%) |
| 2   | A32  | D     | 104 | -    | 35,35,35     | 1.76 | 7 (20%)  | 46,48,48    | 2.98 | 20 (43%) |
| 2   | A32  | E     | 104 | -    | 35,35,35     | 1.86 | 9 (25%)  | 46,48,48    | 3.29 | 17 (36%) |
| 2   | A32  | F     | 104 | -    | 35,35,35     | 1.67 | 7 (20%)  | 46,48,48    | 2.86 | 19 (41%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | A32  | G     | 104 | -    | -       | 3/19/49/49 | 0/3/3/3 |
| 2   | A32  | W     | 104 | -    | -       | 8/19/49/49 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | A32  | P     | 104 | -    | -       | 9/19/49/49 | 0/3/3/3 |
| 2   | A32  | O     | 104 | -    | -       | 8/19/49/49 | 0/3/3/3 |
| 2   | A32  | Y     | 104 | -    | -       | 6/19/49/49 | 0/3/3/3 |
| 2   | A32  | Z     | 104 | -    | -       | 6/19/49/49 | 0/3/3/3 |
| 2   | A32  | H     | 104 | -    | -       | 5/19/49/49 | 0/3/3/3 |
| 2   | A32  | X     | 104 | -    | -       | 3/19/49/49 | 0/3/3/3 |
| 2   | A32  | V     | 104 | -    | 1/1/8/9 | 5/19/49/49 | 0/3/3/3 |
| 2   | A32  | M     | 104 | -    | -       | 3/19/49/49 | 0/3/3/3 |
| 2   | A32  | L     | 104 | -    | -       | 6/19/49/49 | 0/3/3/3 |
| 2   | A32  | D     | 104 | -    | -       | 7/19/49/49 | 0/3/3/3 |
| 2   | A32  | E     | 104 | -    | -       | 7/19/49/49 | 0/3/3/3 |
| 2   | A32  | F     | 104 | -    | -       | 3/19/49/49 | 0/3/3/3 |

All (120) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 104 | A32  | O1-C1   | 4.48  | 1.48        | 1.41     |
| 2   | E     | 104 | A32  | O2'-N1' | 4.43  | 1.30        | 1.22     |
| 2   | D     | 104 | A32  | C7'-N2' | -4.38 | 1.24        | 1.33     |
| 2   | V     | 104 | A32  | O1-C1   | 4.32  | 1.47        | 1.41     |
| 2   | V     | 104 | A32  | C7'-N2' | -4.19 | 1.24        | 1.33     |
| 2   | H     | 104 | A32  | C7'-N2' | -4.17 | 1.24        | 1.33     |
| 2   | Y     | 104 | A32  | O1-C1   | 4.10  | 1.47        | 1.41     |
| 2   | P     | 104 | A32  | C5'-C7' | -4.10 | 1.41        | 1.50     |
| 2   | Z     | 104 | A32  | C7'-N2' | -4.08 | 1.24        | 1.33     |
| 2   | D     | 104 | A32  | O1-C1   | 3.95  | 1.47        | 1.41     |
| 2   | F     | 104 | A32  | O1-C1'  | 3.91  | 1.45        | 1.38     |
| 2   | O     | 104 | A32  | C7'-N2' | -3.90 | 1.25        | 1.33     |
| 2   | L     | 104 | A32  | C7'-N2' | -3.88 | 1.25        | 1.33     |
| 2   | Y     | 104 | A32  | C7'-N2' | -3.77 | 1.25        | 1.33     |
| 2   | Z     | 104 | A32  | C5'-C7' | -3.74 | 1.42        | 1.50     |
| 2   | M     | 104 | A32  | C7'-N2' | -3.70 | 1.25        | 1.33     |
| 2   | Y     | 104 | A32  | O1-C1'  | 3.70  | 1.45        | 1.38     |
| 2   | Y     | 104 | A32  | C5'-C7' | -3.70 | 1.42        | 1.50     |
| 2   | X     | 104 | A32  | C5'-C7' | -3.63 | 1.42        | 1.50     |
| 2   | O     | 104 | A32  | O1-C1'  | 3.63  | 1.45        | 1.38     |
| 2   | V     | 104 | A32  | C5'-C7' | -3.61 | 1.42        | 1.50     |
| 2   | M     | 104 | A32  | O1-C1'  | 3.61  | 1.45        | 1.38     |
| 2   | H     | 104 | A32  | O2'-N1' | 3.61  | 1.29        | 1.22     |
| 2   | P     | 104 | A32  | O1-C1'  | 3.59  | 1.45        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 104 | A32  | O1-C1'  | 3.59  | 1.45        | 1.38     |
| 2   | O     | 104 | A32  | C5'-C7' | -3.58 | 1.42        | 1.50     |
| 2   | H     | 104 | A32  | C5'-C7' | -3.51 | 1.42        | 1.50     |
| 2   | E     | 104 | A32  | C2'-C3' | 3.51  | 1.45        | 1.39     |
| 2   | D     | 104 | A32  | C5'-C7' | -3.46 | 1.42        | 1.50     |
| 2   | G     | 104 | A32  | C5'-C7' | -3.46 | 1.42        | 1.50     |
| 2   | M     | 104 | A32  | C5'-C7' | -3.45 | 1.42        | 1.50     |
| 2   | W     | 104 | A32  | C5'-C7' | -3.44 | 1.42        | 1.50     |
| 2   | L     | 104 | A32  | O1-C1'  | 3.43  | 1.44        | 1.38     |
| 2   | W     | 104 | A32  | O1-C1'  | 3.39  | 1.44        | 1.38     |
| 2   | X     | 104 | A32  | O2'-N1' | 3.35  | 1.28        | 1.22     |
| 2   | G     | 104 | A32  | O1-C1'  | 3.34  | 1.44        | 1.38     |
| 2   | L     | 104 | A32  | C5'-C7' | -3.34 | 1.42        | 1.50     |
| 2   | F     | 104 | A32  | O3'-C7' | 3.24  | 1.30        | 1.23     |
| 2   | P     | 104 | A32  | O1-C1   | 3.23  | 1.46        | 1.41     |
| 2   | E     | 104 | A32  | C5'-C7' | -3.23 | 1.43        | 1.50     |
| 2   | W     | 104 | A32  | O1-C1   | 3.22  | 1.46        | 1.41     |
| 2   | G     | 104 | A32  | C7'-N2' | -3.21 | 1.26        | 1.33     |
| 2   | P     | 104 | A32  | C4'-C5' | 3.19  | 1.44        | 1.39     |
| 2   | V     | 104 | A32  | O1-C1'  | 3.18  | 1.44        | 1.38     |
| 2   | X     | 104 | A32  | C7'-N2' | -3.17 | 1.26        | 1.33     |
| 2   | W     | 104 | A32  | C7'-N2' | -3.16 | 1.26        | 1.33     |
| 2   | H     | 104 | A32  | C2'-C3' | 3.05  | 1.44        | 1.39     |
| 2   | G     | 104 | A32  | O1-C1   | 3.05  | 1.45        | 1.41     |
| 2   | Z     | 104 | A32  | O1-C1'  | 3.04  | 1.44        | 1.38     |
| 2   | F     | 104 | A32  | O2'-N1' | 3.03  | 1.28        | 1.22     |
| 2   | H     | 104 | A32  | O1-C1'  | 3.01  | 1.44        | 1.38     |
| 2   | L     | 104 | A32  | O1-C1   | 2.99  | 1.45        | 1.41     |
| 2   | E     | 104 | A32  | C4'-C3' | 2.96  | 1.44        | 1.39     |
| 2   | F     | 104 | A32  | C4'-C5' | 2.96  | 1.43        | 1.39     |
| 2   | W     | 104 | A32  | C4'-C5' | 2.96  | 1.43        | 1.39     |
| 2   | E     | 104 | A32  | C6'-C5' | 2.95  | 1.43        | 1.39     |
| 2   | H     | 104 | A32  | O3'-C7' | 2.94  | 1.30        | 1.23     |
| 2   | F     | 104 | A32  | C5'-C7' | -2.92 | 1.43        | 1.50     |
| 2   | E     | 104 | A32  | C7'-N2' | -2.89 | 1.27        | 1.33     |
| 2   | F     | 104 | A32  | C2'-C3' | 2.89  | 1.43        | 1.39     |
| 2   | D     | 104 | A32  | C4'-C3' | 2.85  | 1.43        | 1.39     |
| 2   | E     | 104 | A32  | O1-C1'  | 2.82  | 1.43        | 1.38     |
| 2   | Z     | 104 | A32  | O1-C1   | 2.82  | 1.45        | 1.41     |
| 2   | X     | 104 | A32  | C4'-C3' | 2.80  | 1.43        | 1.39     |
| 2   | O     | 104 | A32  | O1-C1   | 2.80  | 1.45        | 1.41     |
| 2   | Z     | 104 | A32  | C5B-N4' | 2.78  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | X     | 104 | A32  | C2'-C3' | 2.70  | 1.43        | 1.39     |
| 2   | W     | 104 | A32  | O2'-N1' | 2.69  | 1.27        | 1.22     |
| 2   | P     | 104 | A32  | C7'-N2' | -2.63 | 1.28        | 1.33     |
| 2   | X     | 104 | A32  | C4'-C5' | 2.61  | 1.43        | 1.39     |
| 2   | F     | 104 | A32  | C7'-N2' | -2.59 | 1.28        | 1.33     |
| 2   | M     | 104 | A32  | O1-C1   | 2.58  | 1.45        | 1.41     |
| 2   | L     | 104 | A32  | C9'-N2' | -2.58 | 1.40        | 1.46     |
| 2   | Z     | 104 | A32  | O2'-N1' | 2.53  | 1.27        | 1.22     |
| 2   | X     | 104 | A32  | C4-C3   | 2.51  | 1.58        | 1.52     |
| 2   | W     | 104 | A32  | C2'-C3' | 2.50  | 1.43        | 1.39     |
| 2   | E     | 104 | A32  | C4'-C5' | 2.49  | 1.43        | 1.39     |
| 2   | D     | 104 | A32  | O3'-C7' | 2.49  | 1.29        | 1.23     |
| 2   | H     | 104 | A32  | C9'-N2' | -2.48 | 1.40        | 1.46     |
| 2   | H     | 104 | A32  | C4-C3   | 2.46  | 1.58        | 1.52     |
| 2   | E     | 104 | A32  | C7B-N4' | 2.44  | 1.53        | 1.47     |
| 2   | V     | 104 | A32  | C4'-C3' | 2.40  | 1.43        | 1.39     |
| 2   | H     | 104 | A32  | C6'-C5' | 2.40  | 1.43        | 1.39     |
| 2   | L     | 104 | A32  | C2'-C3' | 2.39  | 1.43        | 1.39     |
| 2   | H     | 104 | A32  | C4'-C5' | 2.39  | 1.43        | 1.39     |
| 2   | D     | 104 | A32  | C6'-C5' | 2.32  | 1.43        | 1.39     |
| 2   | W     | 104 | A32  | C6'-C5' | 2.32  | 1.43        | 1.39     |
| 2   | X     | 104 | A32  | C7B-N4' | 2.30  | 1.52        | 1.47     |
| 2   | L     | 104 | A32  | O2'-N1' | 2.30  | 1.26        | 1.22     |
| 2   | L     | 104 | A32  | C5B-N4' | 2.30  | 1.53        | 1.46     |
| 2   | Y     | 104 | A32  | C7B-N4' | 2.29  | 1.52        | 1.47     |
| 2   | Z     | 104 | A32  | C2'-C3' | 2.28  | 1.42        | 1.39     |
| 2   | W     | 104 | A32  | C4'-C3' | 2.28  | 1.42        | 1.39     |
| 2   | M     | 104 | A32  | O2'-N1' | 2.25  | 1.26        | 1.22     |
| 2   | Z     | 104 | A32  | C4'-C3' | 2.24  | 1.42        | 1.39     |
| 2   | L     | 104 | A32  | C4'-C5' | 2.23  | 1.42        | 1.39     |
| 2   | P     | 104 | A32  | O2'-N1' | 2.23  | 1.26        | 1.22     |
| 2   | Y     | 104 | A32  | O2'-N1' | 2.21  | 1.26        | 1.22     |
| 2   | X     | 104 | A32  | O1-C1'  | 2.18  | 1.42        | 1.38     |
| 2   | M     | 104 | A32  | C2'-C3' | 2.16  | 1.42        | 1.39     |
| 2   | P     | 104 | A32  | C5B-N4' | 2.16  | 1.52        | 1.46     |
| 2   | Z     | 104 | A32  | O3-C3   | -2.13 | 1.37        | 1.43     |
| 2   | W     | 104 | A32  | O5-C1   | 2.13  | 1.47        | 1.41     |
| 2   | P     | 104 | A32  | C3B-N4' | 2.13  | 1.52        | 1.46     |
| 2   | O     | 104 | A32  | C4'-C3' | 2.12  | 1.42        | 1.39     |
| 2   | M     | 104 | A32  | C9'-N2' | -2.11 | 1.41        | 1.46     |
| 2   | H     | 104 | A32  | C7B-N4' | 2.11  | 1.52        | 1.47     |
| 2   | Z     | 104 | A32  | C3B-N4' | 2.10  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | O     | 104 | A32  | C3B-N4' | 2.10  | 1.52        | 1.46     |
| 2   | H     | 104 | A32  | C3B-N4' | 2.09  | 1.52        | 1.46     |
| 2   | L     | 104 | A32  | C4'-C3' | 2.09  | 1.42        | 1.39     |
| 2   | Z     | 104 | A32  | C9'-N2' | -2.07 | 1.41        | 1.46     |
| 2   | V     | 104 | A32  | C9'-N2' | -2.06 | 1.41        | 1.46     |
| 2   | O     | 104 | A32  | C4'-C5' | 2.06  | 1.42        | 1.39     |
| 2   | O     | 104 | A32  | O2'-N1' | 2.05  | 1.26        | 1.22     |
| 2   | G     | 104 | A32  | C5B-N4' | 2.05  | 1.52        | 1.46     |
| 2   | Y     | 104 | A32  | C5B-N4' | 2.04  | 1.52        | 1.46     |
| 2   | X     | 104 | A32  | C3B-N4' | 2.04  | 1.52        | 1.46     |
| 2   | G     | 104 | A32  | C4'-C3' | 2.03  | 1.42        | 1.39     |
| 2   | W     | 104 | A32  | C7B-N4' | 2.02  | 1.52        | 1.47     |

All (192) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 104 | A32  | C4'-C3'-N1' | 13.89 | 130.70      | 118.74   |
| 2   | E     | 104 | A32  | C1'-O1-C1   | 10.52 | 132.64      | 117.82   |
| 2   | F     | 104 | A32  | C4'-C3'-N1' | 10.51 | 127.79      | 118.74   |
| 2   | E     | 104 | A32  | C4'-C3'-N1' | 9.98  | 127.34      | 118.74   |
| 2   | W     | 104 | A32  | C4'-C3'-N1' | 9.97  | 127.33      | 118.74   |
| 2   | X     | 104 | A32  | C1'-O1-C1   | 9.47  | 131.16      | 117.82   |
| 2   | D     | 104 | A32  | C2'-C3'-N1' | 9.28  | 126.73      | 118.74   |
| 2   | E     | 104 | A32  | O1-C1-C2    | 7.60  | 118.23      | 107.16   |
| 2   | M     | 104 | A32  | O1-C1-C2    | 7.39  | 117.93      | 107.16   |
| 2   | W     | 104 | A32  | O2-C2-C1    | 7.38  | 127.67      | 110.08   |
| 2   | X     | 104 | A32  | C4'-C3'-N1' | 7.25  | 124.98      | 118.74   |
| 2   | O     | 104 | A32  | O1-C1-C2    | 7.08  | 117.47      | 107.16   |
| 2   | H     | 104 | A32  | C2'-C3'-N1' | -6.89 | 112.80      | 118.74   |
| 2   | D     | 104 | A32  | O1-C1-C2    | 6.26  | 116.28      | 107.16   |
| 2   | P     | 104 | A32  | O3'-C7'-C5' | 6.20  | 133.19      | 120.90   |
| 2   | O     | 104 | A32  | C2'-C3'-N1' | 6.20  | 124.08      | 118.74   |
| 2   | D     | 104 | A32  | C2B-C3B-N4' | 6.14  | 119.45      | 110.12   |
| 2   | O     | 104 | A32  | O2-C2-C1    | 5.92  | 124.19      | 110.08   |
| 2   | H     | 104 | A32  | C5'-C4'-C3' | 5.90  | 126.59      | 119.79   |
| 2   | F     | 104 | A32  | C5'-C6'-C1' | 5.89  | 125.65      | 119.56   |
| 2   | E     | 104 | A32  | O3'-C7'-N2' | -5.81 | 111.27      | 122.59   |
| 2   | V     | 104 | A32  | C2'-C3'-N1' | 5.74  | 123.69      | 118.74   |
| 2   | X     | 104 | A32  | O1-C1-C2    | 5.73  | 115.52      | 107.16   |
| 2   | Z     | 104 | A32  | C4'-C3'-N1' | 5.70  | 123.65      | 118.74   |
| 2   | F     | 104 | A32  | C1'-O1-C1   | 5.64  | 125.77      | 117.82   |
| 2   | H     | 104 | A32  | C6'-C5'-C4' | -5.54 | 113.17      | 119.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 104 | A32  | C5'-C7'-N2' | 5.42  | 128.38      | 117.12   |
| 2   | Z     | 104 | A32  | O3-C3-C2    | 5.42  | 123.14      | 110.38   |
| 2   | X     | 104 | A32  | C6'-C5'-C4' | -5.33 | 113.41      | 119.65   |
| 2   | F     | 104 | A32  | C6'-C5'-C4' | -5.20 | 113.56      | 119.65   |
| 2   | D     | 104 | A32  | C9'-N2'-C7' | 5.19  | 133.84      | 122.11   |
| 2   | F     | 104 | A32  | O1-C1-C2    | 5.12  | 114.62      | 107.16   |
| 2   | E     | 104 | A32  | O5-C1-O1    | 5.07  | 121.41      | 108.42   |
| 2   | H     | 104 | A32  | C9'-N2'-C7' | 5.03  | 133.49      | 122.11   |
| 2   | W     | 104 | A32  | C1'-O1-C1   | 4.85  | 124.66      | 117.82   |
| 2   | L     | 104 | A32  | O1-C1-C2    | 4.82  | 114.18      | 107.16   |
| 2   | P     | 104 | A32  | O3'-C7'-N2' | -4.71 | 113.41      | 122.59   |
| 2   | W     | 104 | A32  | O1-C1-C2    | 4.61  | 113.88      | 107.16   |
| 2   | P     | 104 | A32  | O1-C1-C2    | 4.60  | 113.86      | 107.16   |
| 2   | P     | 104 | A32  | C4'-C3'-N1' | 4.59  | 122.69      | 118.74   |
| 2   | D     | 104 | A32  | O1B-C2B-C3B | 4.59  | 121.66      | 111.77   |
| 2   | E     | 104 | A32  | C6'-C5'-C4' | -4.53 | 114.35      | 119.65   |
| 2   | X     | 104 | A32  | C5'-C6'-C1' | 4.50  | 124.21      | 119.56   |
| 2   | D     | 104 | A32  | O3'-C7'-C5' | -4.47 | 112.04      | 120.90   |
| 2   | E     | 104 | A32  | C5'-C7'-N2' | 4.45  | 126.38      | 117.12   |
| 2   | V     | 104 | A32  | O2-C2-C1    | 4.45  | 120.67      | 110.08   |
| 2   | D     | 104 | A32  | C5'-C4'-C3' | 4.27  | 124.71      | 119.79   |
| 2   | E     | 104 | A32  | C5'-C6'-C1' | 4.26  | 123.96      | 119.56   |
| 2   | F     | 104 | A32  | C2'-C3'-N1' | -4.23 | 115.09      | 118.74   |
| 2   | E     | 104 | A32  | C5'-C4'-C3' | 4.20  | 124.63      | 119.79   |
| 2   | H     | 104 | A32  | C1'-O1-C1   | -4.20 | 111.91      | 117.82   |
| 2   | H     | 104 | A32  | O3'-C7'-N2' | -4.19 | 114.42      | 122.59   |
| 2   | D     | 104 | A32  | C1'-O1-C1   | -4.14 | 111.98      | 117.82   |
| 2   | D     | 104 | A32  | C6'-C1'-C2' | 4.12  | 127.23      | 120.98   |
| 2   | F     | 104 | A32  | C7B-N4'-C3B | 4.05  | 122.04      | 111.24   |
| 2   | X     | 104 | A32  | O5-C1-O1    | 3.92  | 118.45      | 108.42   |
| 2   | M     | 104 | A32  | C1'-O1-C1   | 3.82  | 123.20      | 117.82   |
| 2   | Z     | 104 | A32  | C1'-O1-C1   | 3.79  | 123.16      | 117.82   |
| 2   | X     | 104 | A32  | C4-C3-C2    | -3.79 | 104.18      | 110.83   |
| 2   | W     | 104 | A32  | C2'-C3'-N1' | -3.79 | 115.47      | 118.74   |
| 2   | Z     | 104 | A32  | C6'-C5'-C4' | -3.76 | 115.25      | 119.65   |
| 2   | L     | 104 | A32  | C9'-N2'-C7' | 3.73  | 130.55      | 122.11   |
| 2   | X     | 104 | A32  | O3'-C7'-N2' | -3.71 | 115.36      | 122.59   |
| 2   | Y     | 104 | A32  | C5'-C4'-C3' | 3.66  | 124.01      | 119.79   |
| 2   | V     | 104 | A32  | O3'-C7'-C5' | -3.60 | 113.76      | 120.90   |
| 2   | M     | 104 | A32  | C4'-C3'-N1' | 3.60  | 121.84      | 118.74   |
| 2   | D     | 104 | A32  | C5'-C6'-C1' | -3.57 | 115.86      | 119.56   |
| 2   | M     | 104 | A32  | C5B-N4'-C3B | 3.53  | 116.45      | 108.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 104 | A32  | C5'-C7'-N2' | 3.52  | 124.44      | 117.12   |
| 2   | W     | 104 | A32  | C6'-C5'-C4' | -3.52 | 115.54      | 119.65   |
| 2   | H     | 104 | A32  | C4'-C5'-C7' | 3.51  | 132.01      | 120.40   |
| 2   | L     | 104 | A32  | C4'-C3'-N1' | 3.51  | 121.76      | 118.74   |
| 2   | E     | 104 | A32  | C5B-N4'-C3B | 3.50  | 116.39      | 108.84   |
| 2   | H     | 104 | A32  | C6'-C1'-C2' | 3.50  | 126.28      | 120.98   |
| 2   | F     | 104 | A32  | O3'-C7'-C5' | 3.49  | 127.82      | 120.90   |
| 2   | P     | 104 | A32  | C6'-C5'-C4' | -3.44 | 115.63      | 119.65   |
| 2   | Y     | 104 | A32  | C1'-O1-C1   | -3.44 | 112.98      | 117.82   |
| 2   | X     | 104 | A32  | C5'-C4'-C3' | 3.42  | 123.73      | 119.79   |
| 2   | F     | 104 | A32  | C2B-C3B-N4' | -3.38 | 104.98      | 110.12   |
| 2   | L     | 104 | A32  | C1'-O1-C1   | 3.38  | 122.58      | 117.82   |
| 2   | D     | 104 | A32  | O2'-N1'-C3' | 3.38  | 123.47      | 118.82   |
| 2   | P     | 104 | A32  | O2-C2-C1    | 3.35  | 118.06      | 110.08   |
| 2   | P     | 104 | A32  | C5'-C4'-C3' | 3.35  | 123.64      | 119.79   |
| 2   | E     | 104 | A32  | C4'-C3'-C2' | -3.35 | 115.56      | 120.80   |
| 2   | M     | 104 | A32  | O3'-C7'-C5' | -3.35 | 114.27      | 120.90   |
| 2   | Y     | 104 | A32  | C4'-C3'-N1' | 3.33  | 121.61      | 118.74   |
| 2   | L     | 104 | A32  | O4-C4-C3    | 3.32  | 118.21      | 110.38   |
| 2   | G     | 104 | A32  | O5-C1-O1    | 3.31  | 116.90      | 108.42   |
| 2   | F     | 104 | A32  | C5'-C4'-C3' | 3.29  | 123.58      | 119.79   |
| 2   | Z     | 104 | A32  | O1-C1-C2    | 3.27  | 111.92      | 107.16   |
| 2   | L     | 104 | A32  | C5'-C6'-C1' | 3.26  | 122.93      | 119.56   |
| 2   | D     | 104 | A32  | C6B-C5B-N4' | 3.24  | 115.05      | 110.12   |
| 2   | X     | 104 | A32  | O3-C3-C4    | -3.23 | 102.77      | 110.38   |
| 2   | H     | 104 | A32  | C2B-C3B-N4' | 3.22  | 115.01      | 110.12   |
| 2   | Y     | 104 | A32  | C5'-C7'-N2' | 3.20  | 123.77      | 117.12   |
| 2   | H     | 104 | A32  | O2'-N1'-C3' | -3.18 | 114.44      | 118.82   |
| 2   | Z     | 104 | A32  | C2B-C3B-N4' | -3.18 | 105.29      | 110.12   |
| 2   | V     | 104 | A32  | C9'-N2'-C7' | 3.17  | 129.28      | 122.11   |
| 2   | W     | 104 | A32  | C5'-C4'-C3' | 3.15  | 123.42      | 119.79   |
| 2   | D     | 104 | A32  | C4-C3-C2    | -3.14 | 105.32      | 110.83   |
| 2   | V     | 104 | A32  | C1-O5-C5    | -3.13 | 107.61      | 113.72   |
| 2   | Z     | 104 | A32  | C5'-C4'-C3' | 3.12  | 123.39      | 119.79   |
| 2   | L     | 104 | A32  | C6B-C5B-N4' | -3.11 | 105.39      | 110.12   |
| 2   | Y     | 104 | A32  | C6'-C5'-C4' | -3.10 | 116.02      | 119.65   |
| 2   | V     | 104 | A32  | C6'-C1'-C2' | 3.06  | 125.62      | 120.98   |
| 2   | M     | 104 | A32  | O2-C2-C1    | 3.04  | 117.31      | 110.08   |
| 2   | G     | 104 | A32  | C8'-C7B-N4' | -3.01 | 105.46      | 113.93   |
| 2   | O     | 104 | A32  | O3'-C7'-C5' | -2.99 | 114.98      | 120.90   |
| 2   | H     | 104 | A32  | C5B-N4'-C3B | 2.95  | 115.20      | 108.84   |
| 2   | D     | 104 | A32  | C4'-C3'-C2' | -2.91 | 116.23      | 120.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | M     | 104 | A32  | O5-C1-O1    | 2.91  | 115.88      | 108.42   |
| 2   | P     | 104 | A32  | C6'-C5'-C7' | 2.86  | 129.85      | 120.40   |
| 2   | O     | 104 | A32  | C7B-N4'-C3B | 2.84  | 118.82      | 111.24   |
| 2   | E     | 104 | A32  | C8'-C7B-N4' | -2.81 | 106.02      | 113.93   |
| 2   | P     | 104 | A32  | C2B-C3B-N4' | -2.78 | 105.90      | 110.12   |
| 2   | E     | 104 | A32  | C3'-C2'-C1' | 2.77  | 122.28      | 119.00   |
| 2   | Y     | 104 | A32  | O3-C3-C4    | 2.77  | 116.90      | 110.38   |
| 2   | G     | 104 | A32  | C6'-C5'-C4' | -2.76 | 116.42      | 119.65   |
| 2   | L     | 104 | A32  | O2-C2-C3    | 2.76  | 116.88      | 110.38   |
| 2   | F     | 104 | A32  | O5-C1-O1    | 2.75  | 115.46      | 108.42   |
| 2   | H     | 104 | A32  | C4'-C3'-C2' | -2.75 | 116.50      | 120.80   |
| 2   | Z     | 104 | A32  | C3-C4-C5    | -2.75 | 105.25      | 110.23   |
| 2   | H     | 104 | A32  | O5-C1-O1    | 2.74  | 115.43      | 108.42   |
| 2   | L     | 104 | A32  | C7B-N4'-C3B | 2.74  | 118.54      | 111.24   |
| 2   | M     | 104 | A32  | C6'-C5'-C4' | -2.71 | 116.48      | 119.65   |
| 2   | H     | 104 | A32  | C6B-C5B-N4' | 2.69  | 114.20      | 110.12   |
| 2   | O     | 104 | A32  | C5'-C4'-C3' | 2.67  | 122.86      | 119.79   |
| 2   | V     | 104 | A32  | C6B-C5B-N4' | -2.67 | 106.07      | 110.12   |
| 2   | L     | 104 | A32  | O5-C1-O1    | 2.66  | 115.22      | 108.42   |
| 2   | Y     | 104 | A32  | C6'-C1'-C2' | 2.64  | 124.99      | 120.98   |
| 2   | V     | 104 | A32  | O3-C3-C4    | 2.64  | 116.61      | 110.38   |
| 2   | P     | 104 | A32  | O2-C2-C3    | 2.64  | 116.59      | 110.38   |
| 2   | D     | 104 | A32  | C7B-N4'-C3B | 2.61  | 118.18      | 111.24   |
| 2   | Z     | 104 | A32  | C5'-C7'-N2' | 2.59  | 122.51      | 117.12   |
| 2   | O     | 104 | A32  | C9'-N2'-C7' | 2.56  | 127.89      | 122.11   |
| 2   | H     | 104 | A32  | O3-C3-C2    | -2.56 | 104.35      | 110.38   |
| 2   | L     | 104 | A32  | C6'-C5'-C4' | -2.54 | 116.68      | 119.65   |
| 2   | G     | 104 | A32  | C5B-N4'-C3B | 2.53  | 114.28      | 108.84   |
| 2   | O     | 104 | A32  | C4'-C3'-C2' | -2.52 | 116.86      | 120.80   |
| 2   | L     | 104 | A32  | C2B-C3B-N4' | -2.52 | 106.30      | 110.12   |
| 2   | Z     | 104 | A32  | C9'-N2'-C7' | 2.50  | 127.75      | 122.11   |
| 2   | Z     | 104 | A32  | O3'-C7'-C5' | -2.49 | 115.96      | 120.90   |
| 2   | E     | 104 | A32  | O2-C2-C3    | -2.48 | 104.54      | 110.38   |
| 2   | F     | 104 | A32  | C8'-C7B-N4' | -2.45 | 107.06      | 113.93   |
| 2   | Z     | 104 | A32  | C7B-N4'-C5B | -2.42 | 104.78      | 111.24   |
| 2   | Y     | 104 | A32  | C2'-C3'-N1' | 2.39  | 120.80      | 118.74   |
| 2   | Y     | 104 | A32  | C6B-C5B-N4' | 2.39  | 113.75      | 110.12   |
| 2   | E     | 104 | A32  | C6B-C5B-N4' | -2.39 | 106.49      | 110.12   |
| 2   | F     | 104 | A32  | C4'-C3'-C2' | -2.35 | 117.12      | 120.80   |
| 2   | V     | 104 | A32  | C6-C5-C4    | 2.35  | 118.79      | 113.02   |
| 2   | F     | 104 | A32  | C4'-C5'-C7' | 2.35  | 128.16      | 120.40   |
| 2   | P     | 104 | A32  | C6'-C1'-C2' | 2.35  | 124.54      | 120.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 104 | A32  | O5-C1-C2    | -2.33 | 105.59      | 110.37   |
| 2   | W     | 104 | A32  | C4'-C3'-C2' | -2.32 | 117.17      | 120.80   |
| 2   | W     | 104 | A32  | C1-O5-C5    | -2.30 | 109.23      | 113.72   |
| 2   | L     | 104 | A32  | C6B-O1B-C2B | 2.30  | 117.30      | 109.88   |
| 2   | D     | 104 | A32  | C6B-O1B-C2B | 2.29  | 117.29      | 109.88   |
| 2   | W     | 104 | A32  | O3'-C7'-N2' | -2.29 | 118.13      | 122.59   |
| 2   | M     | 104 | A32  | O1B-C2B-C3B | -2.28 | 106.87      | 111.77   |
| 2   | F     | 104 | A32  | C3'-C2'-C1' | 2.27  | 121.68      | 119.00   |
| 2   | F     | 104 | A32  | O3'-C7'-N2' | -2.26 | 118.18      | 122.59   |
| 2   | W     | 104 | A32  | C1-C2-C3    | 2.24  | 114.71      | 110.01   |
| 2   | V     | 104 | A32  | C1'-O1-C1   | -2.22 | 114.69      | 117.82   |
| 2   | Z     | 104 | A32  | O5-C5-C4    | -2.21 | 105.72      | 109.70   |
| 2   | Z     | 104 | A32  | C6'-C1'-C2' | 2.19  | 124.31      | 120.98   |
| 2   | F     | 104 | A32  | C6B-C5B-N4' | -2.17 | 106.81      | 110.12   |
| 2   | E     | 104 | A32  | O1B-C2B-C3B | -2.17 | 107.10      | 111.77   |
| 2   | V     | 104 | A32  | O3'-C7'-N2' | 2.17  | 126.82      | 122.59   |
| 2   | M     | 104 | A32  | C5'-C7'-N2' | 2.17  | 121.62      | 117.12   |
| 2   | V     | 104 | A32  | C4-C3-C2    | 2.16  | 114.62      | 110.83   |
| 2   | M     | 104 | A32  | C5'-C6'-C1' | 2.16  | 121.79      | 119.56   |
| 2   | D     | 104 | A32  | C4'-C5'-C7' | 2.15  | 127.50      | 120.40   |
| 2   | X     | 104 | A32  | C5B-N4'-C3B | 2.14  | 113.46      | 108.84   |
| 2   | V     | 104 | A32  | C5B-N4'-C3B | 2.14  | 113.44      | 108.84   |
| 2   | D     | 104 | A32  | O2-C2-C1    | 2.13  | 115.15      | 110.08   |
| 2   | G     | 104 | A32  | C6'-C1'-C2' | 2.11  | 124.18      | 120.98   |
| 2   | F     | 104 | A32  | C6B-O1B-C2B | 2.11  | 116.69      | 109.88   |
| 2   | V     | 104 | A32  | C1-C2-C3    | 2.10  | 114.44      | 110.01   |
| 2   | M     | 104 | A32  | C5'-C4'-C3' | 2.10  | 122.20      | 119.79   |
| 2   | V     | 104 | A32  | O4-C4-C3    | 2.09  | 115.30      | 110.38   |
| 2   | Z     | 104 | A32  | O5-C5-C6    | 2.06  | 111.56      | 106.44   |
| 2   | G     | 104 | A32  | O2-C2-C1    | -2.06 | 105.16      | 110.08   |
| 2   | F     | 104 | A32  | C9'-N2'-C7' | -2.06 | 117.44      | 122.11   |
| 2   | W     | 104 | A32  | C5B-N4'-C3B | 2.05  | 113.25      | 108.84   |
| 2   | Y     | 104 | A32  | C4'-C3'-C2' | -2.05 | 117.59      | 120.80   |
| 2   | G     | 104 | A32  | O5-C5-C6    | 2.05  | 111.51      | 106.44   |
| 2   | O     | 104 | A32  | O5-C1-O1    | 2.04  | 113.65      | 108.42   |
| 2   | L     | 104 | A32  | O2-C2-C1    | 2.04  | 114.94      | 110.08   |
| 2   | W     | 104 | A32  | C5'-C6'-C1' | 2.02  | 121.64      | 119.56   |
| 2   | P     | 104 | A32  | C1'-O1-C1   | -2.01 | 114.98      | 117.82   |
| 2   | D     | 104 | A32  | C4'-C3'-N1' | -2.01 | 117.00      | 118.74   |
| 2   | M     | 104 | A32  | C9'-N2'-C7' | 2.00  | 126.63      | 122.11   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | V     | 104 | A32  | C2   |

All (79) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | E     | 104 | A32  | O5-C1-O1-C1'    |
| 2   | O     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | O     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | X     | 104 | A32  | O5-C1-O1-C1'    |
| 2   | H     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | E     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | W     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | Y     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | M     | 104 | A32  | C8'-C7B-N4'-C5B |
| 2   | W     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | D     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | W     | 104 | A32  | O5-C5-C6-O6     |
| 2   | H     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | E     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | O     | 104 | A32  | C8'-C7B-N4'-C5B |
| 2   | W     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | V     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | W     | 104 | A32  | C4-C5-C6-O6     |
| 2   | W     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | Z     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | D     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | E     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | D     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | Z     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | O     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | L     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | Z     | 104 | A32  | O5-C5-C6-O6     |
| 2   | V     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | Y     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | L     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | E     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | G     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | Y     | 104 | A32  | O5-C5-C6-O6     |
| 2   | V     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | Z     | 104 | A32  | C4-C5-C6-O6     |
| 2   | L     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | D     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | D     | 104 | A32  | C8'-C7B-N4'-C5B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | X     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | M     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | O     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | O     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | P     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | P     | 104 | A32  | C5'-C7'-N2'-C9' |
| 2   | W     | 104 | A32  | C8'-C7B-N4'-C5B |
| 2   | P     | 104 | A32  | O3'-C7'-N2'-C9' |
| 2   | V     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | Y     | 104 | A32  | C4-C5-C6-O6     |
| 2   | L     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | W     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | E     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | P     | 104 | A32  | C8'-C7B-N4'-C5B |
| 2   | Z     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | D     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | Y     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | P     | 104 | A32  | O5-C5-C6-O6     |
| 2   | P     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | P     | 104 | A32  | C4-C5-C6-O6     |
| 2   | M     | 104 | A32  | O5-C1-O1-C1'    |
| 2   | D     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | Y     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | G     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | P     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | F     | 104 | A32  | O5-C1-O1-C1'    |
| 2   | X     | 104 | A32  | C7B-C8'-C9'-N2' |
| 2   | F     | 104 | A32  | C8'-C7B-N4'-C5B |
| 2   | G     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | H     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | F     | 104 | A32  | N4'-C7B-C8'-C9' |
| 2   | P     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | H     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | E     | 104 | A32  | C4'-C3'-N1'-O2' |
| 2   | V     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | L     | 104 | A32  | O5-C1-O1-C1'    |
| 2   | O     | 104 | A32  | C6'-C1'-O1-C1   |
| 2   | L     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | O     | 104 | A32  | C2'-C1'-O1-C1   |
| 2   | Z     | 104 | A32  | C8'-C7B-N4'-C3B |
| 2   | H     | 104 | A32  | C7B-C8'-C9'-N2' |

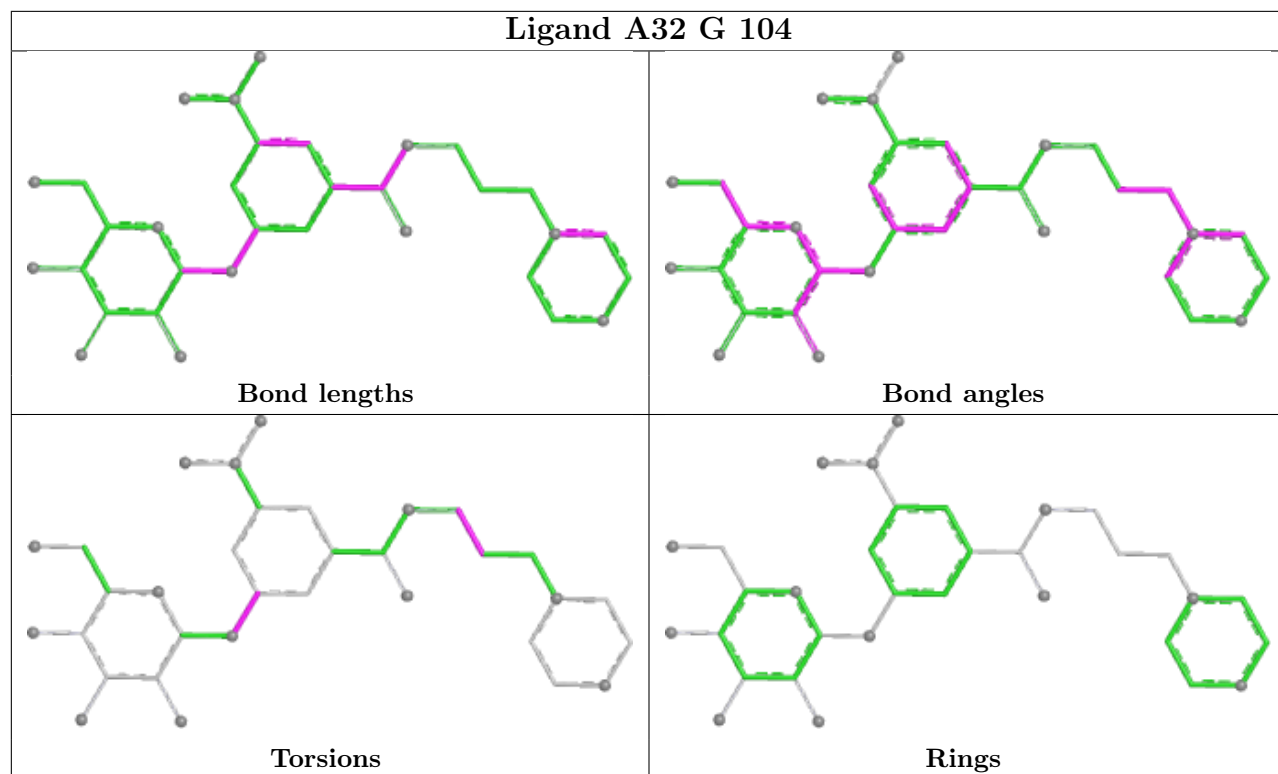
There are no ring outliers.

13 monomers are involved in 57 short contacts:

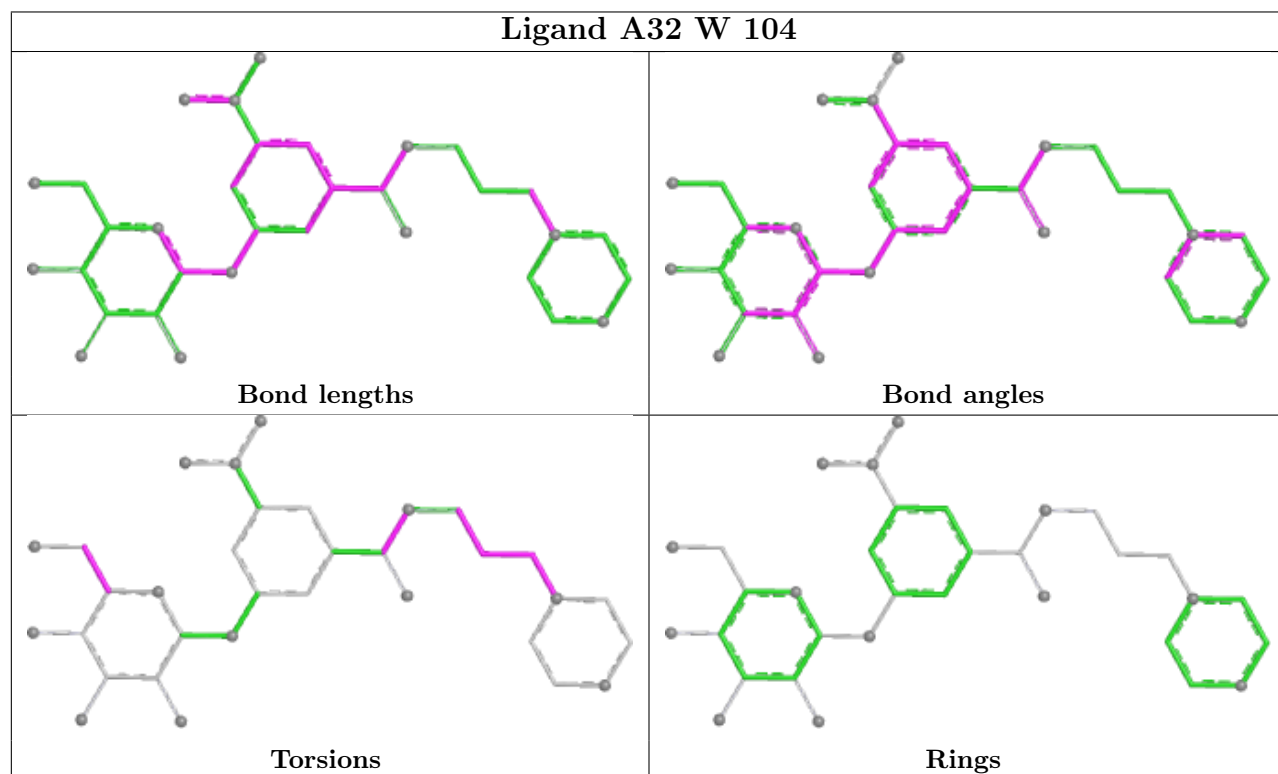
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | G     | 104 | A32  | 2       | 0            |
| 2   | W     | 104 | A32  | 4       | 0            |
| 2   | O     | 104 | A32  | 8       | 0            |
| 2   | Y     | 104 | A32  | 5       | 0            |
| 2   | Z     | 104 | A32  | 9       | 0            |
| 2   | H     | 104 | A32  | 1       | 0            |
| 2   | X     | 104 | A32  | 1       | 0            |
| 2   | V     | 104 | A32  | 6       | 0            |
| 2   | M     | 104 | A32  | 2       | 0            |
| 2   | L     | 104 | A32  | 3       | 0            |
| 2   | D     | 104 | A32  | 9       | 0            |
| 2   | E     | 104 | A32  | 2       | 0            |
| 2   | F     | 104 | A32  | 5       | 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.

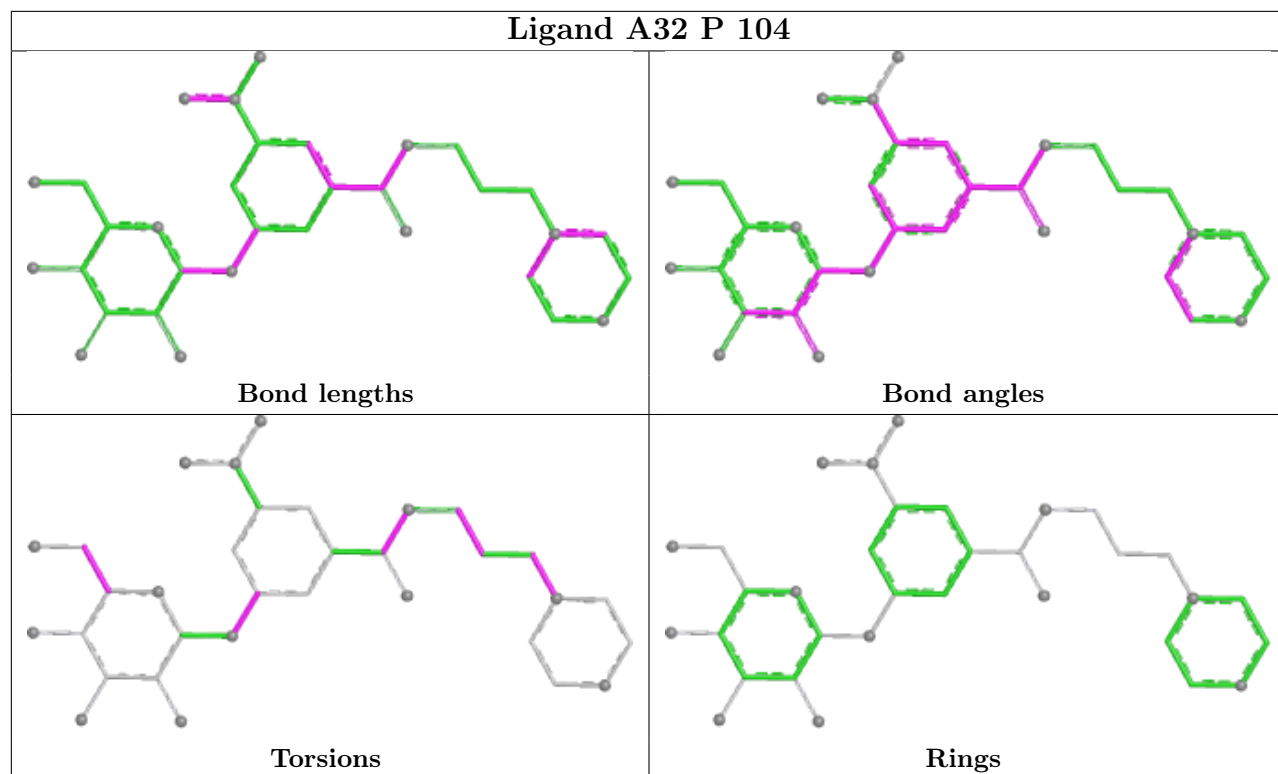
## Ligand A32 G 104



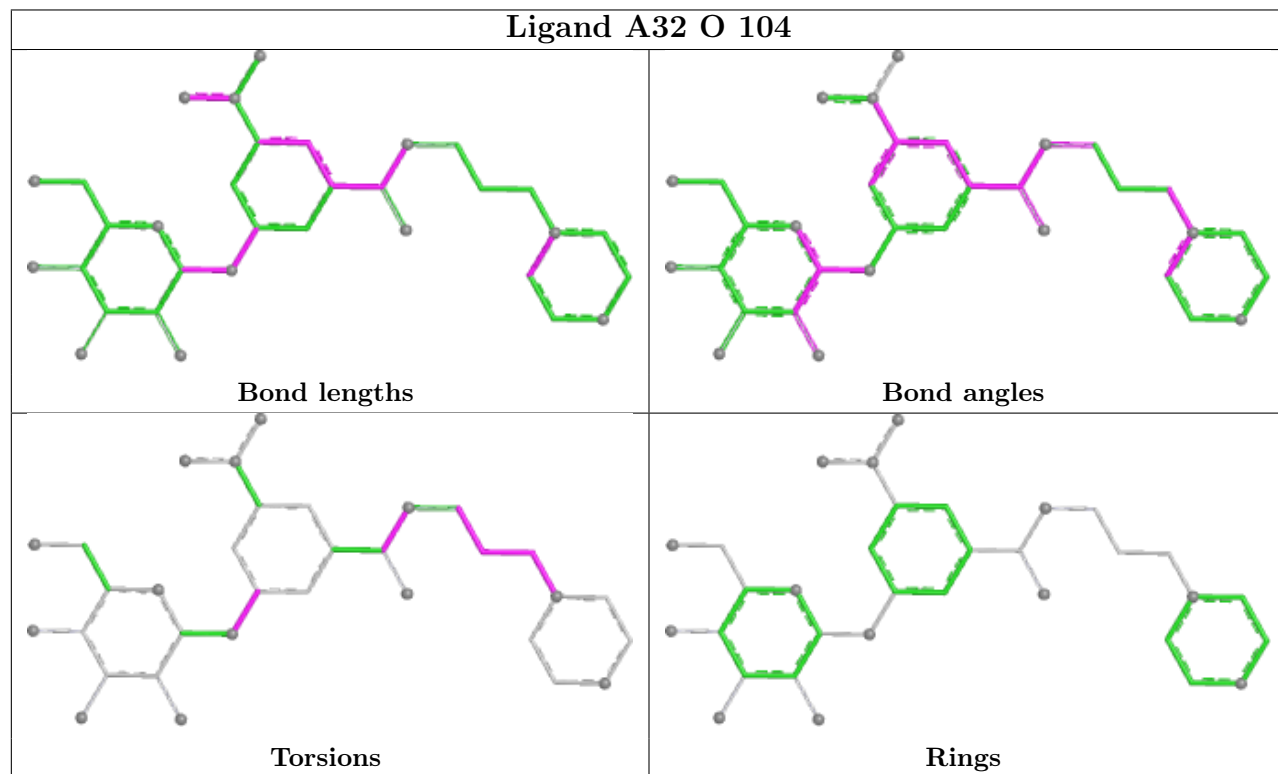
## Ligand A32 W 104



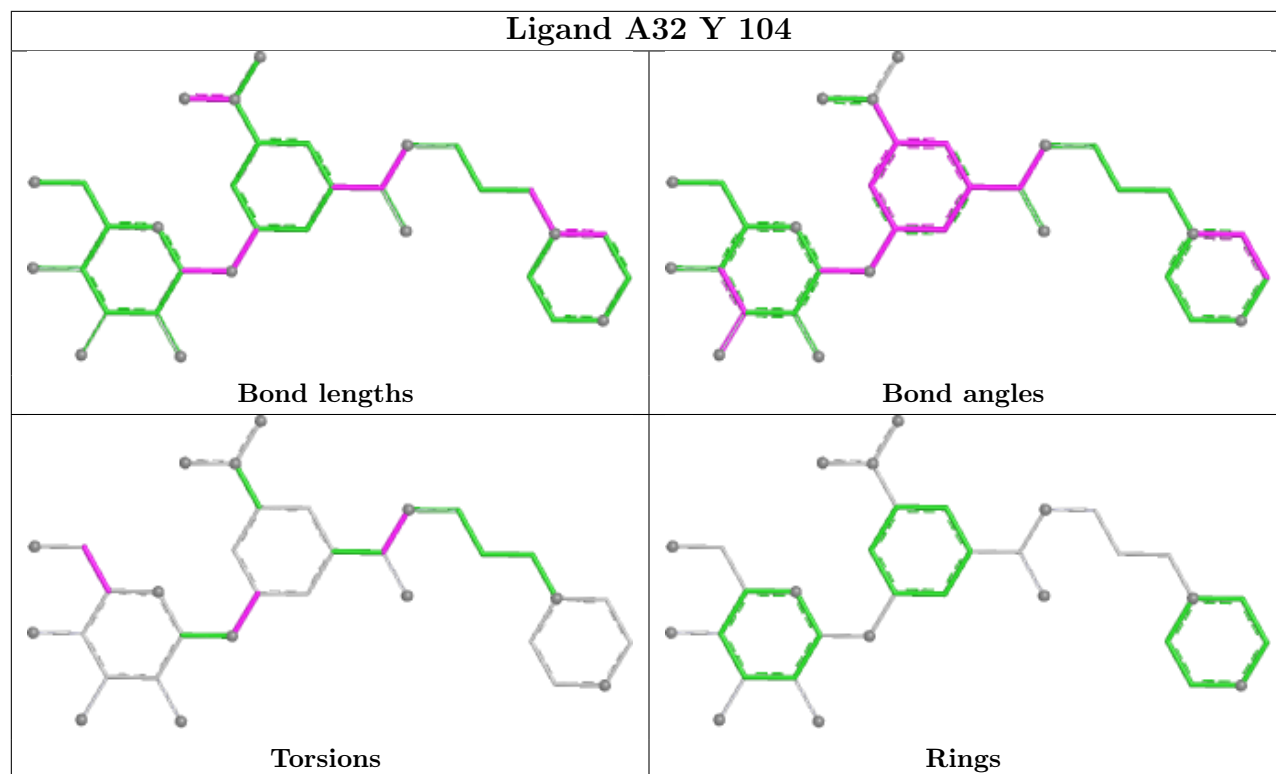
## Ligand A32 P 104



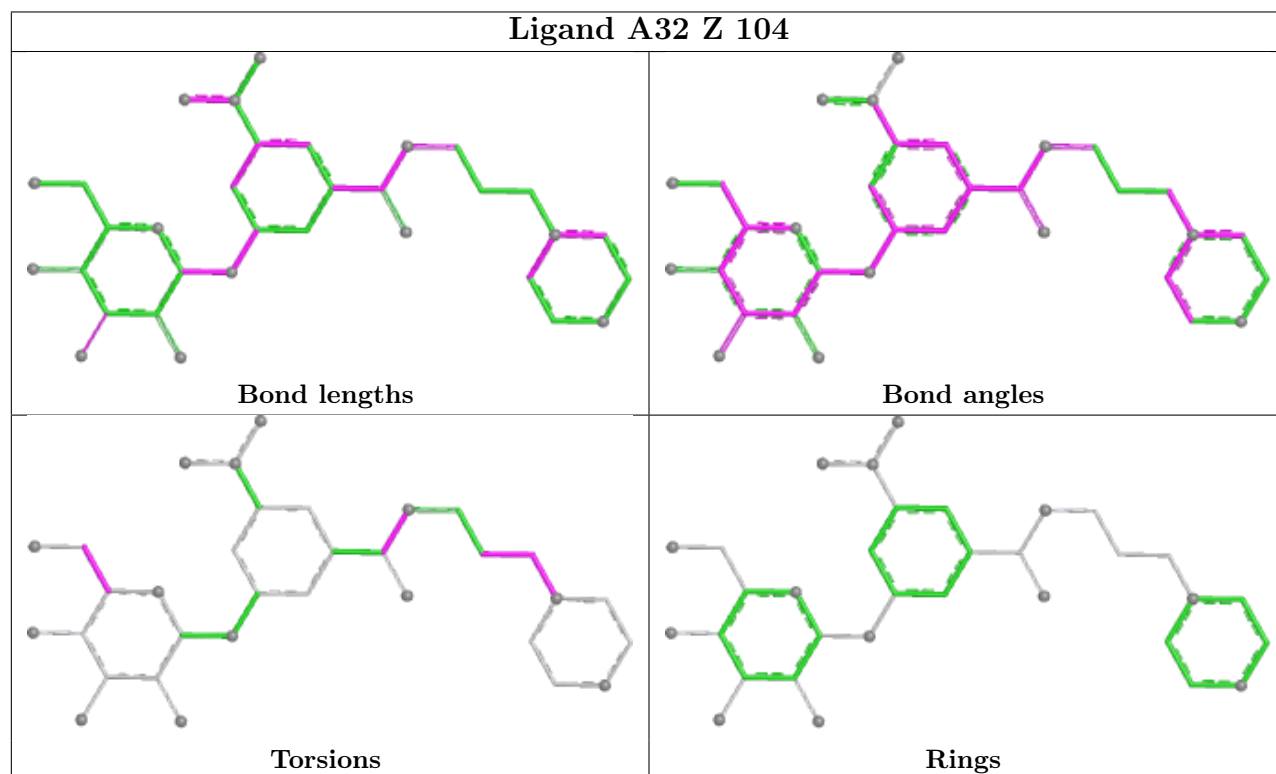
## Ligand A32 O 104



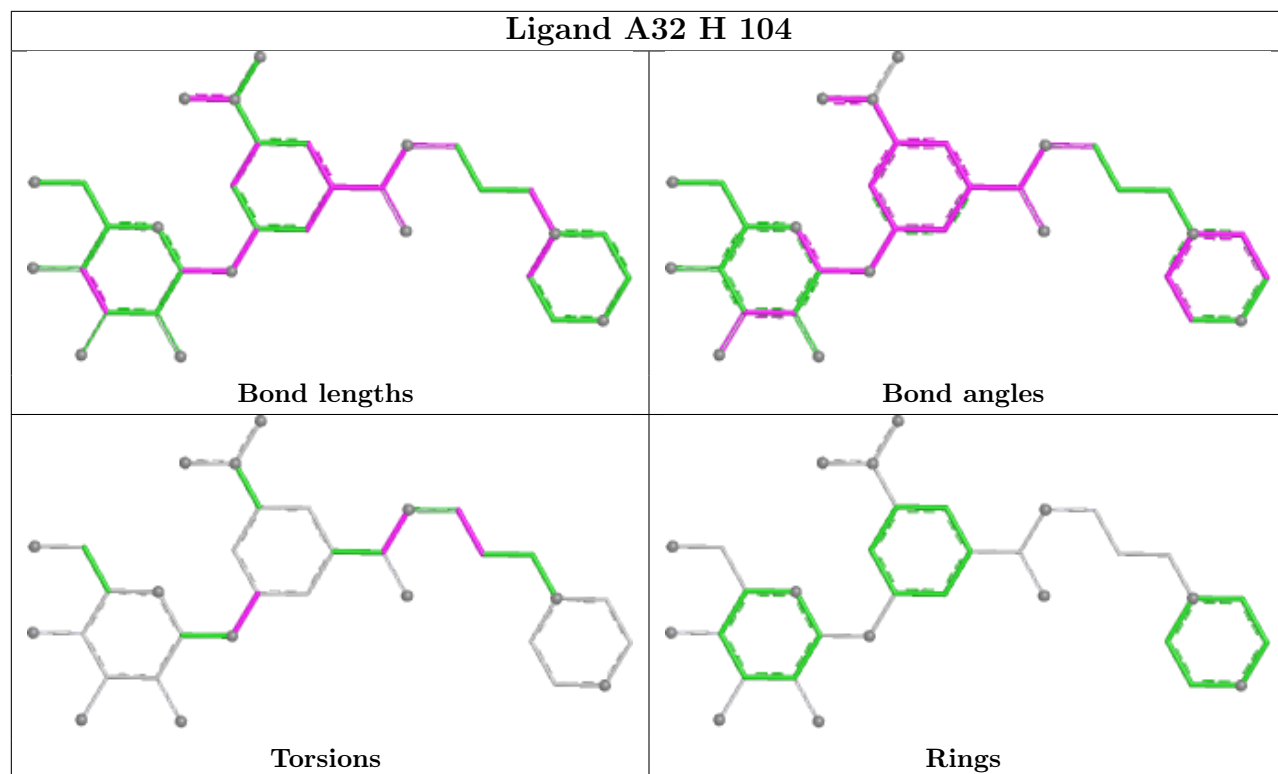
## Ligand A32 Y 104



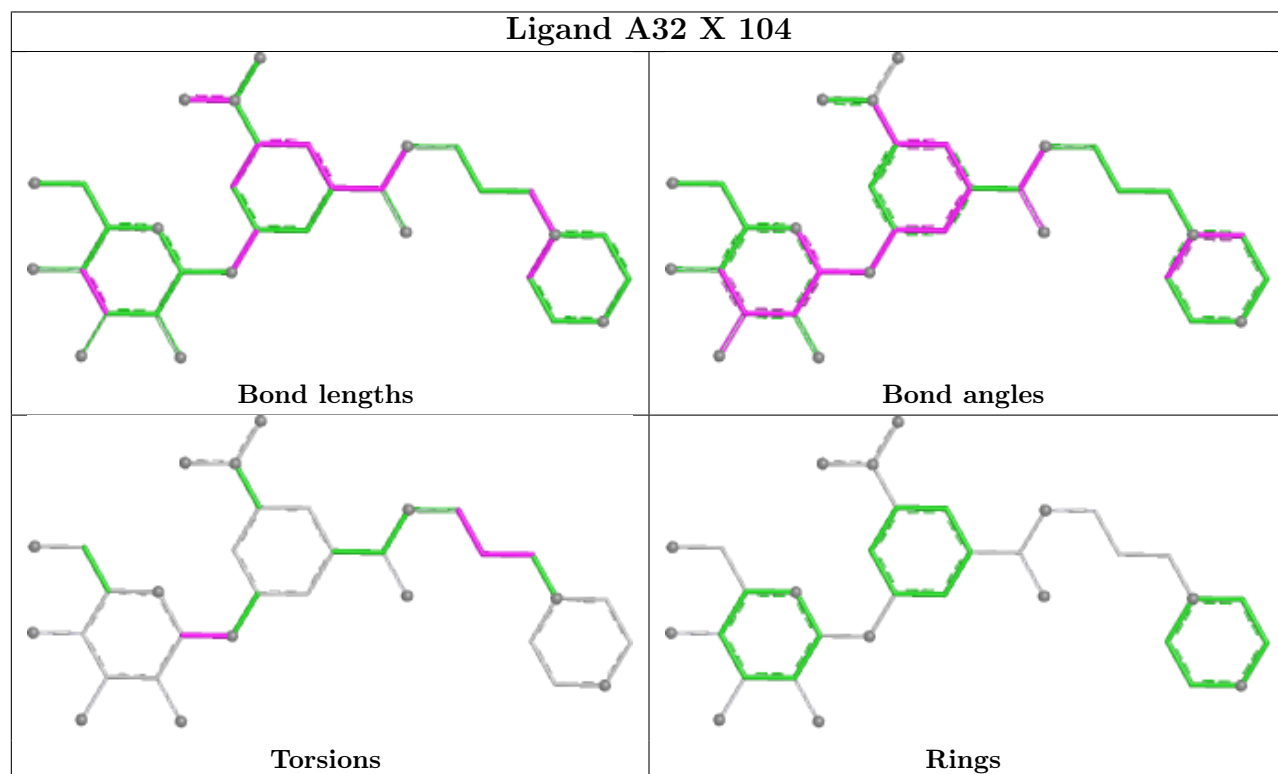
## Ligand A32 Z 104



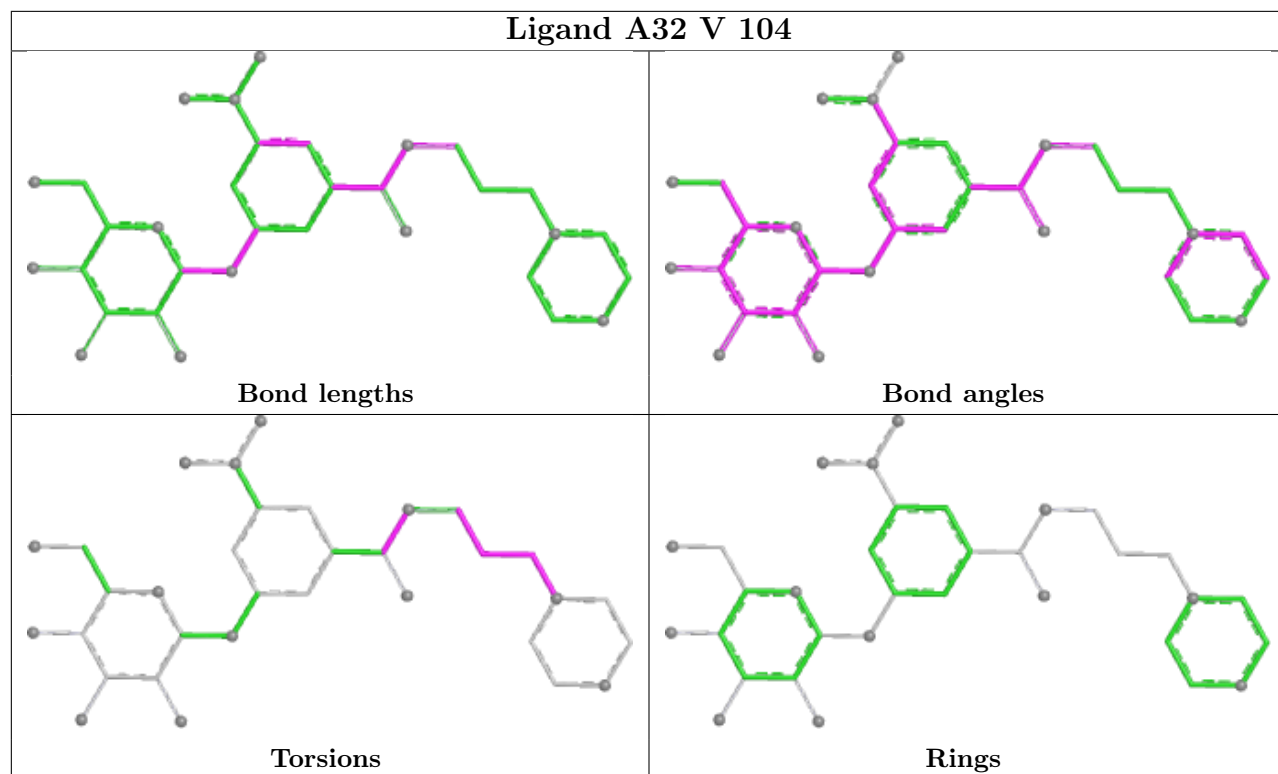
## Ligand A32 H 104



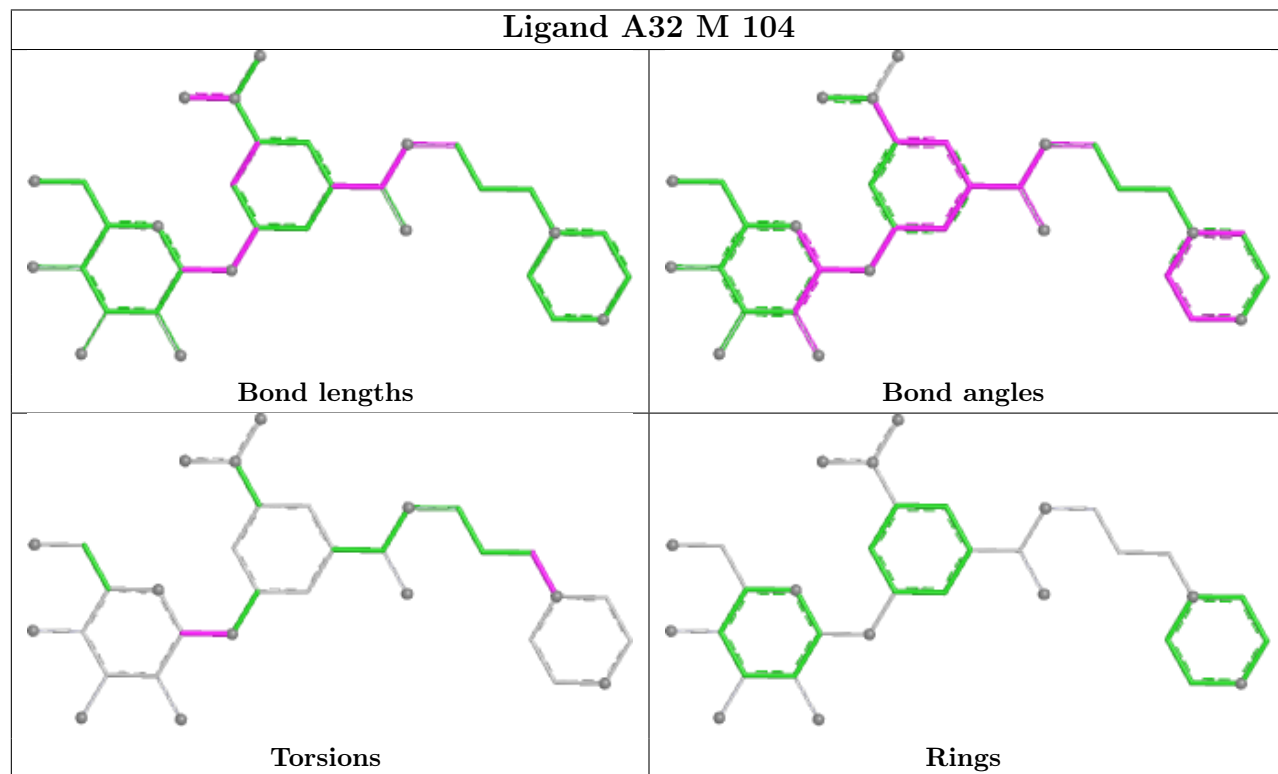
## Ligand A32 X 104



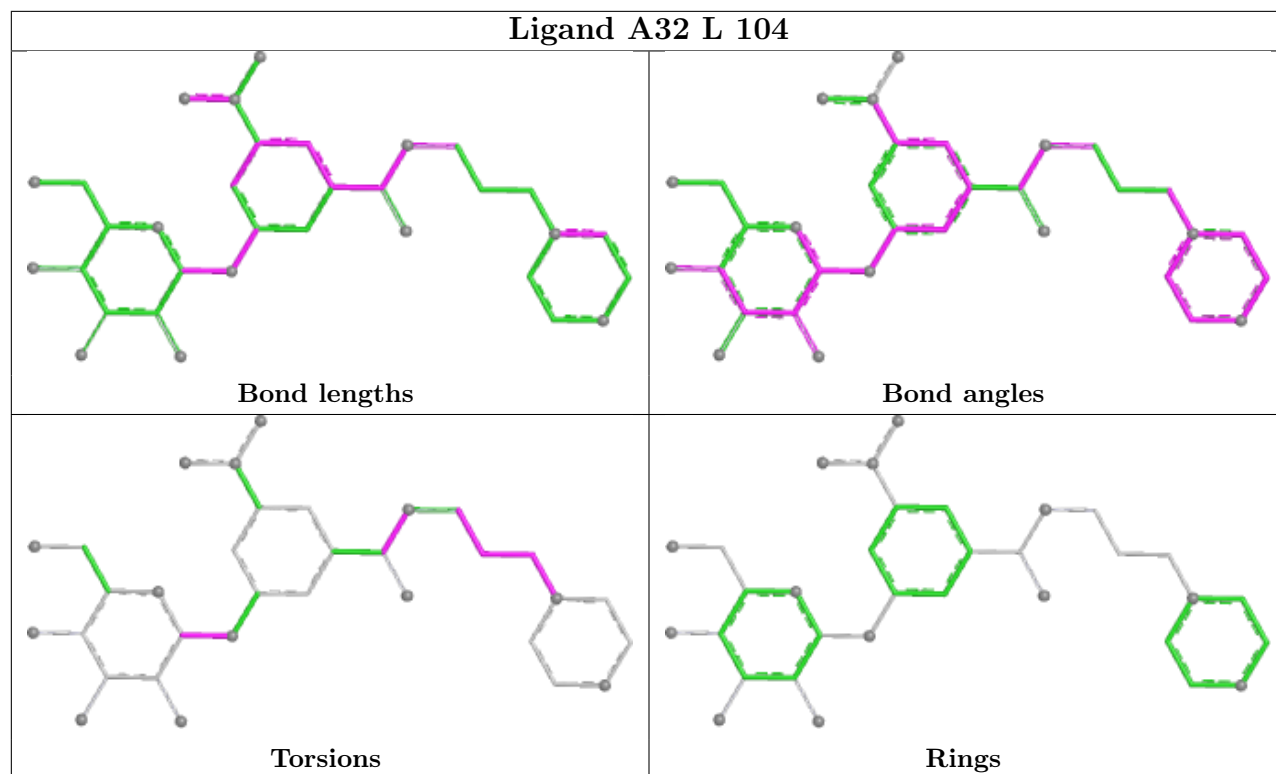
## Ligand A32 V 104



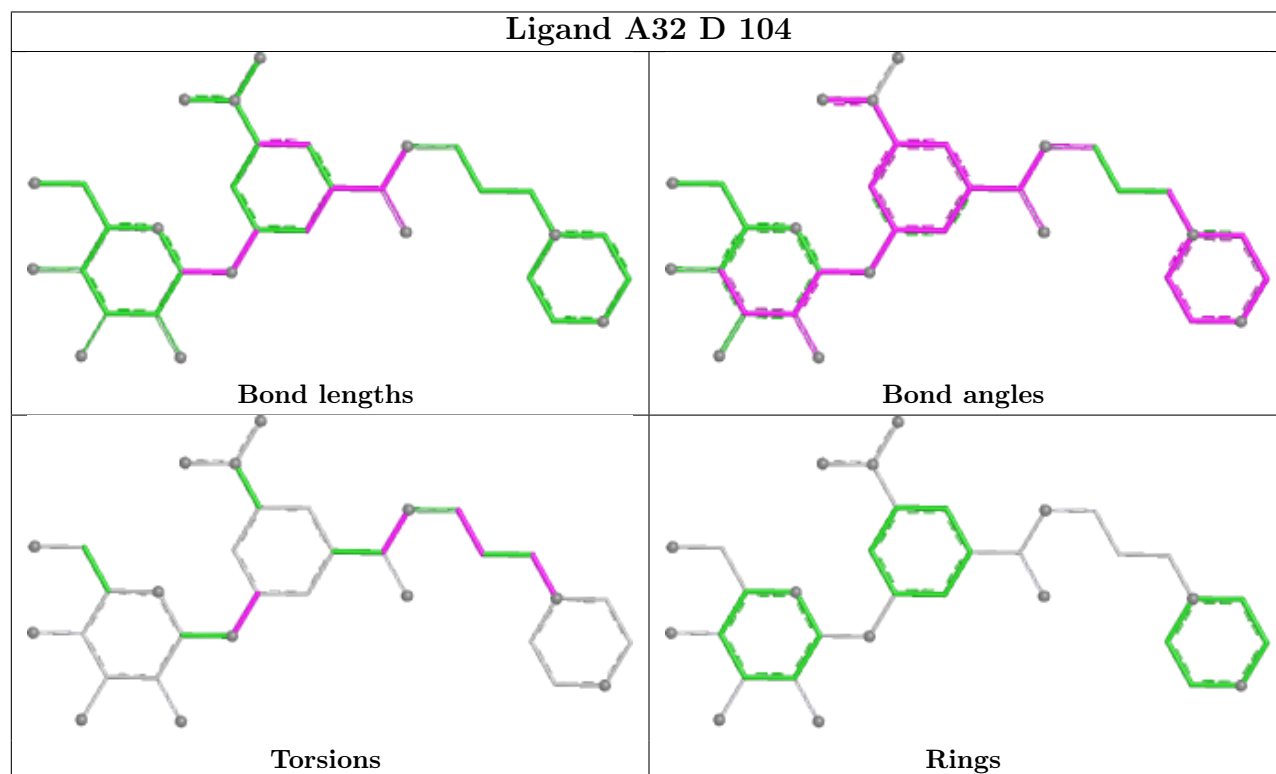
## Ligand A32 M 104

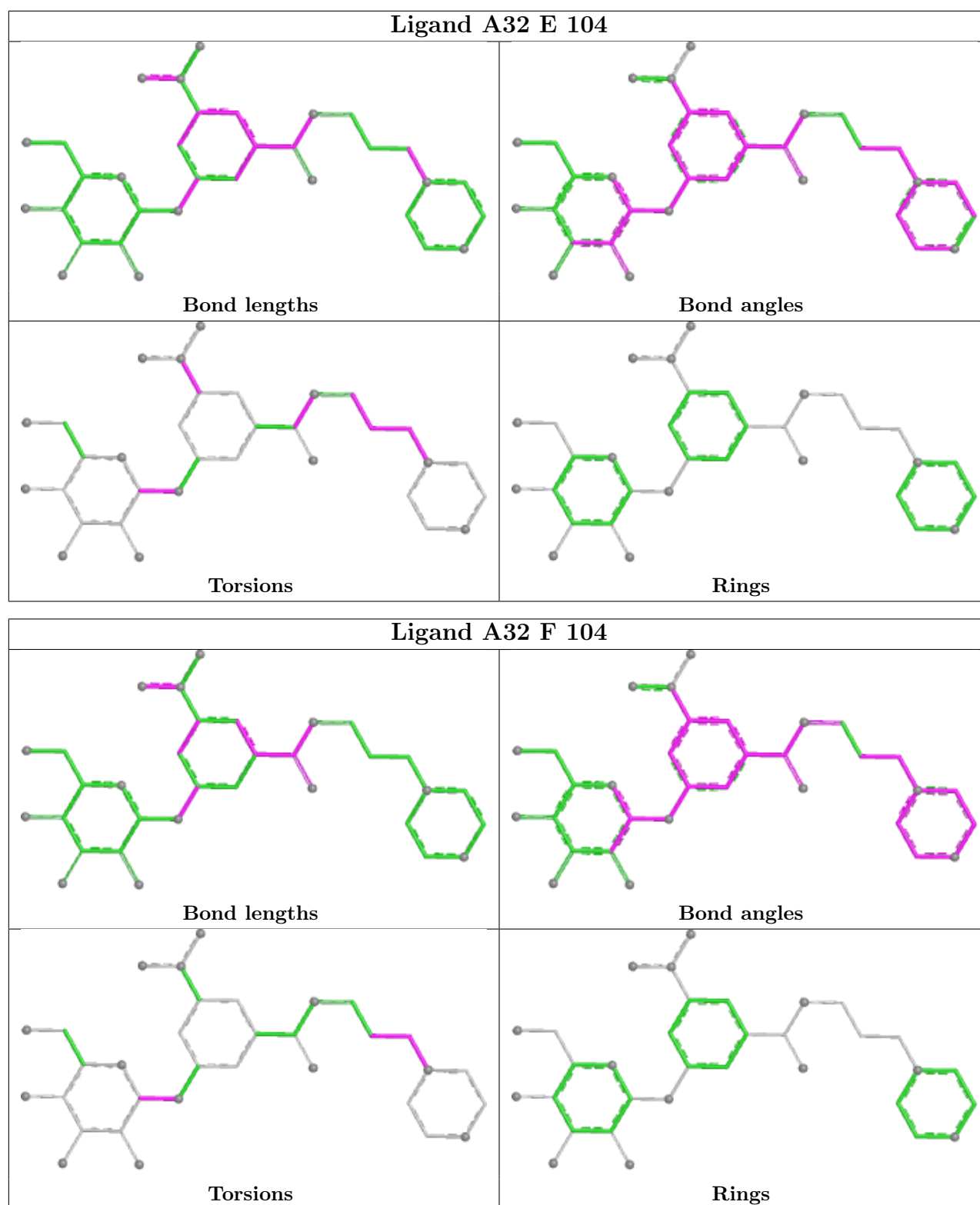


## Ligand A32 L 104



## Ligand A32 D 104





## 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   | D     | 103/103 (100%)   | -0.52  | 1 (0%) 79 83   | 12, 23, 36, 48        | 0       |
| 1   | E     | 103/103 (100%)   | -0.59  | 1 (0%) 79 83   | 12, 21, 40, 54        | 0       |
| 1   | F     | 103/103 (100%)   | -0.64  | 0 100 100      | 12, 21, 33, 50        | 0       |
| 1   | G     | 103/103 (100%)   | -0.36  | 3 (2%) 53 57   | 13, 26, 42, 59        | 0       |
| 1   | H     | 103/103 (100%)   | -0.54  | 1 (0%) 79 83   | 12, 23, 34, 60        | 0       |
| 1   | L     | 103/103 (100%)   | 0.30   | 6 (5%) 29 33   | 18, 37, 70, 84        | 0       |
| 1   | M     | 103/103 (100%)   | 0.69   | 11 (10%) 11 13 | 22, 46, 78, 102       | 0       |
| 1   | N     | 103/103 (100%)   | 0.32   | 1 (0%) 79 83   | 17, 36, 57, 71        | 0       |
| 1   | O     | 103/103 (100%)   | 0.24   | 3 (2%) 53 57   | 18, 36, 60, 83        | 0       |
| 1   | P     | 103/103 (100%)   | -0.23  | 0 100 100      | 17, 28, 46, 62        | 0       |
| 1   | V     | 103/103 (100%)   | 1.88   | 44 (42%) 0 1   | 27, 68, 106, 117      | 0       |
| 1   | W     | 103/103 (100%)   | 1.21   | 24 (23%) 2 2   | 21, 50, 77, 86        | 0       |
| 1   | X     | 103/103 (100%)   | 0.42   | 9 (8%) 16 18   | 16, 36, 64, 77        | 0       |
| 1   | Y     | 103/103 (100%)   | 0.43   | 3 (2%) 53 57   | 17, 37, 62, 79        | 0       |
| 1   | Z     | 103/103 (100%)   | 0.65   | 11 (10%) 11 13 | 19, 42, 72, 93        | 0       |
| All | All   | 1545/1545 (100%) | 0.22   | 118 (7%) 20 23 | 12, 33, 73, 117       | 0       |

All (118) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 88  | TRP  | 6.2  |
| 1   | V     | 17  | ILE  | 5.3  |
| 1   | V     | 85  | LEU  | 4.9  |
| 1   | V     | 8   | LEU  | 4.5  |
| 1   | Z     | 12  | TYR  | 4.3  |
| 1   | V     | 86  | CYS  | 4.3  |
| 1   | V     | 12  | TYR  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 33  | GLY  | 4.1  |
| 1   | V     | 6   | THR  | 4.1  |
| 1   | V     | 15  | THR  | 4.1  |
| 1   | L     | 88  | TRP  | 4.0  |
| 1   | V     | 98  | ALA  | 4.0  |
| 1   | V     | 48  | PHE  | 4.0  |
| 1   | W     | 88  | TRP  | 4.0  |
| 1   | V     | 92  | THR  | 3.9  |
| 1   | V     | 16  | GLN  | 3.8  |
| 1   | M     | 12  | TYR  | 3.7  |
| 1   | W     | 15  | THR  | 3.7  |
| 1   | V     | 47  | THR  | 3.6  |
| 1   | O     | 103 | ASN  | 3.5  |
| 1   | V     | 62  | LYS  | 3.5  |
| 1   | V     | 20  | ILE  | 3.4  |
| 1   | E     | 44  | SER  | 3.4  |
| 1   | H     | 103 | ASN  | 3.4  |
| 1   | Y     | 103 | ASN  | 3.4  |
| 1   | V     | 59  | ASP  | 3.3  |
| 1   | X     | 42  | PHE  | 3.3  |
| 1   | W     | 14  | ASN  | 3.3  |
| 1   | V     | 42  | PHE  | 3.3  |
| 1   | V     | 87  | VAL  | 3.2  |
| 1   | V     | 18  | TYR  | 3.2  |
| 1   | Z     | 14  | ASN  | 3.2  |
| 1   | M     | 10  | SER  | 3.1  |
| 1   | V     | 46  | GLU  | 3.0  |
| 1   | Z     | 17  | ILE  | 3.0  |
| 1   | Z     | 88  | TRP  | 3.0  |
| 1   | V     | 58  | ILE  | 2.9  |
| 1   | V     | 91  | LYS  | 2.9  |
| 1   | V     | 2   | PRO  | 2.9  |
| 1   | V     | 10  | SER  | 2.9  |
| 1   | W     | 17  | ILE  | 2.9  |
| 1   | V     | 93  | PRO  | 2.9  |
| 1   | X     | 17  | ILE  | 2.8  |
| 1   | W     | 103 | ASN  | 2.8  |
| 1   | V     | 14  | ASN  | 2.8  |
| 1   | L     | 12  | TYR  | 2.8  |
| 1   | V     | 96  | ILE  | 2.8  |
| 1   | M     | 88  | TRP  | 2.7  |
| 1   | M     | 15  | THR  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Z     | 11  | GLU  | 2.7  |
| 1   | G     | 13  | ARG  | 2.7  |
| 1   | Z     | 15  | THR  | 2.6  |
| 1   | V     | 90  | ASN  | 2.6  |
| 1   | X     | 18  | TYR  | 2.6  |
| 1   | M     | 17  | ILE  | 2.6  |
| 1   | D     | 59  | ASP  | 2.6  |
| 1   | V     | 52  | VAL  | 2.6  |
| 1   | V     | 19  | THR  | 2.6  |
| 1   | W     | 87  | VAL  | 2.6  |
| 1   | Z     | 86  | CYS  | 2.6  |
| 1   | G     | 46  | GLU  | 2.5  |
| 1   | M     | 11  | GLU  | 2.5  |
| 1   | G     | 103 | ASN  | 2.5  |
| 1   | W     | 47  | THR  | 2.5  |
| 1   | W     | 92  | THR  | 2.5  |
| 1   | L     | 15  | THR  | 2.5  |
| 1   | W     | 85  | LEU  | 2.5  |
| 1   | V     | 9   | CYS  | 2.4  |
| 1   | W     | 12  | TYR  | 2.4  |
| 1   | W     | 18  | TYR  | 2.4  |
| 1   | M     | 13  | ARG  | 2.4  |
| 1   | W     | 48  | PHE  | 2.4  |
| 1   | V     | 53  | PRO  | 2.4  |
| 1   | M     | 103 | ASN  | 2.4  |
| 1   | V     | 89  | ASN  | 2.4  |
| 1   | Z     | 9   | CYS  | 2.4  |
| 1   | W     | 39  | ILE  | 2.4  |
| 1   | W     | 40  | ILE  | 2.4  |
| 1   | W     | 13  | ARG  | 2.4  |
| 1   | V     | 5   | ILE  | 2.3  |
| 1   | V     | 44  | SER  | 2.3  |
| 1   | O     | 88  | TRP  | 2.3  |
| 1   | L     | 59  | ASP  | 2.3  |
| 1   | M     | 102 | LYS  | 2.3  |
| 1   | V     | 24  | ILE  | 2.3  |
| 1   | V     | 45  | GLY  | 2.3  |
| 1   | L     | 10  | SER  | 2.3  |
| 1   | X     | 10  | SER  | 2.3  |
| 1   | O     | 17  | ILE  | 2.3  |
| 1   | W     | 20  | ILE  | 2.3  |
| 1   | X     | 13  | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Z     | 13  | ARG  | 2.3  |
| 1   | N     | 43  | LYS  | 2.3  |
| 1   | W     | 102 | LYS  | 2.3  |
| 1   | V     | 11  | GLU  | 2.2  |
| 1   | Z     | 60  | SER  | 2.2  |
| 1   | V     | 50  | VAL  | 2.2  |
| 1   | X     | 46  | GLU  | 2.2  |
| 1   | M     | 14  | ASN  | 2.2  |
| 1   | X     | 82  | ILE  | 2.2  |
| 1   | V     | 1   | ALA  | 2.2  |
| 1   | W     | 19  | THR  | 2.2  |
| 1   | Z     | 48  | PHE  | 2.2  |
| 1   | Y     | 20  | ILE  | 2.1  |
| 1   | Y     | 13  | ARG  | 2.1  |
| 1   | W     | 90  | ASN  | 2.1  |
| 1   | W     | 4   | THR  | 2.1  |
| 1   | V     | 54  | GLY  | 2.1  |
| 1   | W     | 45  | GLY  | 2.1  |
| 1   | W     | 32  | ALA  | 2.1  |
| 1   | L     | 62  | LYS  | 2.1  |
| 1   | V     | 103 | ASN  | 2.1  |
| 1   | V     | 99  | ILE  | 2.1  |
| 1   | V     | 7   | GLU  | 2.1  |
| 1   | M     | 92  | THR  | 2.1  |
| 1   | W     | 38  | VAL  | 2.1  |
| 1   | X     | 103 | ASN  | 2.0  |
| 1   | X     | 41  | THR  | 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,

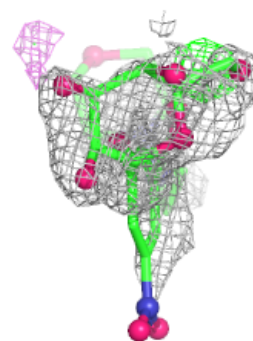
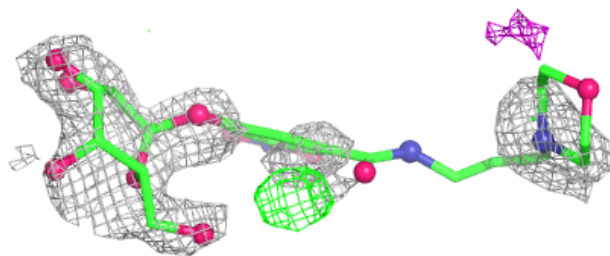
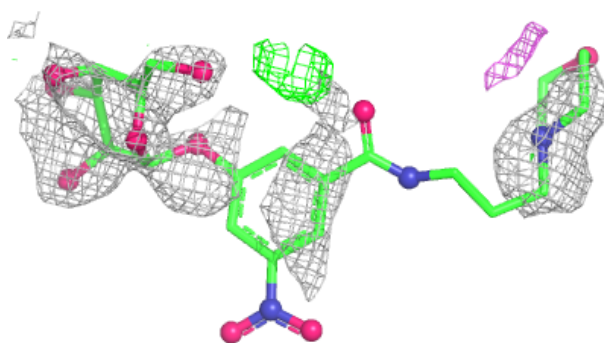
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | A32  | V     | 104 | 33/33 | 0.54 | 0.19 | 86,97,102,103              | 0     |
| 2   | A32  | W     | 104 | 33/33 | 0.63 | 0.20 | 60,87,108,108              | 0     |
| 2   | A32  | Y     | 104 | 33/33 | 0.68 | 0.16 | 65,84,92,94                | 0     |
| 2   | A32  | L     | 104 | 33/33 | 0.69 | 0.19 | 47,77,83,84                | 0     |
| 2   | A32  | O     | 104 | 33/33 | 0.71 | 0.20 | 57,94,111,112              | 0     |
| 2   | A32  | M     | 104 | 33/33 | 0.72 | 0.16 | 64,82,87,87                | 0     |
| 2   | A32  | Z     | 104 | 33/33 | 0.74 | 0.17 | 55,76,87,88                | 0     |
| 2   | A32  | F     | 104 | 33/33 | 0.82 | 0.16 | 24,58,77,77                | 0     |
| 2   | A32  | P     | 104 | 33/33 | 0.83 | 0.14 | 34,72,94,95                | 0     |
| 2   | A32  | D     | 104 | 33/33 | 0.84 | 0.14 | 26,54,80,81                | 0     |
| 2   | A32  | X     | 104 | 33/33 | 0.84 | 0.14 | 25,58,71,72                | 0     |
| 2   | A32  | H     | 104 | 33/33 | 0.85 | 0.14 | 22,58,81,81                | 0     |
| 2   | A32  | G     | 104 | 33/33 | 0.87 | 0.12 | 31,56,78,79                | 0     |
| 2   | A32  | E     | 104 | 33/33 | 0.89 | 0.12 | 23,48,59,59                | 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.

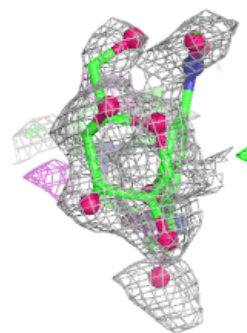
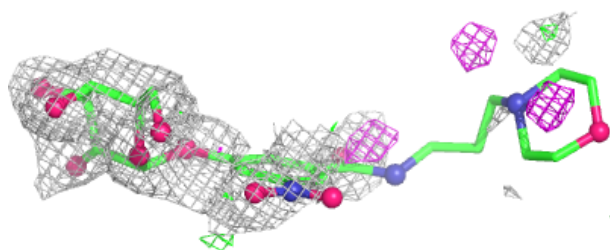
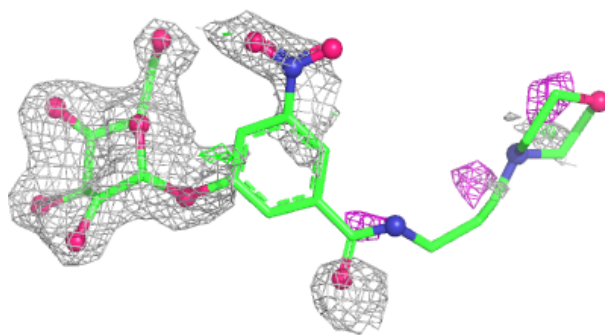
#### Electron density around A32 V 104:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

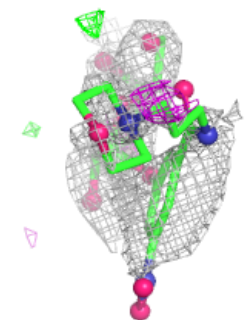
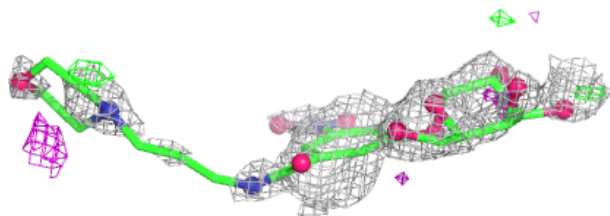
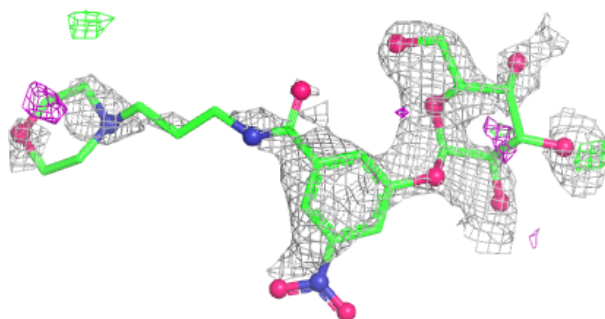


**Electron density around A32 W 104:**

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

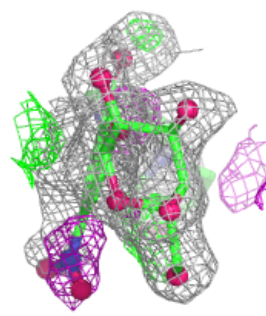
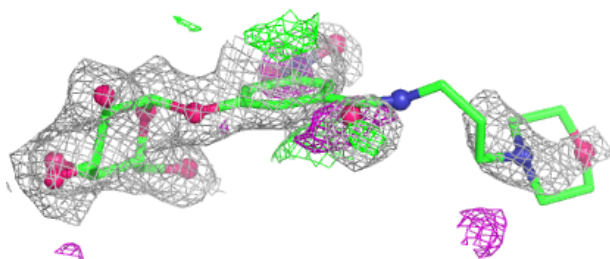
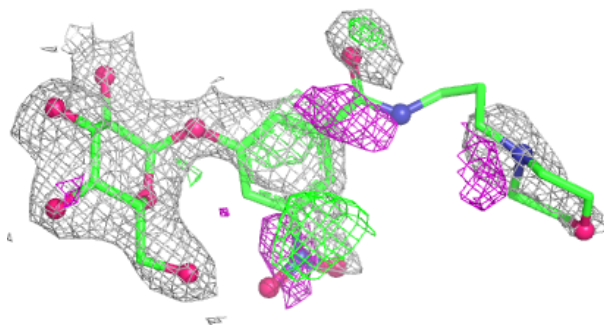
**Electron density around A32 Y 104:**

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

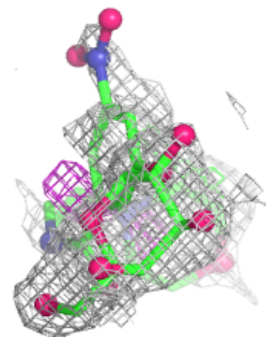
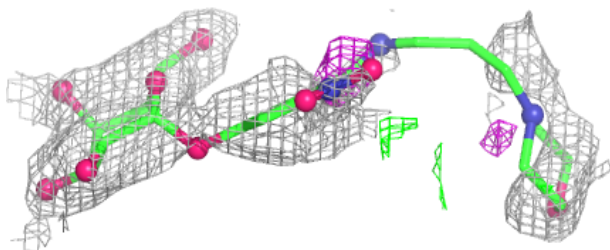
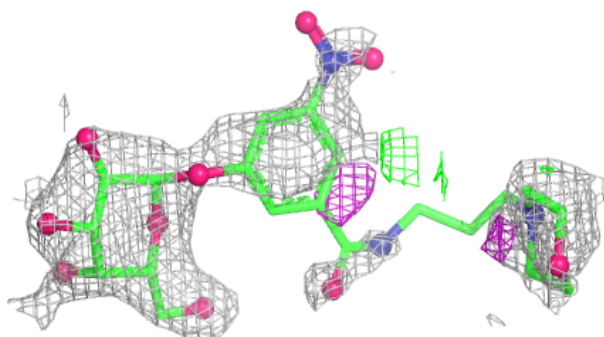


**Electron density around A32 L 104:**

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

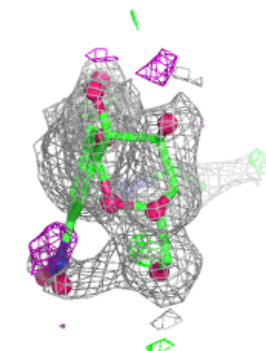
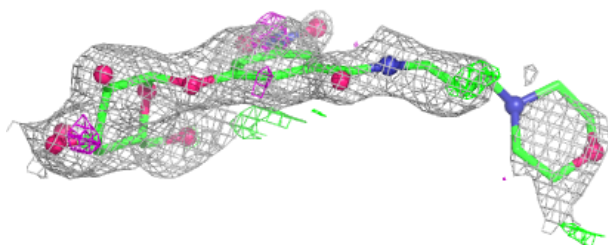
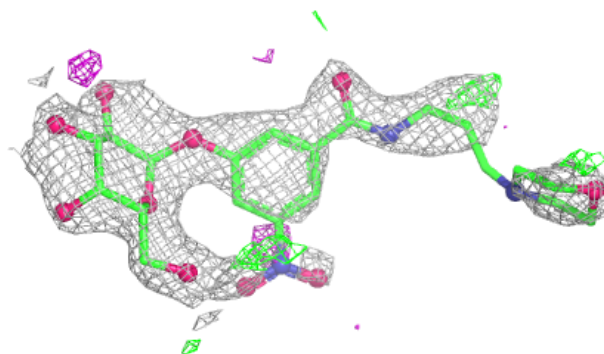
**Electron density around A32 O 104:**

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

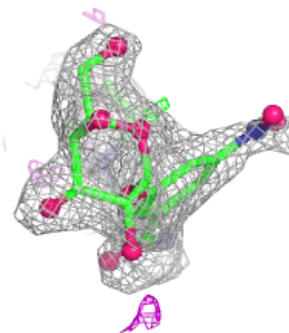
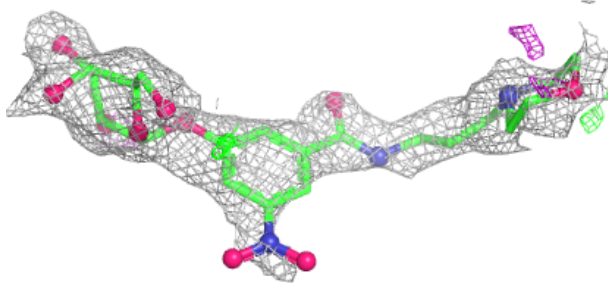
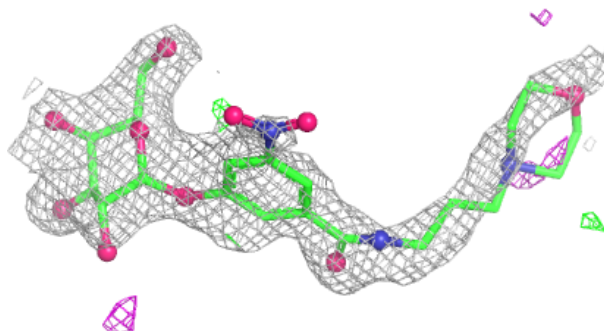


**Electron density around A32 M 104:**

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

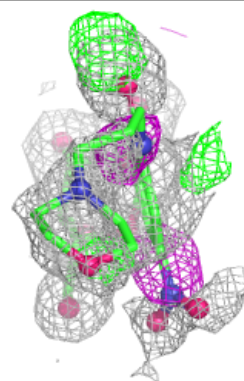
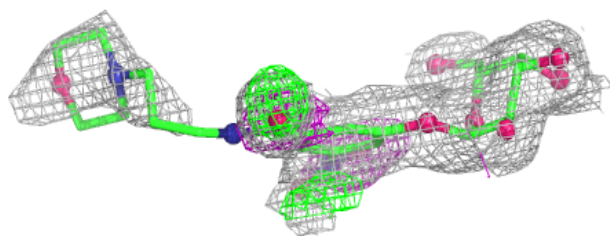
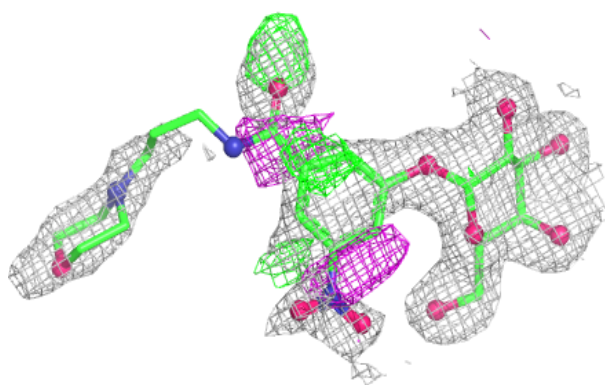
**Electron density around A32 Z 104:**

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

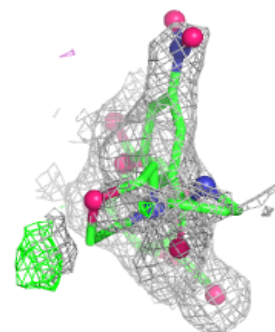
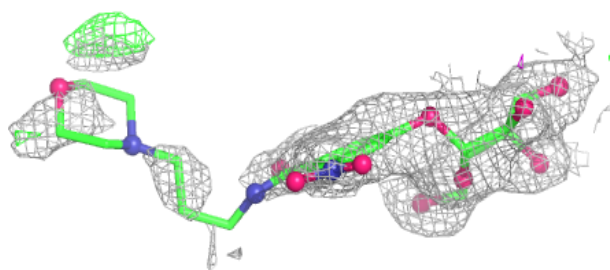
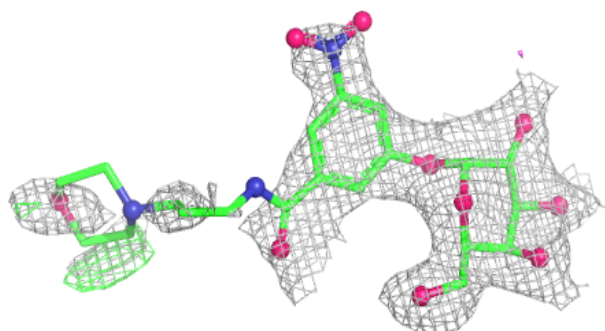


**Electron density around A32 F 104:**

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

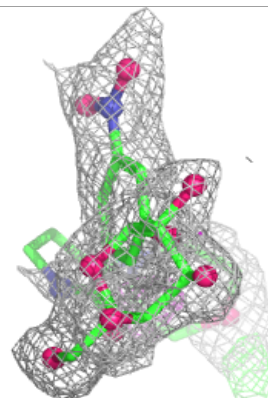
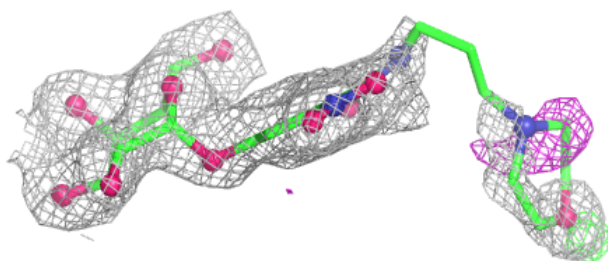
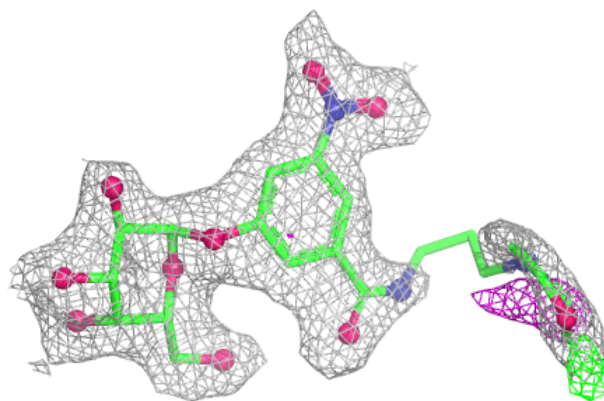
**Electron density around A32 P 104:**

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

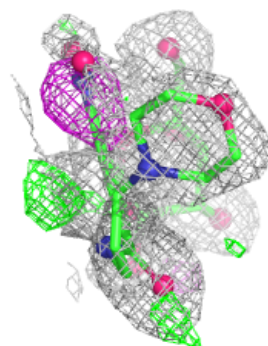
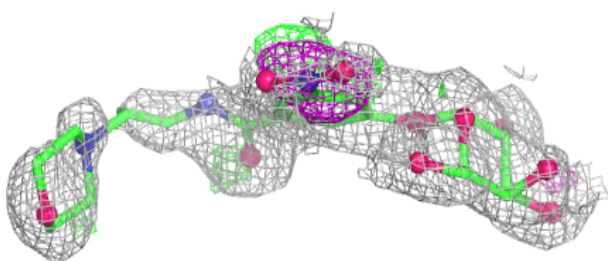
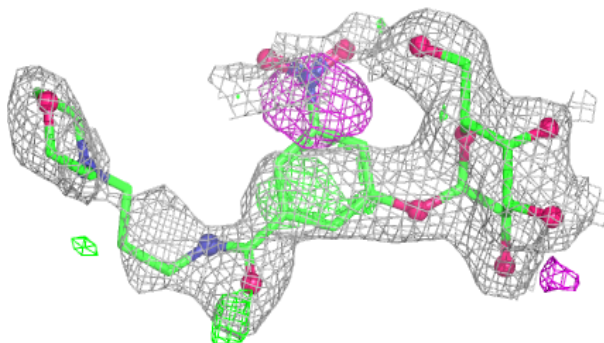


**Electron density around A32 D 104:**

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

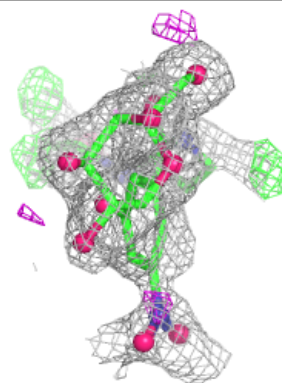
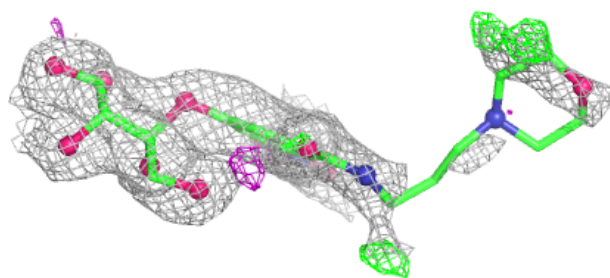
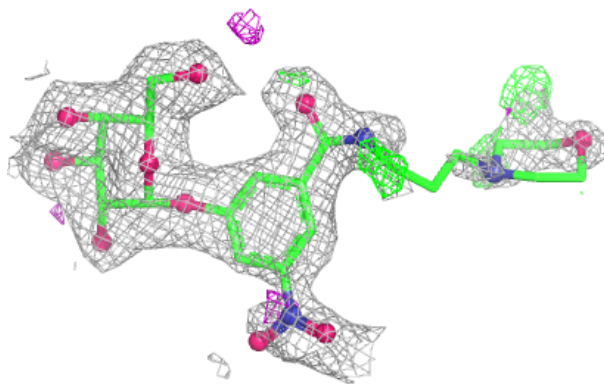
**Electron density around A32 X 104:**

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

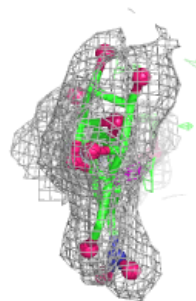
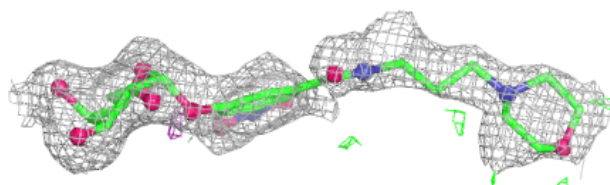
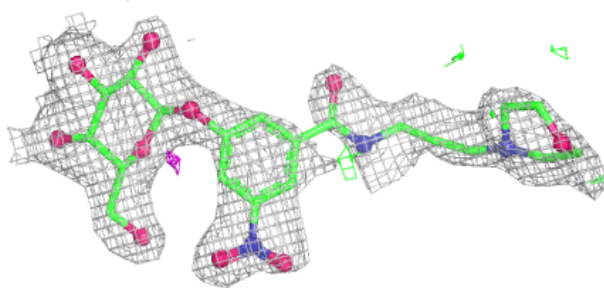


**Electron density around A32 H 104:**

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

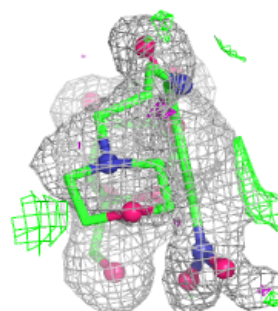
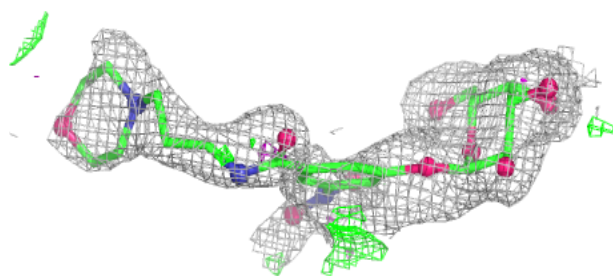
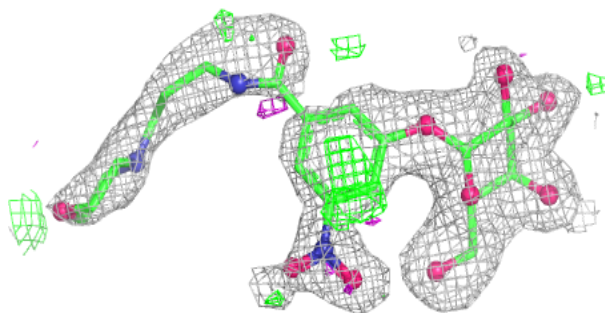
**Electron density around A32 G 104:**

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



**Electron density around A32 E 104:**

$2mF_o-DF_c$  (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.