



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 1UP6 / pdb\_00001up6  
Title : Structure of the 6-phospho-beta glucosidase from *Thermotoga maritima* at 2.55 Angstrom resolution in the tetragonal form with manganese, NAD<sup>+</sup> and glucose-6-phosphate  
Authors : Varrot, A.; Yip, V.L.; Withers, S.G.; Davies, G.J.  
Deposited on : 2003-09-29  
Resolution : 2.55 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:

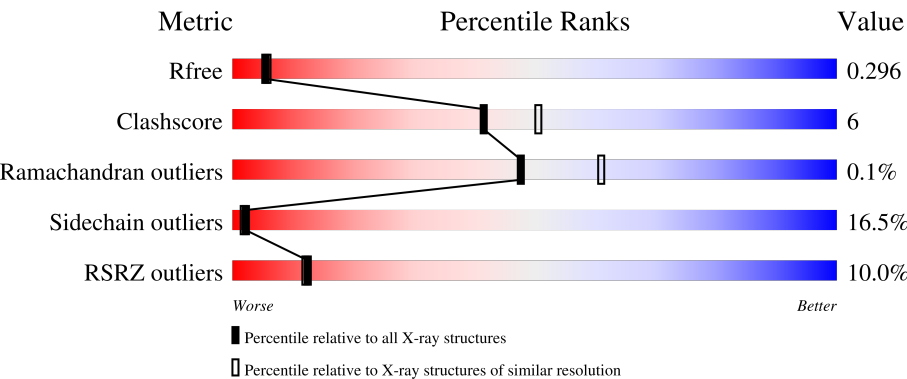
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 2.55 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                      | 1091 (2.54-2.54)                                      |
| Clashscore            | 190562                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers         | 180081                      | 1091 (2.54-2.54)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | A     | 416    | <div><div>9%</div><div><div></div><div>75%</div><div>19%</div><div>5%</div><div>.</div></div></div> |
| 1   | B     | 416    | <div><div>11%</div><div><div></div><div>74%</div><div>22%</div><div>.</div><div>.</div></div></div> |
| 1   | C     | 416    | <div><div>9%</div><div><div></div><div>75%</div><div>18%</div><div>5%</div><div>.</div></div></div> |
| 1   | D     | 416    | <div><div>10%</div><div><div></div><div>74%</div><div>20%</div><div>.</div><div>.</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 416    |                  |
| 1   | F     | 416    |                  |
| 1   | G     | 416    |                  |
| 1   | H     | 416    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | G6P  | A     | 1418 | X         | -        | -       | -                |
| 4   | G6P  | C     | 1418 | X         | -        | -       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26917 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 6-PHOSPHO-BETA-GLUCOSIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 413      | Total | C    | N   | O   | S | Se | 0       | 1       | 0     |
|     |       |          | 3356  | 2164 | 560 | 623 | 2 | 7  |         |         |       |
| 1   | B     | 410      | Total | C    | N   | O   | S | Se | 39      | 0       | 0     |
|     |       |          | 3331  | 2150 | 552 | 620 | 2 | 7  |         |         |       |
| 1   | C     | 407      | Total | C    | N   | O   | S | Se | 14      | 0       | 0     |
|     |       |          | 3303  | 2129 | 548 | 617 | 2 | 7  |         |         |       |
| 1   | D     | 404      | Total | C    | N   | O   | S | Se | 10      | 0       | 0     |
|     |       |          | 3276  | 2113 | 543 | 611 | 2 | 7  |         |         |       |
| 1   | E     | 390      | Total | C    | N   | O   | S | Se | 121     | 0       | 0     |
|     |       |          | 3165  | 2041 | 525 | 591 | 2 | 6  |         |         |       |
| 1   | F     | 399      | Total | C    | N   | O   | S | Se | 80      | 0       | 0     |
|     |       |          | 3240  | 2091 | 539 | 602 | 2 | 6  |         |         |       |
| 1   | G     | 404      | Total | C    | N   | O   | S | Se | 20      | 0       | 0     |
|     |       |          | 3280  | 2117 | 544 | 610 | 2 | 7  |         |         |       |
| 1   | H     | 395      | Total | C    | N   | O   | S | Se | 104     | 0       | 0     |
|     |       |          | 3209  | 2072 | 533 | 596 | 2 | 6  |         |         |       |

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

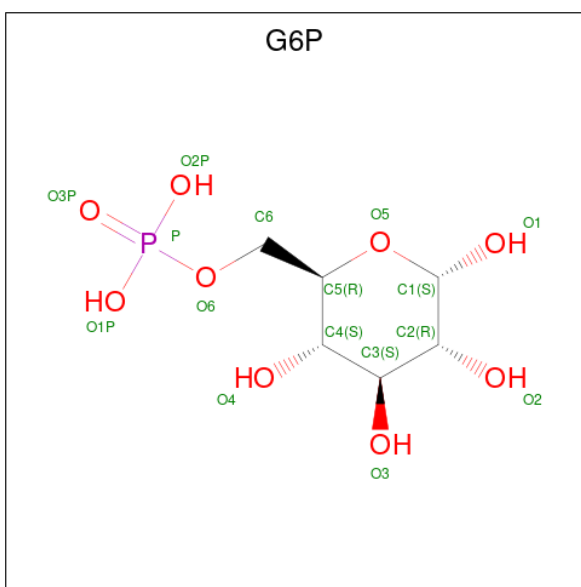


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | C     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 16    | 6 | 9 | 1 |         |         |
| 4   | C     | 1        | Total | C | O | P | 0       | 0       |
|     |       |          | 16    | 6 | 9 | 1 |         |         |

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



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

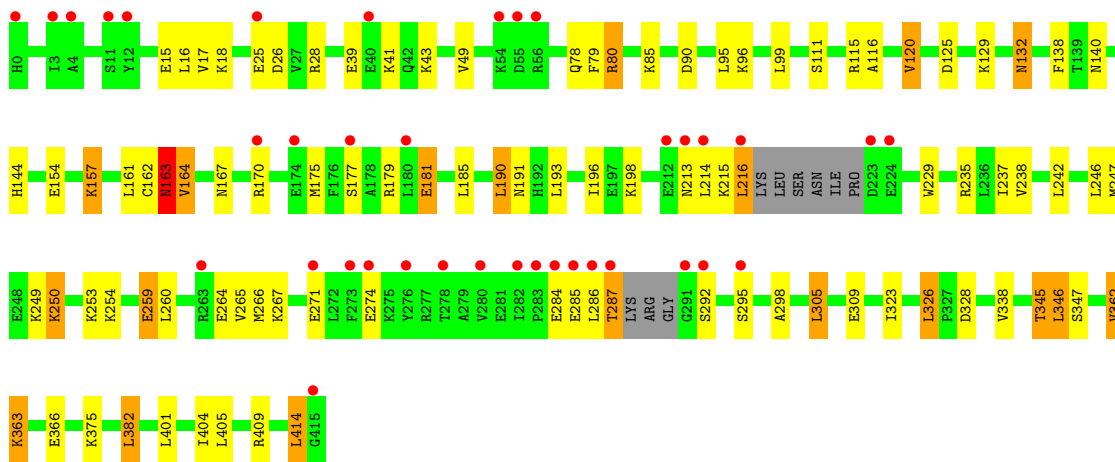
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 136      | Total | O   | 0       | 0       |
|     |       |          | 136   | 136 |         |         |
| 6   | B     | 83       | Total | O   | 0       | 0       |
|     |       |          | 83    | 83  |         |         |
| 6   | C     | 106      | Total | O   | 0       | 0       |
|     |       |          | 106   | 106 |         |         |
| 6   | D     | 95       | Total | O   | 0       | 0       |
|     |       |          | 95    | 95  |         |         |
| 6   | E     | 23       | Total | O   | 0       | 0       |
|     |       |          | 23    | 23  |         |         |
| 6   | F     | 36       | Total | O   | 0       | 0       |
|     |       |          | 36    | 36  |         |         |
| 6   | G     | 59       | Total | O   | 0       | 0       |
|     |       |          | 59    | 59  |         |         |
| 6   | H     | 30       | Total | O   | 0       | 0       |
|     |       |          | 30    | 30  |         |         |

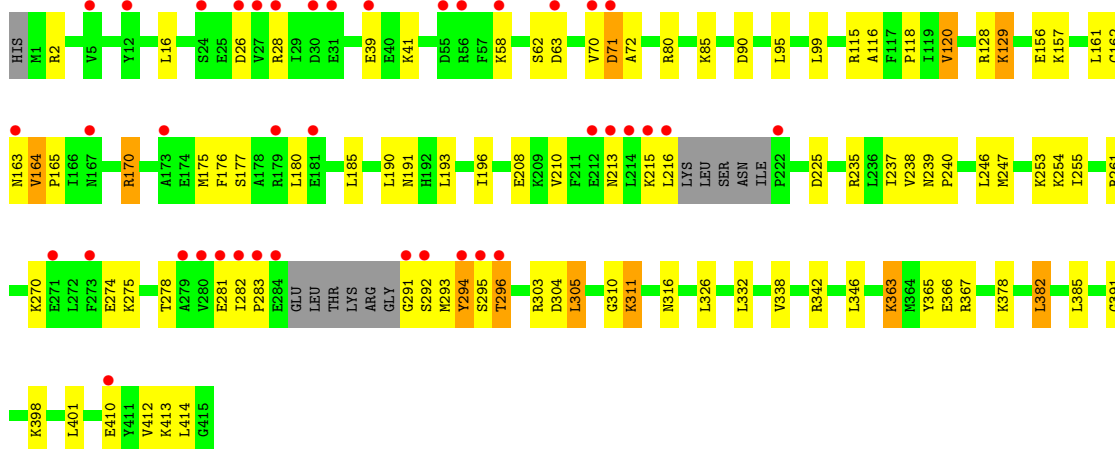
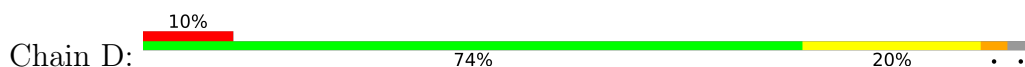


● Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

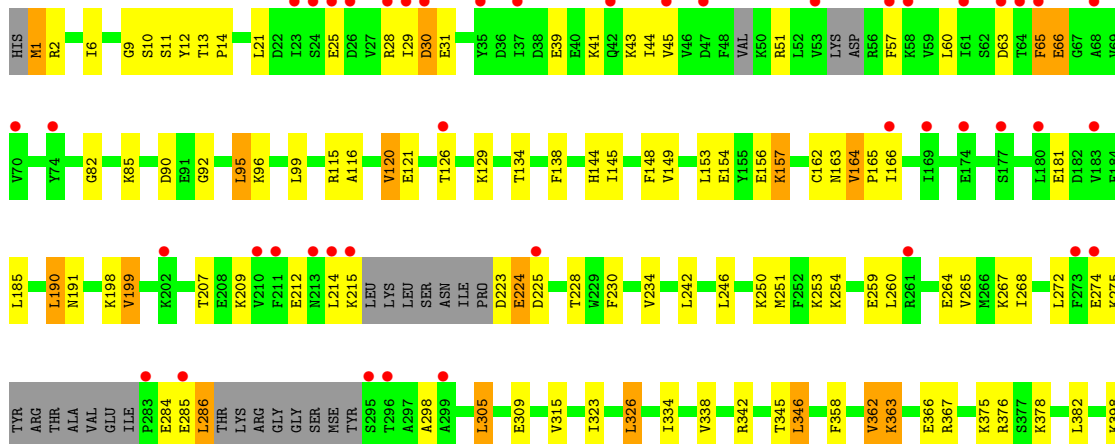




• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

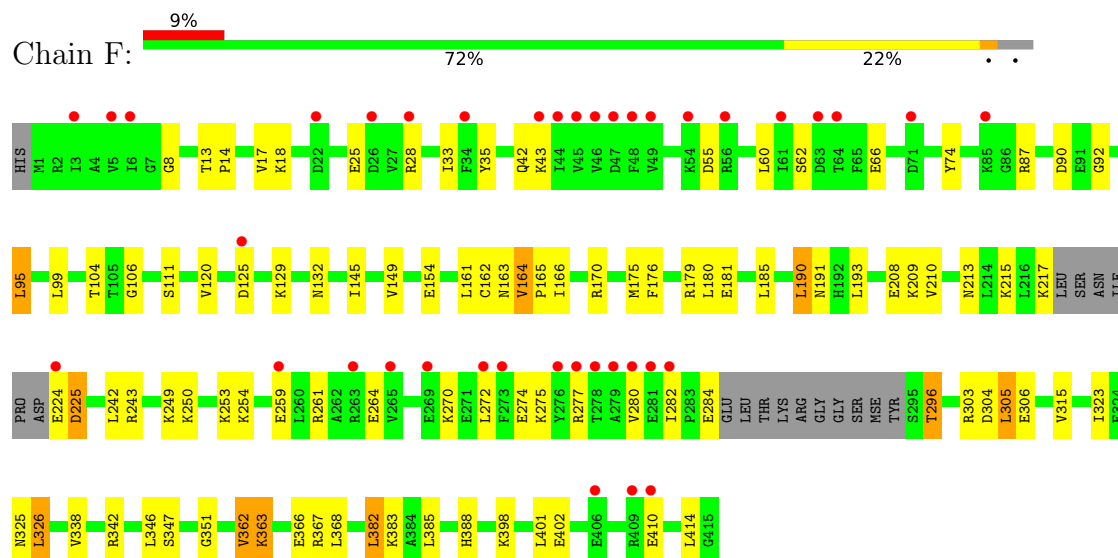


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

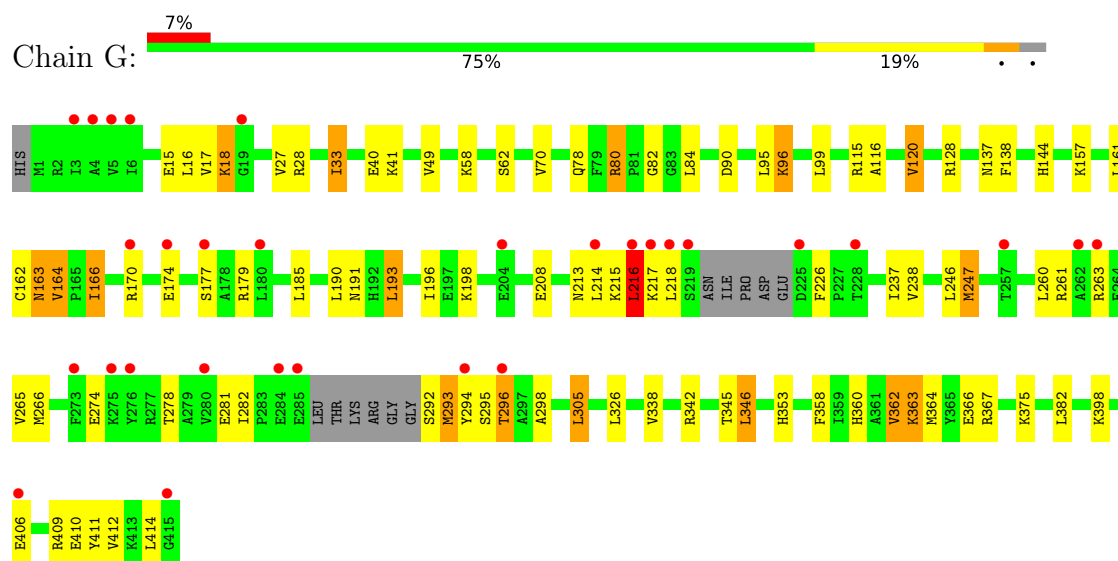




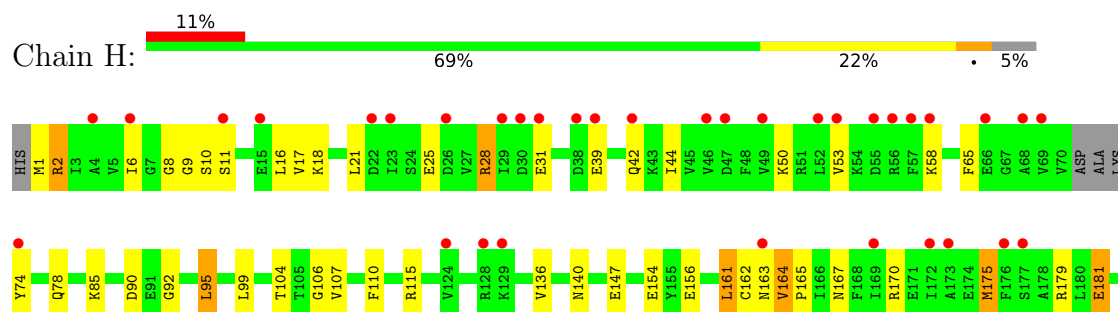
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

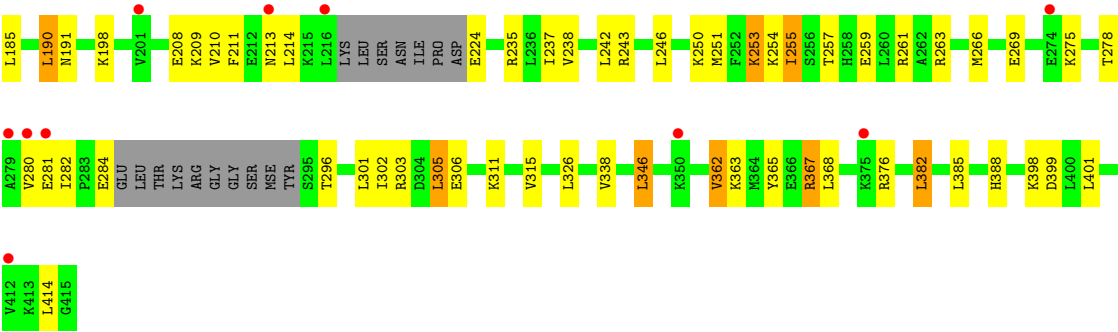


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 179.44Å 179.44Å 282.91Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.96 – 2.55<br>19.96 – 2.55                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (19.96-2.55)<br>99.5 (19.96-2.55)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.95 (at 2.56Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.1.24                                               | Depositor        |
| R, $R_{free}$                                                           | 0.200 , 0.250<br>0.264 , 0.296                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 14357 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.225                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 34.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 26917                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 20.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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: MN, G6P, NAD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.89         | 3/3420 (0.1%)  | 1.04        | 5/4595 (0.1%)   |
| 1   | B     | 0.79         | 0/3390         | 0.99        | 1/4558 (0.0%)   |
| 1   | C     | 0.84         | 2/3361 (0.1%)  | 1.02        | 1/4518 (0.0%)   |
| 1   | D     | 0.81         | 0/3335         | 1.01        | 2/4484 (0.0%)   |
| 1   | E     | 0.60         | 0/3219         | 0.93        | 0/4323          |
| 1   | F     | 0.62         | 0/3298         | 0.94        | 1/4435 (0.0%)   |
| 1   | G     | 0.72         | 0/3338         | 0.96        | 1/4487 (0.0%)   |
| 1   | H     | 0.59         | 0/3266         | 0.91        | 1/4392 (0.0%)   |
| All | All   | 0.74         | 5/26627 (0.0%) | 0.97        | 12/35792 (0.0%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 251 | MSE  | SE-CE  | -6.46 | 1.76        | 1.95     |
| 1   | A     | 167 | ASN  | CG-OD1 | 6.06  | 1.35        | 1.23     |
| 1   | C     | 167 | ASN  | CG-OD1 | 5.64  | 1.34        | 1.23     |
| 1   | C     | 163 | ASN  | CG-OD1 | 5.64  | 1.34        | 1.23     |
| 1   | A     | 93  | ILE  | CA-CB  | 5.46  | 1.57        | 1.53     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 296 | THR  | N-CA-C | -7.17 | 103.75      | 114.64   |
| 1   | D     | 292 | SER  | N-CA-C | 6.49  | 120.05      | 111.75   |
| 1   | H     | 16  | LEU  | N-CA-C | -5.68 | 104.78      | 110.97   |
| 1   | A     | 289 | ARG  | N-CA-C | 5.67  | 116.88      | 108.60   |
| 1   | C     | 328 | ASP  | N-CA-C | 5.59  | 118.14      | 111.71   |
| 1   | A     | 137 | ASN  | N-CA-C | 5.50  | 117.49      | 108.52   |
| 1   | A     | 324 | GLU  | CA-C-N | 5.28  | 131.88      | 122.06   |
| 1   | A     | 324 | GLU  | C-N-CA | 5.28  | 131.88      | 122.06   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 391 | GLY  | N-CA-C | 5.09  | 118.11      | 112.00   |
| 1   | B     | 294 | TYR  | N-CA-C | -5.08 | 105.92      | 111.82   |
| 1   | A     | 142 | SER  | N-CA-C | 5.06  | 116.79      | 111.28   |
| 1   | G     | 137 | ASN  | N-CA-C | 5.02  | 117.43      | 109.24   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3356  | 0        | 3393     | 54      | 0            |
| 1   | B     | 3331  | 0        | 3362     | 46      | 0            |
| 1   | C     | 3303  | 0        | 3322     | 47      | 0            |
| 1   | D     | 3276  | 0        | 3300     | 36      | 0            |
| 1   | E     | 3165  | 0        | 3184     | 45      | 0            |
| 1   | F     | 3240  | 0        | 3275     | 39      | 0            |
| 1   | G     | 3280  | 0        | 3313     | 39      | 0            |
| 1   | H     | 3209  | 0        | 3239     | 39      | 0            |
| 2   | A     | 44    | 0        | 26       | 5       | 0            |
| 2   | C     | 44    | 0        | 26       | 2       | 0            |
| 2   | G     | 44    | 0        | 26       | 3       | 0            |
| 3   | A     | 3     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 16    | 0        | 9        | 1       | 0            |
| 4   | C     | 16    | 0        | 10       | 1       | 0            |
| 5   | B     | 5     | 0        | 0        | 0       | 0            |
| 5   | D     | 5     | 0        | 0        | 0       | 0            |
| 5   | E     | 5     | 0        | 0        | 0       | 0            |
| 5   | G     | 5     | 0        | 0        | 0       | 0            |
| 6   | A     | 136   | 0        | 0        | 1       | 0            |
| 6   | B     | 83    | 0        | 0        | 1       | 0            |
| 6   | C     | 106   | 0        | 0        | 2       | 0            |
| 6   | D     | 95    | 0        | 0        | 2       | 0            |
| 6   | E     | 23    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | F     | 36    | 0        | 0        | 0       | 0            |
| 6   | G     | 59    | 0        | 0        | 0       | 0            |
| 6   | H     | 30    | 0        | 0        | 0       | 0            |
| All | All   | 26917 | 0        | 26485    | 333     | 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 6.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:175:MSE:HE3  | 1:F:213:ASN:ND2  | 1.62                     | 1.15              |
| 1:F:175:MSE:HE3  | 1:F:213:ASN:HD22 | 1.05                     | 1.15              |
| 1:D:175:MSE:HE3  | 1:D:213:ASN:HD22 | 0.92                     | 1.07              |
| 1:D:175:MSE:HE3  | 1:D:213:ASN:ND2  | 1.72                     | 1.03              |
| 1:F:8:GLY:HA3    | 1:F:42:GLN:HE21  | 1.27                     | 0.99              |
| 1:F:175:MSE:CE   | 1:F:213:ASN:HD22 | 1.87                     | 0.88              |
| 1:C:190:LEU:HD23 | 1:C:362:VAL:HG22 | 1.56                     | 0.88              |
| 1:D:175:MSE:CE   | 1:D:213:ASN:HD22 | 1.84                     | 0.87              |
| 1:D:175:MSE:HE1  | 1:D:210:VAL:HA   | 1.59                     | 0.85              |
| 1:E:190:LEU:HD23 | 1:E:362:VAL:HG22 | 1.60                     | 0.82              |
| 1:B:346:LEU:HD12 | 1:C:346:LEU:HD12 | 1.62                     | 0.81              |
| 1:F:382:LEU:HD13 | 1:F:401:LEU:HD22 | 1.62                     | 0.79              |
| 1:D:2:ARG:HG3    | 1:D:72:ALA:HA    | 1.64                     | 0.77              |
| 1:C:125:ASP:OD1  | 1:C:129:LYS:HE3  | 1.87                     | 0.75              |
| 1:H:190:LEU:HD23 | 1:H:362:VAL:HG22 | 1.70                     | 0.73              |
| 1:A:162:CYS:HB2  | 1:A:191:ASN:ND2  | 2.02                     | 0.73              |
| 1:D:170:ARG:HH22 | 1:D:293:MSE:HB2  | 1.52                     | 0.73              |
| 1:G:80:ARG:HB2   | 2:G:1416:NAD:H3D | 1.71                     | 0.72              |
| 1:A:162:CYS:HB2  | 1:A:191:ASN:HD21 | 1.52                     | 0.71              |
| 1:C:190:LEU:CD2  | 1:C:362:VAL:HG22 | 2.19                     | 0.71              |
| 1:G:305:LEU:HD13 | 1:G:338:VAL:HG13 | 1.72                     | 0.71              |
| 1:A:224:GLU:OE2  | 1:A:254:LYS:HE3  | 1.91                     | 0.70              |
| 1:F:162:CYS:SG   | 1:F:163:ASN:N    | 2.65                     | 0.69              |
| 1:D:175:MSE:HE2  | 1:D:176:PHE:CE2  | 2.28                     | 0.69              |
| 1:F:190:LEU:HD23 | 1:F:362:VAL:HG22 | 1.75                     | 0.69              |
| 1:A:289:ARG:HG3  | 1:A:290:GLY:H    | 1.58                     | 0.68              |
| 1:B:33:ILE:HD11  | 1:B:62:SER:HB2   | 1.76                     | 0.67              |
| 1:G:15:GLU:OE1   | 1:G:18:LYS:NZ    | 2.26                     | 0.67              |
| 1:B:346:LEU:CD1  | 1:C:346:LEU:HD12 | 2.23                     | 0.67              |
| 1:B:138:PHE:CE1  | 1:B:294:TYR:HD2  | 2.13                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:ASP:CG    | 1:C:115:ARG:HH22 | 2.03                     | 0.66              |
| 1:E:1:MSE:O      | 1:E:1:MSE:HG3    | 1.94                     | 0.66              |
| 1:E:9:GLY:HA2    | 1:E:45:VAL:HG21  | 1.78                     | 0.66              |
| 1:H:162:CYS:SG   | 1:H:163:ASN:N    | 2.65                     | 0.66              |
| 1:A:224:GLU:HG2  | 1:A:251:MSE:HE1  | 1.78                     | 0.66              |
| 1:E:162:CYS:HB2  | 1:E:191:ASN:ND2  | 2.10                     | 0.66              |
| 1:E:162:CYS:HB2  | 1:E:191:ASN:HD21 | 1.60                     | 0.65              |
| 1:G:163:ASN:HD22 | 1:G:163:ASN:H    | 1.45                     | 0.65              |
| 1:A:163:ASN:ND2  | 4:A:1418:G6P:O2  | 2.29                     | 0.64              |
| 1:A:162:CYS:CB   | 1:A:191:ASN:HD21 | 2.10                     | 0.64              |
| 1:H:162:CYS:HB2  | 1:H:191:ASN:HD21 | 1.63                     | 0.64              |
| 1:H:162:CYS:HB2  | 1:H:191:ASN:ND2  | 2.12                     | 0.64              |
| 1:D:170:ARG:NH2  | 1:D:293:MSE:HB2  | 2.13                     | 0.64              |
| 1:E:1:MSE:HE3    | 1:E:29:ILE:HG12  | 1.80                     | 0.63              |
| 1:D:163:ASN:ND2  | 1:D:291:GLY:HA2  | 2.14                     | 0.63              |
| 1:C:190:LEU:HD23 | 1:C:362:VAL:CG2  | 2.27                     | 0.63              |
| 1:H:175:MSE:HE1  | 1:H:210:VAL:HA   | 1.81                     | 0.63              |
| 1:C:345:THR:HG22 | 6:C:2081:HOH:O   | 1.97                     | 0.63              |
| 1:B:190:LEU:HD23 | 1:B:362:VAL:HG22 | 1.79                     | 0.62              |
| 1:E:164:VAL:HG22 | 1:E:165:PRO:HD3  | 1.81                     | 0.62              |
| 1:G:116:ALA:O    | 1:G:120:VAL:HG13 | 2.00                     | 0.62              |
| 1:F:259:GLU:OE1  | 1:F:264:GLU:HG3  | 2.00                     | 0.62              |
| 1:E:346:LEU:HD12 | 1:H:346:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:138:PHE:O    | 2:A:1416:NAD:H2N | 2.00                     | 0.61              |
| 1:E:1:MSE:N      | 6:E:2001:HOH:O   | 2.33                     | 0.61              |
| 1:F:346:LEU:HD23 | 1:G:346:LEU:CD1  | 2.31                     | 0.61              |
| 1:C:162:CYS:SG   | 1:C:164:VAL:HG13 | 2.41                     | 0.61              |
| 1:C:80:ARG:HB2   | 2:C:1416:NAD:H3D | 1.82                     | 0.60              |
| 1:C:179:ARG:NH1  | 1:C:181:GLU:OE2  | 2.35                     | 0.60              |
| 1:G:162:CYS:SG   | 1:G:164:VAL:HG13 | 2.42                     | 0.60              |
| 1:E:162:CYS:SG   | 1:E:164:VAL:HG13 | 2.41                     | 0.59              |
| 1:B:224:GLU:HG2  | 1:B:251:MSE:HE1  | 1.83                     | 0.59              |
| 1:F:175:MSE:HE2  | 1:F:176:PHE:CE2  | 2.38                     | 0.59              |
| 1:B:138:PHE:CZ   | 1:B:298:ALA:HB2  | 2.38                     | 0.59              |
| 1:A:261:ARG:HH22 | 1:A:289:ARG:HE   | 1.51                     | 0.59              |
| 1:A:90:ASP:CG    | 1:A:115:ARG:HH22 | 2.10                     | 0.59              |
| 1:E:149:VAL:HG22 | 1:E:153:LEU:HD12 | 1.84                     | 0.59              |
| 1:F:363:LYS:HE3  | 1:F:366:GLU:OE1  | 2.03                     | 0.58              |
| 1:B:303:ARG:NH1  | 1:B:304:ASP:OD1  | 2.35                     | 0.58              |
| 1:C:90:ASP:OD1   | 1:C:115:ARG:NH2  | 2.36                     | 0.58              |
| 1:C:163:ASN:ND2  | 4:C:1418:G6P:O2  | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:305:LEU:HD13 | 1:B:338:VAL:HG13 | 1.83                     | 0.58              |
| 1:H:251:MSE:O    | 1:H:255:ILE:HG13 | 2.04                     | 0.58              |
| 1:G:193:LEU:HD11 | 1:G:358:PHE:HB3  | 1.86                     | 0.58              |
| 1:C:116:ALA:O    | 1:C:120:VAL:HG13 | 2.04                     | 0.57              |
| 1:C:144:HIS:CD2  | 1:C:366:GLU:HB2  | 2.38                     | 0.57              |
| 1:A:305:LEU:HD13 | 1:A:338:VAL:HG13 | 1.86                     | 0.57              |
| 1:E:190:LEU:CD2  | 1:E:362:VAL:HG22 | 2.32                     | 0.57              |
| 1:H:305:LEU:HD13 | 1:H:338:VAL:HG13 | 1.87                     | 0.57              |
| 1:E:284:GLU:C    | 1:E:286:LEU:H    | 2.13                     | 0.57              |
| 1:H:104:THR:OG1  | 1:H:140:ASN:ND2  | 2.38                     | 0.57              |
| 1:H:90:ASP:CG    | 1:H:115:ARG:HH22 | 2.14                     | 0.56              |
| 1:D:303:ARG:HD2  | 1:D:304:ASP:OD1  | 2.06                     | 0.56              |
| 1:D:310:GLY:O    | 1:D:311:LYS:HD2  | 2.06                     | 0.56              |
| 1:H:74:TYR:OH    | 1:H:306:GLU:HG2  | 2.06                     | 0.56              |
| 1:G:406:GLU:OE1  | 1:G:406:GLU:HA   | 2.05                     | 0.55              |
| 1:H:382:LEU:HD13 | 1:H:401:LEU:HD22 | 1.88                     | 0.55              |
| 1:G:16:LEU:HD22  | 1:G:78:GLN:OE1   | 2.07                     | 0.55              |
| 1:A:41:LYS:HD3   | 1:A:273:PHE:CZ   | 2.41                     | 0.55              |
| 1:B:215:LYS:HG2  | 1:B:228:THR:HG23 | 1.87                     | 0.55              |
| 1:C:259:GLU:OE2  | 1:C:264:GLU:HG3  | 2.07                     | 0.55              |
| 1:E:30:ASP:OD1   | 1:E:30:ASP:N     | 2.40                     | 0.55              |
| 1:E:362:VAL:O    | 1:E:366:GLU:HG3  | 2.07                     | 0.55              |
| 1:F:125:ASP:O    | 1:F:129:LYS:HG2  | 2.07                     | 0.55              |
| 1:B:90:ASP:CG    | 1:B:115:ARG:HH22 | 2.13                     | 0.55              |
| 1:C:175:MSE:HE3  | 1:C:213:ASN:ND2  | 2.22                     | 0.55              |
| 1:H:162:CYS:CB   | 1:H:191:ASN:HD21 | 2.20                     | 0.55              |
| 1:H:253:LYS:O    | 1:H:257:THR:HG23 | 2.06                     | 0.55              |
| 1:A:116:ALA:O    | 1:A:120:VAL:HG13 | 2.06                     | 0.55              |
| 1:D:90:ASP:CG    | 1:D:115:ARG:HH22 | 2.15                     | 0.55              |
| 1:E:144:HIS:CD2  | 1:E:366:GLU:HB3  | 2.41                     | 0.55              |
| 1:A:294:TYR:CD1  | 1:A:295:SER:N    | 2.75                     | 0.55              |
| 1:C:163:ASN:H    | 1:C:163:ASN:HD22 | 1.55                     | 0.55              |
| 1:H:21:LEU:HD11  | 1:H:53:VAL:HG12  | 1.88                     | 0.55              |
| 1:B:376:ARG:NH2  | 6:B:2066:HOH:O   | 2.39                     | 0.54              |
| 1:A:261:ARG:HH12 | 1:A:289:ARG:NH2  | 2.05                     | 0.54              |
| 1:E:346:LEU:CD1  | 1:H:346:LEU:HD12 | 2.37                     | 0.54              |
| 1:A:305:LEU:HD13 | 1:A:338:VAL:CG1  | 2.38                     | 0.54              |
| 1:A:162:CYS:CB   | 1:A:191:ASN:ND2  | 2.69                     | 0.54              |
| 1:C:229:TRP:CD1  | 1:D:398:LYS:HD2  | 2.42                     | 0.54              |
| 1:G:90:ASP:OD1   | 1:G:115:ARG:NH2  | 2.41                     | 0.54              |
| 1:C:144:HIS:NE2  | 1:C:366:GLU:HB2  | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:ARG:HB2   | 2:A:1416:NAD:H3D | 1.89                     | 0.53              |
| 1:G:80:ARG:HB2   | 2:G:1416:NAD:C3D | 2.37                     | 0.53              |
| 1:C:305:LEU:HD13 | 1:C:338:VAL:HG13 | 1.91                     | 0.53              |
| 1:D:162:CYS:HB2  | 1:D:191:ASN:ND2  | 2.24                     | 0.53              |
| 1:C:140:ASN:HB3  | 6:C:2026:HOH:O   | 2.08                     | 0.53              |
| 1:F:175:MSE:HE1  | 1:F:210:VAL:HA   | 1.89                     | 0.53              |
| 1:B:164:VAL:HG22 | 1:B:165:PRO:HD3  | 1.91                     | 0.53              |
| 1:C:79:PHE:HB2   | 2:C:1416:NAD:C4A | 2.39                     | 0.53              |
| 1:D:162:CYS:SG   | 1:D:163:ASN:N    | 2.81                     | 0.52              |
| 1:A:132:ASN:O    | 1:A:157:LYS:NZ   | 2.42                     | 0.52              |
| 1:G:33:ILE:HD11  | 1:G:62:SER:HB2   | 1.92                     | 0.52              |
| 1:C:162:CYS:HB2  | 1:C:191:ASN:ND2  | 2.24                     | 0.52              |
| 1:D:305:LEU:HD13 | 1:D:338:VAL:HG13 | 1.92                     | 0.52              |
| 1:E:134:THR:HA   | 1:E:157:LYS:HB3  | 1.92                     | 0.52              |
| 1:B:16:LEU:HA    | 1:B:295:SER:HB2  | 1.92                     | 0.52              |
| 1:C:138:PHE:CZ   | 1:C:298:ALA:HB2  | 2.43                     | 0.52              |
| 1:E:199:VAL:HG13 | 1:E:207:THR:HA   | 1.92                     | 0.52              |
| 1:A:234:VAL:HA   | 1:B:383:LYS:HD2  | 1.92                     | 0.52              |
| 1:D:80:ARG:HD3   | 6:D:2020:HOH:O   | 2.09                     | 0.52              |
| 1:G:305:LEU:HD13 | 1:G:338:VAL:CG1  | 2.38                     | 0.52              |
| 1:G:409:ARG:HB2  | 1:G:409:ARG:NH1  | 2.24                     | 0.52              |
| 1:C:247:MSE:CE   | 1:C:250:LYS:HD2  | 2.39                     | 0.51              |
| 1:C:162:CYS:HB2  | 1:C:191:ASN:HD21 | 1.75                     | 0.51              |
| 1:A:215:LYS:C    | 1:A:217:LYS:H    | 2.19                     | 0.51              |
| 1:D:382:LEU:HD13 | 1:D:401:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:295:SER:OG   | 1:A:296:THR:N    | 2.42                     | 0.51              |
| 1:F:90:ASP:OD1   | 1:F:111:SER:OG   | 2.29                     | 0.51              |
| 1:F:35:TYR:C     | 1:F:42:GLN:HE22  | 2.19                     | 0.51              |
| 1:A:81:PRO:HB3   | 1:A:119:ILE:HD12 | 1.93                     | 0.51              |
| 1:E:65:PHE:HD1   | 1:E:66:GLU:H     | 1.58                     | 0.51              |
| 1:B:138:PHE:HZ   | 1:B:298:ALA:HB2  | 1.76                     | 0.50              |
| 1:A:138:PHE:CZ   | 1:A:298:ALA:HB2  | 2.46                     | 0.50              |
| 1:E:363:LYS:HA   | 1:E:366:GLU:HG3  | 1.93                     | 0.50              |
| 1:B:90:ASP:OD1   | 1:B:111:SER:OG   | 2.24                     | 0.50              |
| 1:G:144:HIS:CD2  | 1:G:366:GLU:HB2  | 2.46                     | 0.50              |
| 1:B:294:TYR:CG   | 1:B:295:SER:N    | 2.80                     | 0.50              |
| 1:B:382:LEU:HD13 | 1:B:401:LEU:HD22 | 1.94                     | 0.50              |
| 1:G:17:VAL:HG11  | 1:G:49:VAL:HG13  | 1.94                     | 0.50              |
| 1:B:90:ASP:OD1   | 1:B:115:ARG:NH2  | 2.42                     | 0.50              |
| 1:A:303:ARG:HD2  | 1:A:304:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:166:ILE:CD1  | 1:A:296:THR:HG22 | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:164:VAL:N    | 1:B:165:PRO:CD   | 2.76                     | 0.49              |
| 1:E:116:ALA:O    | 1:E:120:VAL:HG13 | 2.12                     | 0.49              |
| 1:E:82:GLY:HA2   | 1:E:411:TYR:CZ   | 2.47                     | 0.49              |
| 1:C:405:LEU:HD21 | 1:C:414:LEU:HD22 | 1.95                     | 0.49              |
| 1:D:164:VAL:N    | 1:D:165:PRO:CD   | 2.76                     | 0.49              |
| 1:E:21:LEU:HD23  | 1:E:57:PHE:CE2   | 2.48                     | 0.49              |
| 1:E:230:PHE:CE1  | 1:E:234:VAL:HG21 | 2.48                     | 0.49              |
| 1:H:2:ARG:HB2    | 1:H:31:GLU:HG2   | 1.95                     | 0.48              |
| 1:C:132:ASN:O    | 1:C:157:LYS:NZ   | 2.46                     | 0.48              |
| 1:C:247:MSE:HE2  | 1:C:250:LYS:HD2  | 1.95                     | 0.48              |
| 1:A:289:ARG:HG3  | 1:A:290:GLY:N    | 2.26                     | 0.48              |
| 1:F:368:LEU:HD22 | 1:F:383:LYS:HD3  | 1.95                     | 0.48              |
| 1:E:2:ARG:HG3    | 1:E:31:GLU:HG3   | 1.95                     | 0.48              |
| 1:F:162:CYS:CB   | 1:F:191:ASN:HD21 | 2.27                     | 0.48              |
| 1:F:33:ILE:HD11  | 1:F:62:SER:HB2   | 1.96                     | 0.48              |
| 1:C:138:PHE:HZ   | 1:C:298:ALA:HB2  | 1.78                     | 0.47              |
| 1:C:363:LYS:HE3  | 1:C:366:GLU:OE2  | 2.13                     | 0.47              |
| 1:D:239:ASN:OD1  | 1:D:240:PRO:HD2  | 2.14                     | 0.47              |
| 1:D:294:TYR:C    | 1:D:296:THR:H    | 2.22                     | 0.47              |
| 1:G:215:LYS:C    | 1:G:217:LYS:H    | 2.23                     | 0.47              |
| 1:H:92:GLY:O     | 1:H:95:LEU:HB2   | 2.14                     | 0.47              |
| 1:H:164:VAL:N    | 1:H:165:PRO:CD   | 2.77                     | 0.47              |
| 1:B:346:LEU:CD1  | 1:C:346:LEU:CD1  | 2.92                     | 0.47              |
| 1:C:382:LEU:HD13 | 1:C:401:LEU:HD22 | 1.95                     | 0.47              |
| 1:E:90:ASP:OD2   | 1:E:115:ARG:NH2  | 2.46                     | 0.47              |
| 1:E:212:GLU:HA   | 1:E:215:LYS:HE2  | 1.96                     | 0.47              |
| 1:B:247:MSE:HE2  | 1:B:251:MSE:HE3  | 1.96                     | 0.47              |
| 1:E:9:GLY:HA2    | 1:E:45:VAL:CG2   | 2.43                     | 0.47              |
| 1:H:106:GLY:HA2  | 1:H:388:HIS:CE1  | 2.49                     | 0.47              |
| 1:B:190:LEU:CD2  | 1:B:362:VAL:HG22 | 2.43                     | 0.47              |
| 1:F:382:LEU:HD13 | 1:F:401:LEU:CD2  | 2.38                     | 0.47              |
| 1:G:362:VAL:O    | 1:G:366:GLU:HG2  | 2.15                     | 0.47              |
| 1:G:90:ASP:CG    | 1:G:115:ARG:HH22 | 2.24                     | 0.46              |
| 1:A:170:ARG:HH22 | 1:A:293:MSE:HB3  | 1.80                     | 0.46              |
| 1:H:136:VAL:HG13 | 1:H:161:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:79:PHE:HB2   | 2:A:1416:NAD:C4A | 2.45                     | 0.46              |
| 1:C:17:VAL:HG11  | 1:C:49:VAL:HG13  | 1.97                     | 0.46              |
| 1:D:90:ASP:OD1   | 1:D:115:ARG:NH2  | 2.47                     | 0.46              |
| 1:E:358:PHE:O    | 1:E:362:VAL:HG13 | 2.15                     | 0.46              |
| 1:F:190:LEU:CD2  | 1:F:362:VAL:HG22 | 2.42                     | 0.46              |
| 1:B:13:THR:HB    | 1:B:14:PRO:HD3   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:49:VAL:O     | 1:B:53:VAL:HG23  | 2.15                     | 0.46              |
| 1:F:175:MSE:HE2  | 1:F:176:PHE:CZ   | 2.50                     | 0.46              |
| 1:D:282:ILE:HA   | 1:D:283:PRO:HD3  | 1.84                     | 0.46              |
| 1:E:284:GLU:C    | 1:E:286:LEU:N    | 2.74                     | 0.46              |
| 1:B:162:CYS:HB2  | 1:B:191:ASN:HD21 | 1.80                     | 0.46              |
| 1:D:129:LYS:HE3  | 1:D:129:LYS:HB3  | 1.70                     | 0.46              |
| 1:F:162:CYS:HB2  | 1:F:191:ASN:HD21 | 1.81                     | 0.46              |
| 1:F:305:LEU:HD13 | 1:F:338:VAL:HG13 | 1.98                     | 0.46              |
| 1:H:162:CYS:CB   | 1:H:191:ASN:ND2  | 2.79                     | 0.46              |
| 1:A:175:MSE:HE2  | 1:A:176:PHE:CE2  | 2.51                     | 0.45              |
| 1:E:145:ILE:O    | 1:E:148:PHE:HB3  | 2.16                     | 0.45              |
| 1:D:162:CYS:HB2  | 1:D:191:ASN:HD21 | 1.82                     | 0.45              |
| 1:E:284:GLU:O    | 1:E:286:LEU:N    | 2.49                     | 0.45              |
| 1:F:303:ARG:HD2  | 1:F:304:ASP:OD1  | 2.16                     | 0.45              |
| 1:A:163:ASN:H    | 1:A:163:ASN:HD22 | 1.64                     | 0.45              |
| 1:C:111:SER:HB3  | 1:C:404:ILE:HG23 | 1.99                     | 0.45              |
| 1:D:255:ILE:HG22 | 1:D:255:ILE:O    | 2.15                     | 0.45              |
| 1:H:90:ASP:OD1   | 1:H:115:ARG:NH2  | 2.50                     | 0.45              |
| 1:A:272:LEU:HD21 | 1:A:285:GLU:HG2  | 1.97                     | 0.45              |
| 1:B:149:VAL:HG11 | 1:B:158:PHE:CD2  | 2.52                     | 0.45              |
| 1:E:92:GLY:HA2   | 1:E:95:LEU:HD22  | 1.98                     | 0.45              |
| 1:G:138:PHE:CE1  | 1:G:294:TYR:HD2  | 2.35                     | 0.45              |
| 1:D:164:VAL:HG22 | 1:D:165:PRO:HD3  | 1.99                     | 0.45              |
| 1:H:74:TYR:CD2   | 1:H:302:ILE:HG12 | 2.52                     | 0.45              |
| 1:A:261:ARG:HH22 | 1:A:289:ARG:NE   | 2.14                     | 0.45              |
| 1:E:13:THR:HB    | 1:E:14:PRO:CD    | 2.47                     | 0.45              |
| 1:B:15:GLU:OE1   | 1:B:292:SER:O    | 2.35                     | 0.45              |
| 1:D:175:MSE:HE2  | 1:D:176:PHE:CZ   | 2.52                     | 0.45              |
| 1:H:235:ARG:HG2  | 1:H:235:ARG:HH11 | 1.82                     | 0.45              |
| 1:A:239:ASN:OD1  | 1:A:240:PRO:HD2  | 2.16                     | 0.44              |
| 1:B:85:LYS:HG3   | 1:B:86:GLY:N     | 2.32                     | 0.44              |
| 1:B:147:GLU:HA   | 1:B:331:VAL:HG21 | 1.98                     | 0.44              |
| 1:F:8:GLY:HA3    | 1:F:42:GLN:NE2   | 2.11                     | 0.44              |
| 1:A:261:ARG:HH12 | 1:A:289:ARG:HH21 | 1.63                     | 0.44              |
| 1:H:6:ILE:HD12   | 1:H:65:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:173:ALA:HB1  | 1:A:178:ALA:O    | 2.16                     | 0.44              |
| 1:A:215:LYS:HB2  | 1:A:215:LYS:HE2  | 1.81                     | 0.44              |
| 1:A:382:LEU:HD13 | 1:A:401:LEU:HD22 | 2.00                     | 0.44              |
| 1:B:138:PHE:CZ   | 1:B:161:LEU:HD23 | 2.53                     | 0.44              |
| 1:B:138:PHE:CZ   | 1:B:294:TYR:HD2  | 2.35                     | 0.44              |
| 1:A:88:GLU:OE1   | 1:A:266:MSE:HE1  | 2.16                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:138:PHE:HZ   | 1:A:298:ALA:HB2   | 1.82                     | 0.44              |
| 1:B:162:CYS:CB   | 1:B:191:ASN:HD21  | 2.30                     | 0.44              |
| 1:E:224:GLU:HG2  | 1:E:251:MSE:HE1   | 2.00                     | 0.44              |
| 1:A:78:GLN:O     | 2:A:1416:NAD:H52N | 2.18                     | 0.44              |
| 1:A:90:ASP:OD1   | 1:A:115:ARG:NH2   | 2.49                     | 0.44              |
| 1:C:16:LEU:HD22  | 1:C:78:GLN:OE1    | 2.18                     | 0.44              |
| 1:E:65:PHE:CD1   | 1:E:66:GLU:N      | 2.83                     | 0.44              |
| 1:G:360:HIS:O    | 1:G:364:MSE:HG2   | 2.17                     | 0.44              |
| 1:A:162:CYS:SG   | 1:A:164:VAL:HG13  | 2.58                     | 0.44              |
| 1:A:405:LEU:HD21 | 1:A:414:LEU:HD22  | 1.98                     | 0.44              |
| 1:G:196:ILE:HB   | 1:G:237:ILE:HB    | 2.00                     | 0.44              |
| 1:A:140:ASN:HB3  | 6:A:2035:HOH:O    | 2.17                     | 0.44              |
| 1:F:106:GLY:HA2  | 1:F:388:HIS:CE1   | 2.52                     | 0.44              |
| 1:H:17:VAL:O     | 1:H:18:LYS:C      | 2.59                     | 0.44              |
| 1:D:2:ARG:CG     | 1:D:72:ALA:HA     | 2.41                     | 0.44              |
| 1:F:145:ILE:O    | 1:F:149:VAL:HG23  | 2.18                     | 0.44              |
| 1:B:346:LEU:HD11 | 1:C:346:LEU:CD1   | 2.48                     | 0.43              |
| 1:E:305:LEU:HD13 | 1:E:338:VAL:HG13  | 1.99                     | 0.43              |
| 1:F:87:ARG:O     | 1:F:90:ASP:HB2    | 2.19                     | 0.43              |
| 1:G:170:ARG:HH12 | 1:G:293:MSE:SE    | 2.51                     | 0.43              |
| 1:G:216:LEU:H    | 1:G:216:LEU:HG    | 1.64                     | 0.43              |
| 1:B:87:ARG:NH1   | 1:B:265:VAL:HG21  | 2.33                     | 0.43              |
| 1:E:323:ILE:HG21 | 1:E:326:LEU:HD22  | 1.99                     | 0.43              |
| 1:B:294:TYR:CE1  | 1:B:295:SER:HB3   | 2.54                     | 0.43              |
| 1:E:362:VAL:O    | 1:E:366:GLU:CG    | 2.66                     | 0.43              |
| 1:G:363:LYS:HA   | 1:G:366:GLU:HG2   | 2.00                     | 0.43              |
| 1:C:215:LYS:HG3  | 1:C:216:LEU:N     | 2.32                     | 0.43              |
| 1:D:116:ALA:O    | 1:D:120:VAL:HG13  | 2.19                     | 0.43              |
| 1:F:13:THR:N     | 1:F:14:PRO:CD     | 2.82                     | 0.43              |
| 1:F:92:GLY:O     | 1:F:95:LEU:HB2    | 2.17                     | 0.43              |
| 1:F:363:LYS:CE   | 1:F:366:GLU:OE1   | 2.66                     | 0.43              |
| 1:G:363:LYS:CE   | 1:G:366:GLU:OE2   | 2.66                     | 0.43              |
| 1:B:316:ASN:HA   | 1:B:332:LEU:O     | 2.18                     | 0.43              |
| 1:D:363:LYS:HE3  | 1:D:366:GLU:OE1   | 2.19                     | 0.43              |
| 1:A:175:MSE:HE1  | 1:A:210:VAL:HA    | 2.01                     | 0.43              |
| 1:E:1:MSE:HG2    | 1:E:28:ARG:O      | 2.19                     | 0.43              |
| 1:E:259:GLU:OE2  | 1:E:264:GLU:HG2   | 2.18                     | 0.43              |
| 1:F:346:LEU:HD23 | 1:G:346:LEU:HD13  | 2.00                     | 0.43              |
| 1:H:8:GLY:HA3    | 1:H:42:GLN:OE1    | 2.19                     | 0.43              |
| 1:H:107:VAL:O    | 1:H:110:PHE:HB3   | 2.18                     | 0.43              |
| 1:A:316:ASN:HA   | 1:A:332:LEU:O     | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:234:VAL:HA   | 1:F:383:LYS:HG3  | 2.00                     | 0.42              |
| 1:G:294:TYR:CD1  | 1:G:295:SER:N    | 2.87                     | 0.42              |
| 1:H:235:ARG:HG2  | 1:H:235:ARG:NH1  | 2.33                     | 0.42              |
| 1:H:301:LEU:HG   | 1:H:305:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:93:ILE:N     | 1:A:94:PRO:CD    | 2.81                     | 0.42              |
| 1:B:116:ALA:O    | 1:B:120:VAL:HG13 | 2.19                     | 0.42              |
| 1:C:196:ILE:HB   | 1:C:237:ILE:HB   | 2.01                     | 0.42              |
| 1:H:147:GLU:OE2  | 1:H:367:ARG:NH1  | 2.41                     | 0.42              |
| 1:C:15:GLU:OE2   | 1:C:287:THR:HG23 | 2.19                     | 0.42              |
| 1:B:239:ASN:OD1  | 1:B:240:PRO:HD2  | 2.20                     | 0.42              |
| 1:A:45:VAL:CG2   | 1:A:273:PHE:HE1  | 2.32                     | 0.42              |
| 1:C:144:HIS:CE1  | 1:C:366:GLU:HB2  | 2.54                     | 0.42              |
| 1:D:196:ILE:HB   | 1:D:237:ILE:HB   | 2.02                     | 0.42              |
| 1:B:282:ILE:HA   | 1:B:283:PRO:HD3  | 1.89                     | 0.42              |
| 1:D:316:ASN:HA   | 1:D:332:LEU:O    | 2.19                     | 0.42              |
| 1:B:147:GLU:OE2  | 1:B:367:ARG:HD3  | 2.20                     | 0.42              |
| 1:B:392:PRO:HG3  | 1:B:400:LEU:HD23 | 2.02                     | 0.42              |
| 1:C:16:LEU:HA    | 1:C:295:SER:HB2  | 2.02                     | 0.42              |
| 1:A:261:ARG:O    | 1:A:265:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:166:ILE:CD1  | 1:G:296:THR:HG22 | 2.50                     | 0.41              |
| 1:G:226:PHE:CD1  | 1:G:247:MSE:HE3  | 2.55                     | 0.41              |
| 1:F:325:ASN:ND2  | 1:F:351:GLY:O    | 2.53                     | 0.41              |
| 1:B:49:VAL:HA    | 1:B:52:LEU:HD12  | 2.03                     | 0.41              |
| 1:B:162:CYS:SG   | 1:B:191:ASN:ND2  | 2.90                     | 0.41              |
| 1:C:323:ILE:HG21 | 1:C:326:LEU:HD22 | 2.02                     | 0.41              |
| 1:D:2:ARG:HG2    | 1:D:71:ASP:O     | 2.21                     | 0.41              |
| 1:F:164:VAL:HG22 | 1:F:165:PRO:HD3  | 2.03                     | 0.41              |
| 1:G:353:HIS:HB2  | 1:H:368:LEU:HD21 | 2.03                     | 0.41              |
| 1:H:181:GLU:H    | 1:H:181:GLU:HG3  | 1.65                     | 0.41              |
| 1:C:80:ARG:O     | 1:C:80:ARG:HG3   | 2.19                     | 0.41              |
| 1:C:162:CYS:CB   | 1:C:191:ASN:HD21 | 2.34                     | 0.41              |
| 1:A:326:LEU:HD21 | 1:A:356:LEU:HG   | 2.02                     | 0.41              |
| 1:B:221:ILE:HA   | 1:B:222:PRO:HD3  | 1.66                     | 0.41              |
| 1:D:16:LEU:HA    | 1:D:295:SER:HB3  | 2.03                     | 0.41              |
| 1:G:138:PHE:CE2  | 1:G:298:ALA:HB2  | 2.56                     | 0.41              |
| 1:A:97:TYR:HB2   | 1:A:99:LEU:HD22  | 2.03                     | 0.41              |
| 1:A:282:ILE:HA   | 1:A:283:PRO:HD3  | 1.95                     | 0.41              |
| 1:G:84:LEU:HD13  | 1:G:266:MSE:HG3  | 2.02                     | 0.41              |
| 1:G:162:CYS:HB2  | 1:G:191:ASN:ND2  | 2.36                     | 0.41              |
| 1:H:243:ARG:HB3  | 1:H:251:MSE:HE3  | 2.03                     | 0.41              |
| 1:E:138:PHE:HE2  | 1:E:298:ALA:HB2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:96:LYS:HZ2   | 1:G:96:LYS:HG2   | 1.77                     | 0.41              |
| 1:H:1:MSE:HE3    | 1:H:28:ARG:O     | 2.21                     | 0.41              |
| 1:H:9:GLY:O      | 1:H:10:SER:C     | 2.62                     | 0.41              |
| 1:E:10:SER:C     | 1:E:12:TYR:N     | 2.79                     | 0.40              |
| 1:C:249:LYS:HB2  | 1:C:249:LYS:HE3  | 1.96                     | 0.40              |
| 1:F:225:ASP:OD1  | 1:F:225:ASP:N    | 2.54                     | 0.40              |
| 1:F:17:VAL:O     | 1:F:18:LYS:C     | 2.65                     | 0.40              |
| 1:F:74:TYR:OH    | 1:F:306:GLU:OE2  | 2.27                     | 0.40              |
| 1:F:323:ILE:HG21 | 1:F:326:LEU:HD22 | 2.02                     | 0.40              |
| 1:G:80:ARG:NH2   | 2:G:1416:NAD:O1N | 2.54                     | 0.40              |
| 1:G:82:GLY:HA2   | 1:G:411:TYR:CZ   | 2.56                     | 0.40              |
| 1:G:166:ILE:HD13 | 1:G:296:THR:HG22 | 2.03                     | 0.40              |
| 1:H:211:PHE:CE1  | 1:H:237:ILE:HG13 | 2.56                     | 0.40              |
| 1:A:79:PHE:HB2   | 2:A:1416:NAD:C5A | 2.51                     | 0.40              |
| 1:D:118:PRO:HG2  | 6:D:2023:HOH:O   | 2.21                     | 0.40              |
| 1:H:10:SER:HB3   | 1:H:78:GLN:NE2   | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 410/416 (99%) | 398 (97%) | 10 (2%) | 2 (0%)   | 24          | 34  |
| 1   | B     | 404/416 (97%) | 393 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | C     | 401/416 (96%) | 395 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | D     | 398/416 (96%) | 387 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | E     | 378/416 (91%) | 372 (98%) | 5 (1%)  | 1 (0%)   | 36          | 45  |
| 1   | F     | 393/416 (94%) | 383 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | G     | 398/416 (96%) | 386 (97%) | 11 (3%) | 1 (0%)   | 36          | 45  |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | H     | 387/416 (93%)   | 379 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| All | All   | 3169/3328 (95%) | 3093 (98%) | 72 (2%) | 4 (0%)   | 48          | 61  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 216 | LEU  |
| 1   | A     | 290 | GLY  |
| 1   | E     | 285 | GLU  |
| 1   | G     | 216 | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | A     | 366/361 (101%)  | 322 (88%)  | 44 (12%)  | 5           | 5 |
| 1   | B     | 364/361 (101%)  | 306 (84%)  | 58 (16%)  | 2           | 2 |
| 1   | C     | 360/361 (100%)  | 301 (84%)  | 59 (16%)  | 2           | 2 |
| 1   | D     | 357/361 (99%)   | 299 (84%)  | 58 (16%)  | 2           | 2 |
| 1   | E     | 345/361 (96%)   | 274 (79%)  | 71 (21%)  | 1           | 1 |
| 1   | F     | 353/361 (98%)   | 295 (84%)  | 58 (16%)  | 2           | 2 |
| 1   | G     | 358/361 (99%)   | 299 (84%)  | 59 (16%)  | 2           | 2 |
| 1   | H     | 350/361 (97%)   | 287 (82%)  | 63 (18%)  | 2           | 1 |
| All | All   | 2853/2888 (99%) | 2383 (84%) | 470 (16%) | 2           | 2 |

All (470) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | ARG  |
| 1   | A     | 39  | GLU  |
| 1   | A     | 41  | LYS  |
| 1   | A     | 58  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | ARG  |
| 1   | A     | 85  | LYS  |
| 1   | A     | 95  | LEU  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 120 | VAL  |
| 1   | A     | 154 | GLU  |
| 1   | A     | 156 | GLU  |
| 1   | A     | 157 | LYS  |
| 1   | A     | 161 | LEU  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 164 | VAL  |
| 1   | A     | 174 | GLU  |
| 1   | A     | 185 | LEU  |
| 1   | A     | 190 | LEU  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 198 | LYS  |
| 1   | A     | 213 | ASN  |
| 1   | A     | 214 | LEU  |
| 1   | A     | 215 | LYS  |
| 1   | A     | 216 | LEU  |
| 1   | A     | 217 | LYS  |
| 1   | A     | 235 | ARG  |
| 1   | A     | 238 | VAL  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 282 | ILE  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 287 | THR  |
| 1   | A     | 294 | TYR  |
| 1   | A     | 303 | ARG  |
| 1   | A     | 305 | LEU  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 342 | ARG  |
| 1   | A     | 345 | THR  |
| 1   | A     | 346 | LEU  |
| 1   | A     | 367 | ARG  |
| 1   | A     | 375 | LYS  |
| 1   | A     | 378 | LYS  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 402 | GLU  |
| 1   | A     | 414 | LEU  |
| 1   | B     | 25  | GLU  |
| 1   | B     | 26  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 27  | VAL  |
| 1   | B     | 43  | LYS  |
| 1   | B     | 44  | ILE  |
| 1   | B     | 54  | LYS  |
| 1   | B     | 55  | ASP  |
| 1   | B     | 58  | LYS  |
| 1   | B     | 85  | LYS  |
| 1   | B     | 95  | LEU  |
| 1   | B     | 99  | LEU  |
| 1   | B     | 120 | VAL  |
| 1   | B     | 154 | GLU  |
| 1   | B     | 161 | LEU  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 164 | VAL  |
| 1   | B     | 170 | ARG  |
| 1   | B     | 177 | SER  |
| 1   | B     | 180 | LEU  |
| 1   | B     | 185 | LEU  |
| 1   | B     | 190 | LEU  |
| 1   | B     | 202 | LYS  |
| 1   | B     | 208 | GLU  |
| 1   | B     | 212 | GLU  |
| 1   | B     | 217 | LYS  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 221 | ILE  |
| 1   | B     | 223 | ASP  |
| 1   | B     | 225 | ASP  |
| 1   | B     | 238 | VAL  |
| 1   | B     | 246 | LEU  |
| 1   | B     | 247 | MSE  |
| 1   | B     | 253 | LYS  |
| 1   | B     | 261 | ARG  |
| 1   | B     | 266 | MSE  |
| 1   | B     | 268 | ILE  |
| 1   | B     | 270 | LYS  |
| 1   | B     | 274 | GLU  |
| 1   | B     | 275 | LYS  |
| 1   | B     | 278 | THR  |
| 1   | B     | 280 | VAL  |
| 1   | B     | 286 | LEU  |
| 1   | B     | 293 | MSE  |
| 1   | B     | 296 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 305 | LEU  |
| 1   | B     | 311 | LYS  |
| 1   | B     | 322 | SER  |
| 1   | B     | 326 | LEU  |
| 1   | B     | 342 | ARG  |
| 1   | B     | 346 | LEU  |
| 1   | B     | 362 | VAL  |
| 1   | B     | 363 | LYS  |
| 1   | B     | 365 | TYR  |
| 1   | B     | 367 | ARG  |
| 1   | B     | 376 | ARG  |
| 1   | B     | 382 | LEU  |
| 1   | B     | 385 | LEU  |
| 1   | B     | 414 | LEU  |
| 1   | C     | 18  | LYS  |
| 1   | C     | 25  | GLU  |
| 1   | C     | 26  | ASP  |
| 1   | C     | 28  | ARG  |
| 1   | C     | 39  | GLU  |
| 1   | C     | 41  | LYS  |
| 1   | C     | 43  | LYS  |
| 1   | C     | 80  | ARG  |
| 1   | C     | 85  | LYS  |
| 1   | C     | 95  | LEU  |
| 1   | C     | 96  | LYS  |
| 1   | C     | 99  | LEU  |
| 1   | C     | 120 | VAL  |
| 1   | C     | 132 | ASN  |
| 1   | C     | 154 | GLU  |
| 1   | C     | 157 | LYS  |
| 1   | C     | 161 | LEU  |
| 1   | C     | 163 | ASN  |
| 1   | C     | 164 | VAL  |
| 1   | C     | 170 | ARG  |
| 1   | C     | 177 | SER  |
| 1   | C     | 181 | GLU  |
| 1   | C     | 185 | LEU  |
| 1   | C     | 190 | LEU  |
| 1   | C     | 193 | LEU  |
| 1   | C     | 198 | LYS  |
| 1   | C     | 214 | LEU  |
| 1   | C     | 216 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 235 | ARG  |
| 1   | C     | 238 | VAL  |
| 1   | C     | 242 | LEU  |
| 1   | C     | 246 | LEU  |
| 1   | C     | 250 | LYS  |
| 1   | C     | 253 | LYS  |
| 1   | C     | 254 | LYS  |
| 1   | C     | 259 | GLU  |
| 1   | C     | 260 | LEU  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 266 | MSE  |
| 1   | C     | 267 | LYS  |
| 1   | C     | 271 | GLU  |
| 1   | C     | 274 | GLU  |
| 1   | C     | 284 | GLU  |
| 1   | C     | 285 | GLU  |
| 1   | C     | 286 | LEU  |
| 1   | C     | 287 | THR  |
| 1   | C     | 292 | SER  |
| 1   | C     | 305 | LEU  |
| 1   | C     | 309 | GLU  |
| 1   | C     | 326 | LEU  |
| 1   | C     | 345 | THR  |
| 1   | C     | 346 | LEU  |
| 1   | C     | 347 | SER  |
| 1   | C     | 362 | VAL  |
| 1   | C     | 363 | LYS  |
| 1   | C     | 375 | LYS  |
| 1   | C     | 382 | LEU  |
| 1   | C     | 409 | ARG  |
| 1   | C     | 414 | LEU  |
| 1   | D     | 26  | ASP  |
| 1   | D     | 28  | ARG  |
| 1   | D     | 39  | GLU  |
| 1   | D     | 41  | LYS  |
| 1   | D     | 58  | LYS  |
| 1   | D     | 62  | SER  |
| 1   | D     | 63  | ASP  |
| 1   | D     | 70  | VAL  |
| 1   | D     | 71  | ASP  |
| 1   | D     | 85  | LYS  |
| 1   | D     | 95  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 99  | LEU  |
| 1   | D     | 120 | VAL  |
| 1   | D     | 128 | ARG  |
| 1   | D     | 129 | LYS  |
| 1   | D     | 156 | GLU  |
| 1   | D     | 157 | LYS  |
| 1   | D     | 161 | LEU  |
| 1   | D     | 164 | VAL  |
| 1   | D     | 170 | ARG  |
| 1   | D     | 177 | SER  |
| 1   | D     | 180 | LEU  |
| 1   | D     | 185 | LEU  |
| 1   | D     | 190 | LEU  |
| 1   | D     | 193 | LEU  |
| 1   | D     | 208 | GLU  |
| 1   | D     | 215 | LYS  |
| 1   | D     | 216 | LEU  |
| 1   | D     | 225 | ASP  |
| 1   | D     | 235 | ARG  |
| 1   | D     | 238 | VAL  |
| 1   | D     | 246 | LEU  |
| 1   | D     | 247 | MSE  |
| 1   | D     | 253 | LYS  |
| 1   | D     | 254 | LYS  |
| 1   | D     | 261 | ARG  |
| 1   | D     | 270 | LYS  |
| 1   | D     | 274 | GLU  |
| 1   | D     | 275 | LYS  |
| 1   | D     | 278 | THR  |
| 1   | D     | 281 | GLU  |
| 1   | D     | 294 | TYR  |
| 1   | D     | 296 | THR  |
| 1   | D     | 305 | LEU  |
| 1   | D     | 311 | LYS  |
| 1   | D     | 326 | LEU  |
| 1   | D     | 342 | ARG  |
| 1   | D     | 346 | LEU  |
| 1   | D     | 363 | LYS  |
| 1   | D     | 365 | TYR  |
| 1   | D     | 367 | ARG  |
| 1   | D     | 378 | LYS  |
| 1   | D     | 382 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 385 | LEU  |
| 1   | D     | 410 | GLU  |
| 1   | D     | 412 | VAL  |
| 1   | D     | 413 | LYS  |
| 1   | D     | 414 | LEU  |
| 1   | E     | 1   | MSE  |
| 1   | E     | 6   | ILE  |
| 1   | E     | 11  | SER  |
| 1   | E     | 25  | GLU  |
| 1   | E     | 30  | ASP  |
| 1   | E     | 39  | GLU  |
| 1   | E     | 41  | LYS  |
| 1   | E     | 43  | LYS  |
| 1   | E     | 44  | ILE  |
| 1   | E     | 51  | ARG  |
| 1   | E     | 60  | LEU  |
| 1   | E     | 63  | ASP  |
| 1   | E     | 65  | PHE  |
| 1   | E     | 66  | GLU  |
| 1   | E     | 85  | LYS  |
| 1   | E     | 95  | LEU  |
| 1   | E     | 96  | LYS  |
| 1   | E     | 99  | LEU  |
| 1   | E     | 120 | VAL  |
| 1   | E     | 121 | GLU  |
| 1   | E     | 126 | THR  |
| 1   | E     | 129 | LYS  |
| 1   | E     | 154 | GLU  |
| 1   | E     | 156 | GLU  |
| 1   | E     | 157 | LYS  |
| 1   | E     | 163 | ASN  |
| 1   | E     | 164 | VAL  |
| 1   | E     | 166 | ILE  |
| 1   | E     | 181 | GLU  |
| 1   | E     | 185 | LEU  |
| 1   | E     | 190 | LEU  |
| 1   | E     | 198 | LYS  |
| 1   | E     | 199 | VAL  |
| 1   | E     | 209 | LYS  |
| 1   | E     | 214 | LEU  |
| 1   | E     | 223 | ASP  |
| 1   | E     | 224 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 225 | ASP  |
| 1   | E     | 228 | THR  |
| 1   | E     | 242 | LEU  |
| 1   | E     | 246 | LEU  |
| 1   | E     | 250 | LYS  |
| 1   | E     | 253 | LYS  |
| 1   | E     | 254 | LYS  |
| 1   | E     | 260 | LEU  |
| 1   | E     | 265 | VAL  |
| 1   | E     | 267 | LYS  |
| 1   | E     | 268 | ILE  |
| 1   | E     | 272 | LEU  |
| 1   | E     | 274 | GLU  |
| 1   | E     | 275 | LYS  |
| 1   | E     | 286 | LEU  |
| 1   | E     | 305 | LEU  |
| 1   | E     | 309 | GLU  |
| 1   | E     | 315 | VAL  |
| 1   | E     | 326 | LEU  |
| 1   | E     | 334 | ILE  |
| 1   | E     | 342 | ARG  |
| 1   | E     | 345 | THR  |
| 1   | E     | 346 | LEU  |
| 1   | E     | 362 | VAL  |
| 1   | E     | 363 | LYS  |
| 1   | E     | 367 | ARG  |
| 1   | E     | 375 | LYS  |
| 1   | E     | 376 | ARG  |
| 1   | E     | 378 | LYS  |
| 1   | E     | 382 | LEU  |
| 1   | E     | 398 | LYS  |
| 1   | E     | 402 | GLU  |
| 1   | E     | 410 | GLU  |
| 1   | E     | 414 | LEU  |
| 1   | F     | 25  | GLU  |
| 1   | F     | 28  | ARG  |
| 1   | F     | 43  | LYS  |
| 1   | F     | 55  | ASP  |
| 1   | F     | 60  | LEU  |
| 1   | F     | 66  | GLU  |
| 1   | F     | 95  | LEU  |
| 1   | F     | 99  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 104 | THR  |
| 1   | F     | 120 | VAL  |
| 1   | F     | 132 | ASN  |
| 1   | F     | 154 | GLU  |
| 1   | F     | 161 | LEU  |
| 1   | F     | 164 | VAL  |
| 1   | F     | 166 | ILE  |
| 1   | F     | 170 | ARG  |
| 1   | F     | 179 | ARG  |
| 1   | F     | 180 | LEU  |
| 1   | F     | 181 | GLU  |
| 1   | F     | 185 | LEU  |
| 1   | F     | 190 | LEU  |
| 1   | F     | 193 | LEU  |
| 1   | F     | 208 | GLU  |
| 1   | F     | 209 | LYS  |
| 1   | F     | 215 | LYS  |
| 1   | F     | 217 | LYS  |
| 1   | F     | 224 | GLU  |
| 1   | F     | 225 | ASP  |
| 1   | F     | 242 | LEU  |
| 1   | F     | 243 | ARG  |
| 1   | F     | 249 | LYS  |
| 1   | F     | 250 | LYS  |
| 1   | F     | 253 | LYS  |
| 1   | F     | 254 | LYS  |
| 1   | F     | 261 | ARG  |
| 1   | F     | 270 | LYS  |
| 1   | F     | 272 | LEU  |
| 1   | F     | 274 | GLU  |
| 1   | F     | 275 | LYS  |
| 1   | F     | 277 | ARG  |
| 1   | F     | 280 | VAL  |
| 1   | F     | 282 | ILE  |
| 1   | F     | 284 | GLU  |
| 1   | F     | 296 | THR  |
| 1   | F     | 305 | LEU  |
| 1   | F     | 315 | VAL  |
| 1   | F     | 326 | LEU  |
| 1   | F     | 342 | ARG  |
| 1   | F     | 347 | SER  |
| 1   | F     | 362 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 363 | LYS  |
| 1   | F     | 367 | ARG  |
| 1   | F     | 382 | LEU  |
| 1   | F     | 385 | LEU  |
| 1   | F     | 398 | LYS  |
| 1   | F     | 402 | GLU  |
| 1   | F     | 410 | GLU  |
| 1   | F     | 414 | LEU  |
| 1   | G     | 18  | LYS  |
| 1   | G     | 27  | VAL  |
| 1   | G     | 28  | ARG  |
| 1   | G     | 33  | ILE  |
| 1   | G     | 40  | GLU  |
| 1   | G     | 41  | LYS  |
| 1   | G     | 58  | LYS  |
| 1   | G     | 70  | VAL  |
| 1   | G     | 80  | ARG  |
| 1   | G     | 95  | LEU  |
| 1   | G     | 96  | LYS  |
| 1   | G     | 99  | LEU  |
| 1   | G     | 120 | VAL  |
| 1   | G     | 128 | ARG  |
| 1   | G     | 157 | LYS  |
| 1   | G     | 161 | LEU  |
| 1   | G     | 163 | ASN  |
| 1   | G     | 164 | VAL  |
| 1   | G     | 166 | ILE  |
| 1   | G     | 174 | GLU  |
| 1   | G     | 177 | SER  |
| 1   | G     | 179 | ARG  |
| 1   | G     | 185 | LEU  |
| 1   | G     | 190 | LEU  |
| 1   | G     | 193 | LEU  |
| 1   | G     | 198 | LYS  |
| 1   | G     | 208 | GLU  |
| 1   | G     | 213 | ASN  |
| 1   | G     | 214 | LEU  |
| 1   | G     | 216 | LEU  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 238 | VAL  |
| 1   | G     | 246 | LEU  |
| 1   | G     | 247 | MSE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 260 | LEU  |
| 1   | G     | 261 | ARG  |
| 1   | G     | 263 | ARG  |
| 1   | G     | 265 | VAL  |
| 1   | G     | 274 | GLU  |
| 1   | G     | 278 | THR  |
| 1   | G     | 281 | GLU  |
| 1   | G     | 282 | ILE  |
| 1   | G     | 292 | SER  |
| 1   | G     | 293 | MSE  |
| 1   | G     | 296 | THR  |
| 1   | G     | 305 | LEU  |
| 1   | G     | 326 | LEU  |
| 1   | G     | 342 | ARG  |
| 1   | G     | 345 | THR  |
| 1   | G     | 346 | LEU  |
| 1   | G     | 362 | VAL  |
| 1   | G     | 363 | LYS  |
| 1   | G     | 367 | ARG  |
| 1   | G     | 375 | LYS  |
| 1   | G     | 382 | LEU  |
| 1   | G     | 398 | LYS  |
| 1   | G     | 410 | GLU  |
| 1   | G     | 412 | VAL  |
| 1   | G     | 414 | LEU  |
| 1   | H     | 2   | ARG  |
| 1   | H     | 11  | SER  |
| 1   | H     | 25  | GLU  |
| 1   | H     | 28  | ARG  |
| 1   | H     | 39  | GLU  |
| 1   | H     | 44  | ILE  |
| 1   | H     | 50  | LYS  |
| 1   | H     | 58  | LYS  |
| 1   | H     | 85  | LYS  |
| 1   | H     | 95  | LEU  |
| 1   | H     | 99  | LEU  |
| 1   | H     | 154 | GLU  |
| 1   | H     | 156 | GLU  |
| 1   | H     | 161 | LEU  |
| 1   | H     | 164 | VAL  |
| 1   | H     | 167 | ASN  |
| 1   | H     | 170 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 175 | MSE  |
| 1   | H     | 179 | ARG  |
| 1   | H     | 181 | GLU  |
| 1   | H     | 185 | LEU  |
| 1   | H     | 190 | LEU  |
| 1   | H     | 198 | LYS  |
| 1   | H     | 208 | GLU  |
| 1   | H     | 209 | LYS  |
| 1   | H     | 213 | ASN  |
| 1   | H     | 214 | LEU  |
| 1   | H     | 224 | GLU  |
| 1   | H     | 238 | VAL  |
| 1   | H     | 242 | LEU  |
| 1   | H     | 246 | LEU  |
| 1   | H     | 250 | LYS  |
| 1   | H     | 253 | LYS  |
| 1   | H     | 254 | LYS  |
| 1   | H     | 255 | ILE  |
| 1   | H     | 259 | GLU  |
| 1   | H     | 261 | ARG  |
| 1   | H     | 263 | ARG  |
| 1   | H     | 266 | MSE  |
| 1   | H     | 269 | GLU  |
| 1   | H     | 275 | LYS  |
| 1   | H     | 278 | THR  |
| 1   | H     | 280 | VAL  |
| 1   | H     | 281 | GLU  |
| 1   | H     | 282 | ILE  |
| 1   | H     | 284 | GLU  |
| 1   | H     | 296 | THR  |
| 1   | H     | 303 | ARG  |
| 1   | H     | 305 | LEU  |
| 1   | H     | 311 | LYS  |
| 1   | H     | 315 | VAL  |
| 1   | H     | 326 | LEU  |
| 1   | H     | 346 | LEU  |
| 1   | H     | 362 | VAL  |
| 1   | H     | 363 | LYS  |
| 1   | H     | 365 | TYR  |
| 1   | H     | 367 | ARG  |
| 1   | H     | 376 | ARG  |
| 1   | H     | 382 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 385 | LEU  |
| 1   | H     | 398 | LYS  |
| 1   | H     | 399 | ASP  |
| 1   | H     | 414 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 132 | ASN  |
| 1   | A     | 191 | ASN  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 191 | ASN  |
| 1   | B     | 213 | ASN  |
| 1   | B     | 320 | ASN  |
| 1   | C     | 0   | HIS  |
| 1   | C     | 191 | ASN  |
| 1   | C     | 300 | HIS  |
| 1   | C     | 320 | ASN  |
| 1   | D     | 78  | GLN  |
| 1   | D     | 89  | ASN  |
| 1   | D     | 144 | HIS  |
| 1   | D     | 167 | ASN  |
| 1   | D     | 191 | ASN  |
| 1   | D     | 213 | ASN  |
| 1   | D     | 320 | ASN  |
| 1   | E     | 191 | ASN  |
| 1   | E     | 320 | ASN  |
| 1   | F     | 42  | GLN  |
| 1   | F     | 144 | HIS  |
| 1   | F     | 213 | ASN  |
| 1   | F     | 320 | ASN  |
| 1   | F     | 353 | HIS  |
| 1   | G     | 163 | ASN  |
| 1   | G     | 320 | ASN  |
| 1   | H     | 140 | ASN  |
| 1   | H     | 167 | ASN  |
| 1   | H     | 191 | ASN  |
| 1   | H     | 213 | ASN  |
| 1   | H     | 300 | HIS  |
| 1   | H     | 320 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | SO4  | G     | 1418 | -    | 4,4,4        | 0.37 | 0           | 6,6,6       | 0.30 | 0           |
| 4   | G6P  | C     | 1418 | 3    | 16,16,16     | 0.53 | 0           | 23,24,24    | 1.03 | 2 (8%)      |
| 2   | NAD  | G     | 1416 | 3    | 46,48,48     | 1.77 | 6 (13%)     | 64,73,73    | 1.62 | 8 (12%)     |
| 2   | NAD  | A     | 1416 | 3    | 46,48,48     | 1.81 | 5 (10%)     | 64,73,73    | 1.60 | 11 (17%)    |
| 5   | SO4  | E     | 1416 | -    | 4,4,4        | 0.40 | 0           | 6,6,6       | 0.45 | 0           |
| 2   | NAD  | C     | 1416 | 3    | 46,48,48     | 1.76 | 5 (10%)     | 64,73,73    | 1.52 | 10 (15%)    |
| 4   | G6P  | A     | 1418 | 3    | 16,16,16     | 0.97 | 1 (6%)      | 23,24,24    | 1.21 | 3 (13%)     |
| 5   | SO4  | B     | 1416 | -    | 4,4,4        | 0.76 | 0           | 6,6,6       | 0.45 | 0           |
| 5   | SO4  | D     | 1416 | -    | 4,4,4        | 0.84 | 0           | 6,6,6       | 0.37 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 4   | G6P  | C     | 1418 | 3    | 1/1/6/6 | 2/6/26/26   | 0/1/1/1 |
| 2   | NAD  | G     | 1416 | 3    | -       | 10/30/62/62 | 0/5/5/5 |
| 2   | NAD  | A     | 1416 | 3    | -       | 8/30/62/62  | 0/5/5/5 |
| 2   | NAD  | C     | 1416 | 3    | -       | 11/30/62/62 | 0/5/5/5 |
| 4   | G6P  | A     | 1418 | 3    | 1/1/6/6 | 3/6/26/26   | 0/1/1/1 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1416 | NAD  | O7N-C7N | 9.84  | 1.42        | 1.24     |
| 2   | C     | 1416 | NAD  | O7N-C7N | 9.46  | 1.41        | 1.24     |
| 2   | G     | 1416 | NAD  | O7N-C7N | 9.42  | 1.41        | 1.24     |
| 2   | C     | 1416 | NAD  | C2A-N1A | 2.69  | 1.38        | 1.33     |
| 2   | A     | 1416 | NAD  | C2A-N1A | 2.65  | 1.38        | 1.33     |
| 2   | C     | 1416 | NAD  | C8A-N7A | 2.59  | 1.36        | 1.31     |
| 2   | C     | 1416 | NAD  | C2A-N3A | 2.59  | 1.38        | 1.33     |
| 2   | G     | 1416 | NAD  | C2A-N3A | 2.58  | 1.38        | 1.33     |
| 2   | A     | 1416 | NAD  | C2A-N3A | 2.54  | 1.38        | 1.33     |
| 2   | A     | 1416 | NAD  | C8A-N7A | 2.52  | 1.36        | 1.31     |
| 2   | G     | 1416 | NAD  | C2A-N1A | 2.52  | 1.38        | 1.33     |
| 2   | G     | 1416 | NAD  | PN-O3   | 2.48  | 1.62        | 1.59     |
| 2   | A     | 1416 | NAD  | PA-O3   | 2.46  | 1.62        | 1.59     |
| 2   | G     | 1416 | NAD  | PA-O3   | 2.46  | 1.62        | 1.59     |
| 2   | C     | 1416 | NAD  | C5A-N7A | -2.38 | 1.34        | 1.39     |
| 2   | G     | 1416 | NAD  | C8A-N7A | 2.22  | 1.35        | 1.31     |
| 4   | A     | 1418 | G6P  | P-O2P   | -2.22 | 1.46        | 1.54     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | G     | 1416 | NAD  | N3A-C2A-N1A | -5.94 | 119.59      | 128.58   |
| 2   | A     | 1416 | NAD  | N3A-C2A-N1A | -4.81 | 121.30      | 128.58   |
| 2   | C     | 1416 | NAD  | N3A-C2A-N1A | -4.71 | 121.45      | 128.58   |
| 2   | G     | 1416 | NAD  | C5A-C4A-N3A | -4.54 | 120.47      | 126.72   |
| 2   | C     | 1416 | NAD  | C5A-C4A-N3A | -4.41 | 120.64      | 126.72   |
| 2   | G     | 1416 | NAD  | N9A-C8A-N7A | -4.37 | 107.74      | 113.94   |
| 2   | A     | 1416 | NAD  | C5A-C4A-N3A | -4.19 | 120.95      | 126.72   |
| 2   | A     | 1416 | NAD  | N9A-C8A-N7A | -4.03 | 108.22      | 113.94   |
| 2   | G     | 1416 | NAD  | C5A-N7A-C8A | 3.97  | 109.69      | 103.45   |
| 2   | G     | 1416 | NAD  | C2A-N3A-C4A | 3.61  | 120.65      | 111.83   |
| 2   | A     | 1416 | NAD  | C5A-N7A-C8A | 3.50  | 108.95      | 103.45   |
| 2   | A     | 1416 | NAD  | O7N-C7N-C3N | -3.11 | 115.79      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1416 | NAD  | N9A-C8A-N7A | -3.08 | 109.57      | 113.94   |
| 2   | C     | 1416 | NAD  | O7N-C7N-C3N | -3.01 | 115.91      | 119.60   |
| 2   | G     | 1416 | NAD  | N3A-C4A-N9A | 3.00  | 132.27      | 127.17   |
| 2   | A     | 1416 | NAD  | C2A-N3A-C4A | 2.99  | 119.12      | 111.83   |
| 2   | C     | 1416 | NAD  | C5A-N7A-C8A | 2.93  | 108.06      | 103.45   |
| 2   | C     | 1416 | NAD  | C2A-N3A-C4A | 2.92  | 118.96      | 111.83   |
| 2   | C     | 1416 | NAD  | N3A-C4A-N9A | 2.89  | 132.08      | 127.17   |
| 2   | A     | 1416 | NAD  | N3A-C4A-N9A | 2.88  | 132.06      | 127.17   |
| 4   | A     | 1418 | G6P  | O2P-P-O6    | 2.83  | 114.05      | 106.67   |
| 2   | G     | 1416 | NAD  | C4A-C5A-N7A | -2.82 | 107.36      | 110.58   |
| 2   | A     | 1416 | NAD  | O3-PA-O1A   | -2.55 | 103.05      | 110.70   |
| 2   | A     | 1416 | NAD  | C4A-C5A-N7A | -2.42 | 107.82      | 110.58   |
| 2   | C     | 1416 | NAD  | C2N-C3N-C4N | 2.41  | 121.06      | 118.26   |
| 2   | A     | 1416 | NAD  | C4D-O4D-C1D | -2.32 | 107.80      | 109.92   |
| 4   | A     | 1418 | G6P  | O1P-P-O3P   | -2.32 | 101.81      | 110.83   |
| 4   | C     | 1418 | G6P  | C4-C3-C2    | -2.26 | 106.86      | 110.83   |
| 2   | C     | 1416 | NAD  | O5B-C5B-C4B | 2.26  | 116.70      | 108.99   |
| 2   | C     | 1416 | NAD  | O7N-C7N-N7N | 2.25  | 125.87      | 122.62   |
| 4   | A     | 1418 | G6P  | O6-P-O3P    | 2.23  | 112.47      | 106.44   |
| 2   | A     | 1416 | NAD  | C4A-N9A-C8A | 2.17  | 108.02      | 105.74   |
| 2   | G     | 1416 | NAD  | C4A-N9A-C8A | 2.11  | 107.95      | 105.74   |
| 4   | C     | 1418 | G6P  | O5-C5-C6    | 2.00  | 110.67      | 106.69   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 4   | A     | 1418 | G6P  | C1   |
| 4   | C     | 1418 | G6P  | C1   |

All (34) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1416 | NAD  | PN-O3-PA-O5B    |
| 2   | A     | 1416 | NAD  | PA-O3-PN-O5D    |
| 2   | A     | 1416 | NAD  | C5D-O5D-PN-O3   |
| 2   | A     | 1416 | NAD  | O4D-C1D-N1N-C6N |
| 2   | C     | 1416 | NAD  | C5B-O5B-PA-O2A  |
| 2   | C     | 1416 | NAD  | C5B-O5B-PA-O3   |
| 2   | C     | 1416 | NAD  | C5D-O5D-PN-O1N  |
| 2   | C     | 1416 | NAD  | O4D-C1D-N1N-C6N |
| 2   | G     | 1416 | NAD  | C5B-O5B-PA-O1A  |
| 2   | G     | 1416 | NAD  | C5B-O5B-PA-O2A  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | G     | 1416 | NAD  | C5B-O5B-PA-O3   |
| 2   | G     | 1416 | NAD  | C5D-O5D-PN-O3   |
| 4   | C     | 1418 | G6P  | C4-C5-C6-O6     |
| 4   | C     | 1418 | G6P  | O5-C5-C6-O6     |
| 2   | A     | 1416 | NAD  | O4D-C4D-C5D-O5D |
| 2   | C     | 1416 | NAD  | O4D-C4D-C5D-O5D |
| 2   | G     | 1416 | NAD  | O4D-C4D-C5D-O5D |
| 2   | C     | 1416 | NAD  | C3D-C4D-C5D-O5D |
| 2   | A     | 1416 | NAD  | C3D-C4D-C5D-O5D |
| 2   | G     | 1416 | NAD  | C3D-C4D-C5D-O5D |
| 4   | A     | 1418 | G6P  | C4-C5-C6-O6     |
| 4   | A     | 1418 | G6P  | O5-C5-C6-O6     |
| 2   | C     | 1416 | NAD  | PN-O3-PA-O5B    |
| 2   | G     | 1416 | NAD  | PN-O3-PA-O5B    |
| 2   | A     | 1416 | NAD  | C5D-O5D-PN-O1N  |
| 2   | C     | 1416 | NAD  | C5B-O5B-PA-O1A  |
| 2   | C     | 1416 | NAD  | C5D-O5D-PN-O3   |
| 2   | G     | 1416 | NAD  | C5D-O5D-PN-O1N  |
| 2   | G     | 1416 | NAD  | C4B-C5B-O5B-PA  |
| 2   | C     | 1416 | NAD  | C4B-C5B-O5B-PA  |
| 2   | A     | 1416 | NAD  | O4D-C1D-N1N-C2N |
| 2   | C     | 1416 | NAD  | O4D-C1D-N1N-C2N |
| 2   | G     | 1416 | NAD  | PA-O3-PN-O2N    |
| 4   | A     | 1418 | G6P  | C6-O6-P-O1P     |

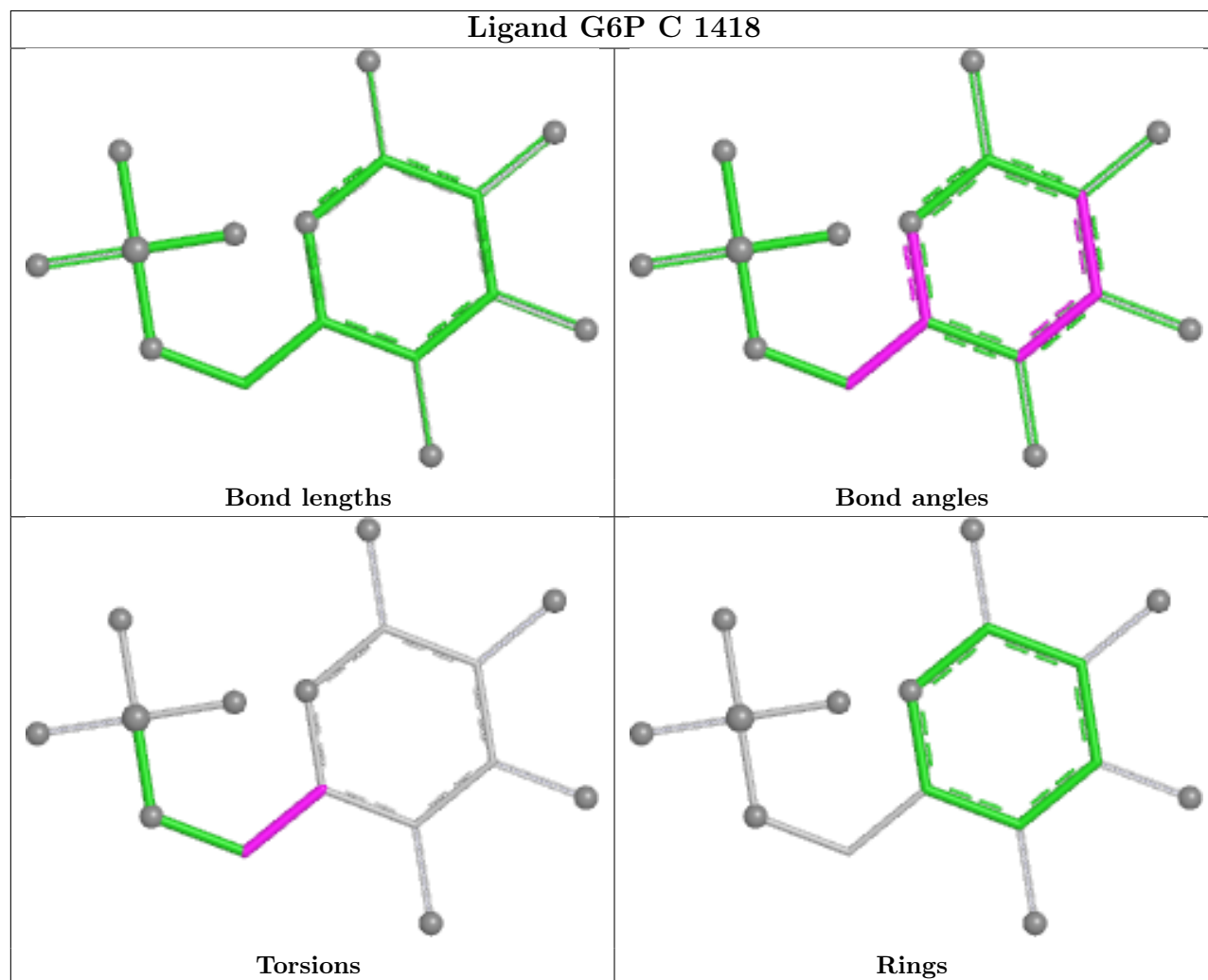
There are no ring outliers.

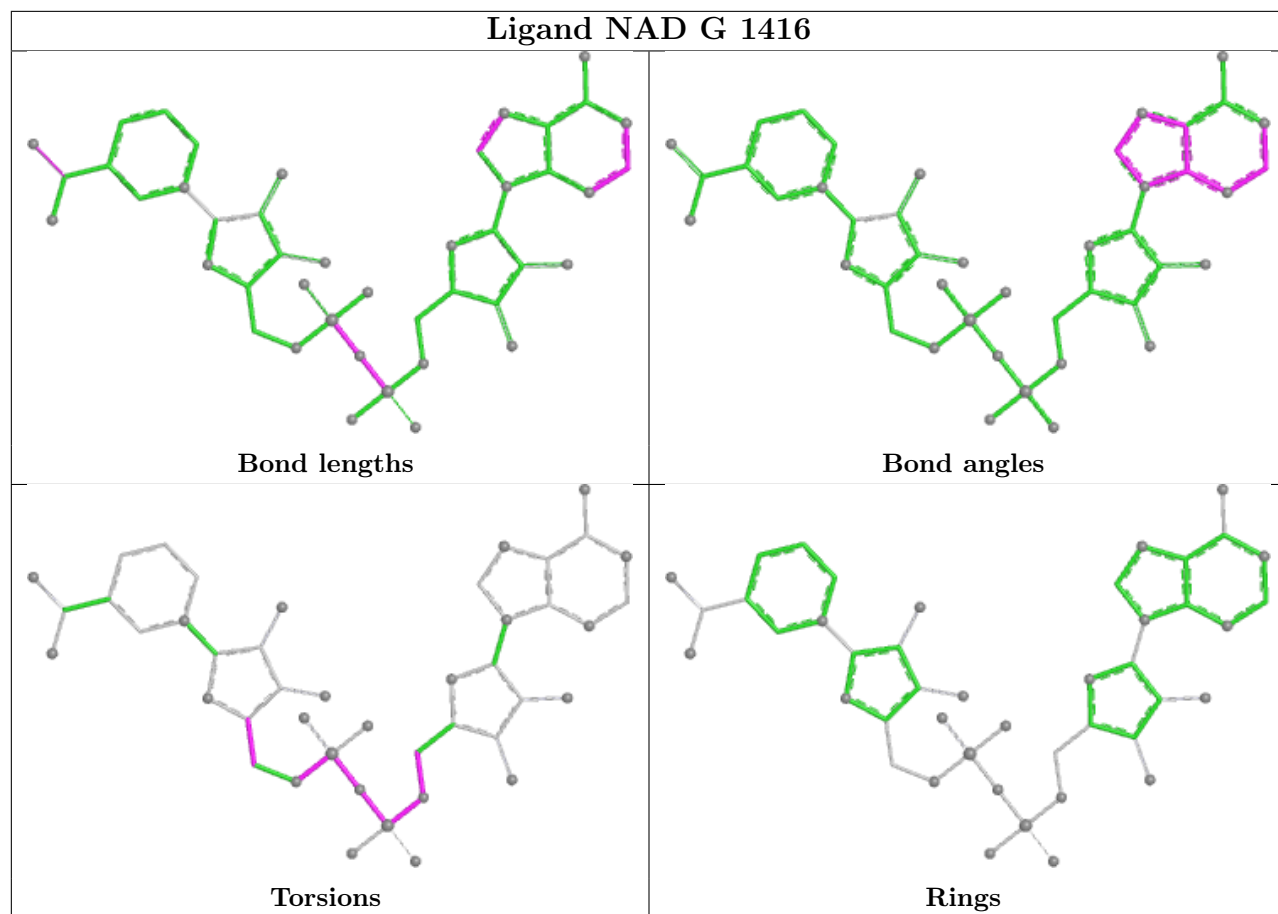
5 monomers are involved in 12 short contacts:

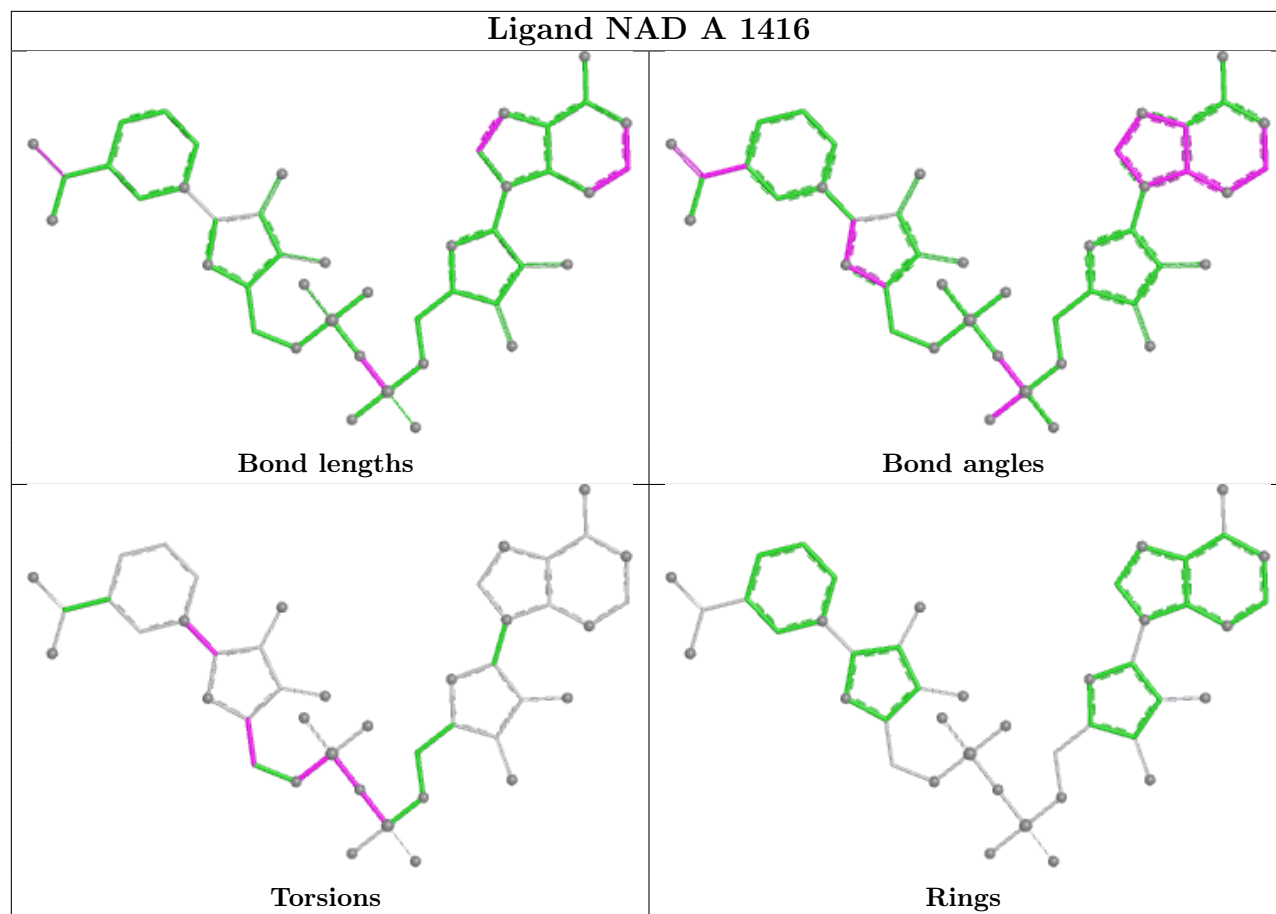
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | C     | 1418 | G6P  | 1       | 0            |
| 2   | G     | 1416 | NAD  | 3       | 0            |
| 2   | A     | 1416 | NAD  | 5       | 0            |
| 2   | C     | 1416 | NAD  | 2       | 0            |
| 4   | A     | 1418 | G6P  | 1       | 0            |

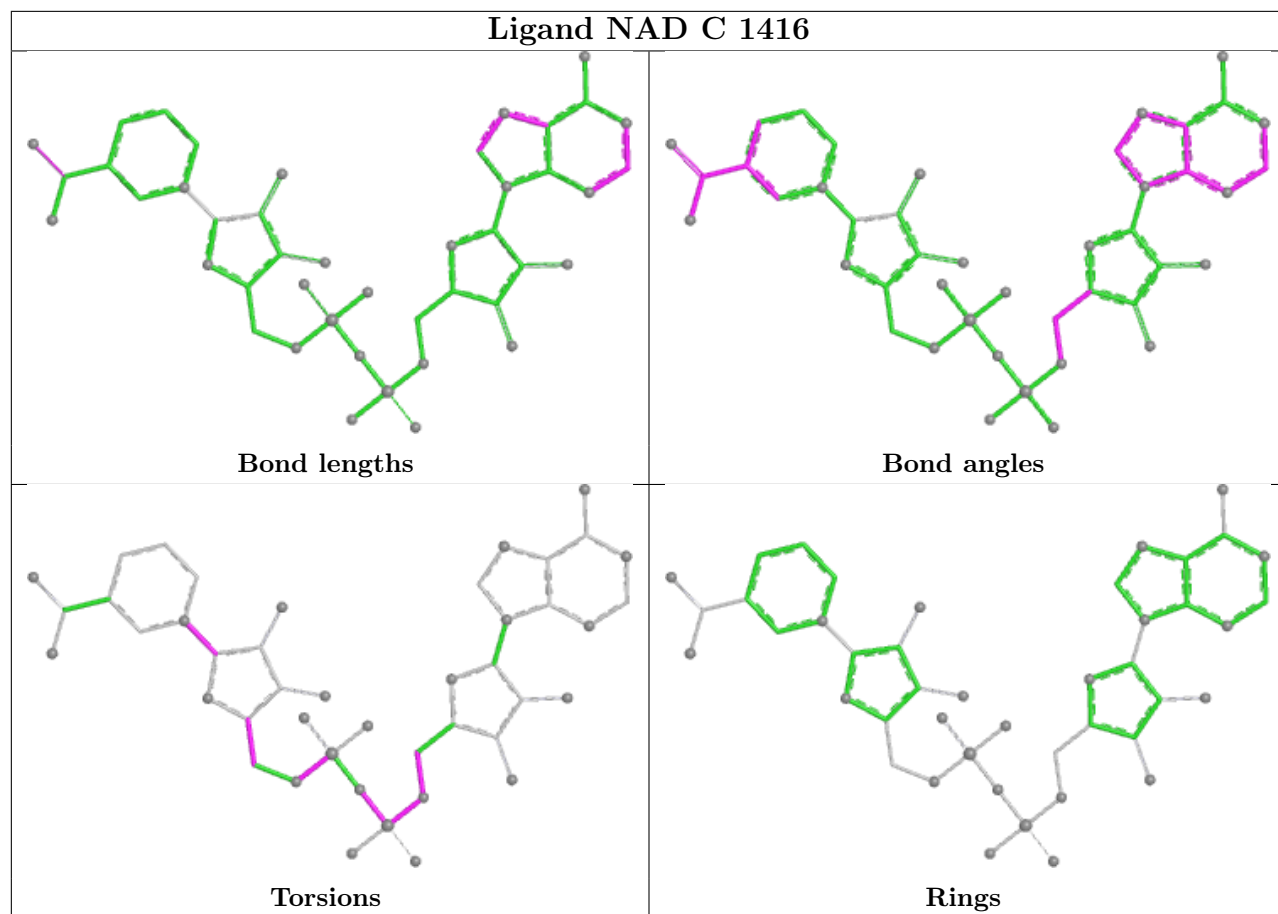
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

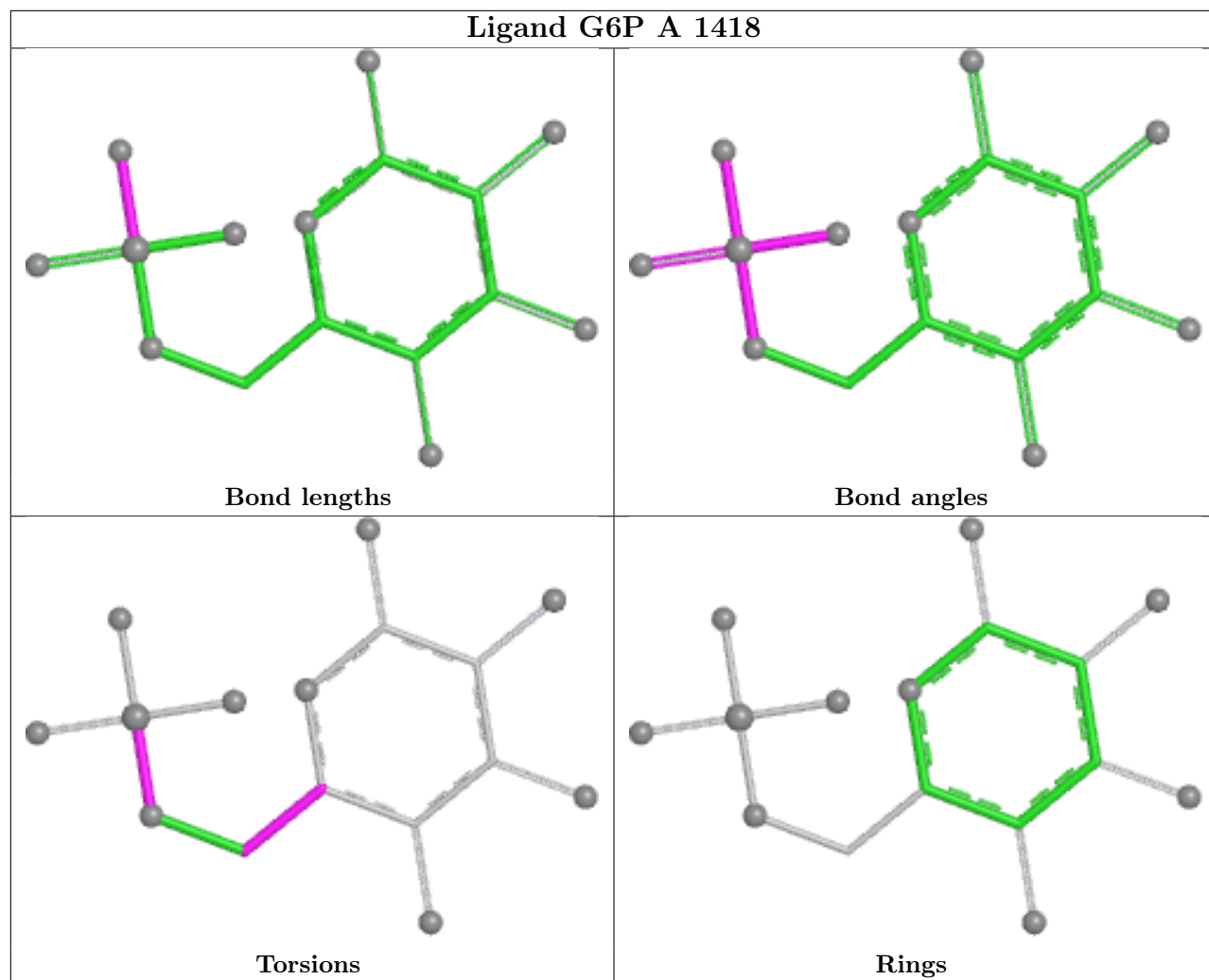
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9  |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|----------|
| 1   | A     | 406/416 (97%)   | 0.83   | 39 (9%)   | 13 13 | 13, 19, 32, 51        | 4 (0%)   |
| 1   | B     | 403/416 (96%)   | 0.80   | 44 (10%)  | 10 10 | 10, 19, 30, 54        | 18 (4%)  |
| 1   | C     | 400/416 (96%)   | 0.72   | 37 (9%)   | 14 13 | 10, 19, 29, 52        | 11 (2%)  |
| 1   | D     | 397/416 (95%)   | 0.76   | 40 (10%)  | 12 11 | 11, 19, 29, 45        | 11 (2%)  |
| 1   | E     | 384/416 (92%)   | 0.99   | 44 (11%)  | 9 8   | 4, 19, 28, 47         | 42 (10%) |
| 1   | F     | 393/416 (94%)   | 0.76   | 39 (9%)   | 13 12 | 7, 19, 29, 49         | 36 (9%)  |
| 1   | G     | 397/416 (95%)   | 0.60   | 30 (7%)   | 20 19 | 9, 19, 37, 46         | 26 (6%)  |
| 1   | H     | 389/416 (93%)   | 0.95   | 45 (11%)  | 9 8   | 7, 19, 28, 49         | 47 (12%) |
| All | All   | 3169/3328 (95%) | 0.80   | 318 (10%) | 12 12 | 4, 19, 32, 54         | 195 (6%) |

All (318) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 286 | LEU  | 6.9  |
| 1   | C     | 287 | THR  | 5.8  |
| 1   | A     | 290 | GLY  | 5.7  |
| 1   | E     | 214 | LEU  | 5.5  |
| 1   | A     | 294 | TYR  | 5.4  |
| 1   | A     | 287 | THR  | 5.4  |
| 1   | A     | 289 | ARG  | 5.1  |
| 1   | H     | 128 | ARG  | 4.9  |
| 1   | A     | 218 | LEU  | 4.8  |
| 1   | B     | 273 | PHE  | 4.8  |
| 1   | A     | 285 | GLU  | 4.6  |
| 1   | G     | 218 | LEU  | 4.6  |
| 1   | B     | 276 | TYR  | 4.5  |
| 1   | D     | 63  | ASP  | 4.4  |
| 1   | A     | 216 | LEU  | 4.4  |
| 1   | A     | 222 | PRO  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 288 | LYS  | 4.3  |
| 1   | H     | 29  | ILE  | 4.3  |
| 1   | A     | 286 | LEU  | 4.2  |
| 1   | G     | 257 | THR  | 4.2  |
| 1   | B     | 280 | VAL  | 4.1  |
| 1   | D     | 292 | SER  | 4.1  |
| 1   | E     | 215 | LYS  | 4.1  |
| 1   | H     | 58  | LYS  | 4.1  |
| 1   | E     | 42  | GLN  | 4.1  |
| 1   | B     | 177 | SER  | 4.0  |
| 1   | F     | 71  | ASP  | 4.0  |
| 1   | C     | 223 | ASP  | 4.0  |
| 1   | D     | 55  | ASP  | 3.9  |
| 1   | B     | 282 | ILE  | 3.9  |
| 1   | E     | 273 | PHE  | 3.8  |
| 1   | E     | 213 | ASN  | 3.8  |
| 1   | H     | 31  | GLU  | 3.8  |
| 1   | D     | 280 | VAL  | 3.8  |
| 1   | A     | 213 | ASN  | 3.8  |
| 1   | B     | 222 | PRO  | 3.8  |
| 1   | C     | 291 | GLY  | 3.8  |
| 1   | D     | 281 | GLU  | 3.8  |
| 1   | B     | 272 | LEU  | 3.7  |
| 1   | B     | 278 | THR  | 3.7  |
| 1   | B     | 285 | GLU  | 3.7  |
| 1   | D     | 279 | ALA  | 3.7  |
| 1   | F     | 85  | LYS  | 3.7  |
| 1   | F     | 280 | VAL  | 3.6  |
| 1   | A     | 39  | GLU  | 3.6  |
| 1   | D     | 71  | ASP  | 3.6  |
| 1   | C     | 216 | LEU  | 3.6  |
| 1   | E     | 166 | ILE  | 3.6  |
| 1   | F     | 276 | TYR  | 3.6  |
| 1   | F     | 265 | VAL  | 3.6  |
| 1   | H     | 173 | ALA  | 3.6  |
| 1   | B     | 286 | LEU  | 3.6  |
| 1   | B     | 268 | ILE  | 3.6  |
| 1   | H     | 38  | ASP  | 3.6  |
| 1   | A     | 0   | HIS  | 3.5  |
| 1   | A     | 225 | ASP  | 3.5  |
| 1   | A     | 217 | LYS  | 3.5  |
| 1   | B     | 294 | TYR  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 259 | GLU  | 3.4  |
| 1   | B     | 295 | SER  | 3.4  |
| 1   | E     | 63  | ASP  | 3.4  |
| 1   | H     | 177 | SER  | 3.4  |
| 1   | B     | 174 | GLU  | 3.4  |
| 1   | H     | 56  | ARG  | 3.4  |
| 1   | E     | 25  | GLU  | 3.4  |
| 1   | F     | 45  | VAL  | 3.3  |
| 1   | D     | 271 | GLU  | 3.3  |
| 1   | D     | 179 | ARG  | 3.3  |
| 1   | G     | 285 | GLU  | 3.3  |
| 1   | B     | 274 | GLU  | 3.2  |
| 1   | B     | 24  | SER  | 3.2  |
| 1   | C     | 170 | ARG  | 3.2  |
| 1   | G     | 415 | GLY  | 3.2  |
| 1   | E     | 299 | ALA  | 3.2  |
| 1   | E     | 295 | SER  | 3.2  |
| 1   | E     | 283 | PRO  | 3.2  |
| 1   | B     | 52  | LEU  | 3.2  |
| 1   | H     | 201 | VAL  | 3.1  |
| 1   | E     | 285 | GLU  | 3.1  |
| 1   | F     | 272 | LEU  | 3.1  |
| 1   | A     | 325 | ASN  | 3.1  |
| 1   | E     | 37  | ILE  | 3.1  |
| 1   | C     | 284 | GLU  | 3.1  |
| 1   | A     | 291 | GLY  | 3.1  |
| 1   | E     | 45  | VAL  | 3.1  |
| 1   | B     | 213 | ASN  | 3.1  |
| 1   | G     | 263 | ARG  | 3.1  |
| 1   | B     | 166 | ILE  | 3.1  |
| 1   | E     | 126 | THR  | 3.0  |
| 1   | B     | 53  | VAL  | 3.0  |
| 1   | C     | 213 | ASN  | 3.0  |
| 1   | E     | 261 | ARG  | 3.0  |
| 1   | E     | 177 | SER  | 3.0  |
| 1   | G     | 217 | LYS  | 3.0  |
| 1   | C     | 285 | GLU  | 3.0  |
| 1   | G     | 228 | THR  | 3.0  |
| 1   | F     | 47  | ASP  | 3.0  |
| 1   | D     | 295 | SER  | 3.0  |
| 1   | C     | 271 | GLU  | 2.9  |
| 1   | C     | 280 | VAL  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 53  | VAL  | 2.9  |
| 1   | H     | 53  | VAL  | 2.9  |
| 1   | A     | 223 | ASP  | 2.9  |
| 1   | H     | 55  | ASP  | 2.9  |
| 1   | F     | 282 | ILE  | 2.9  |
| 1   | A     | 55  | ASP  | 2.9  |
| 1   | C     | 224 | GLU  | 2.9  |
| 1   | H     | 281 | GLU  | 2.9  |
| 1   | F     | 409 | ARG  | 2.9  |
| 1   | D     | 214 | LEU  | 2.9  |
| 1   | E     | 274 | GLU  | 2.9  |
| 1   | E     | 210 | VAL  | 2.9  |
| 1   | D     | 216 | LEU  | 2.9  |
| 1   | C     | 273 | PHE  | 2.9  |
| 1   | D     | 294 | TYR  | 2.9  |
| 1   | D     | 212 | GLU  | 2.9  |
| 1   | D     | 284 | GLU  | 2.9  |
| 1   | C     | 56  | ARG  | 2.8  |
| 1   | H     | 216 | LEU  | 2.8  |
| 1   | A     | 181 | GLU  | 2.8  |
| 1   | A     | 212 | GLU  | 2.8  |
| 1   | B     | 269 | GLU  | 2.8  |
| 1   | A     | 5   | VAL  | 2.8  |
| 1   | G     | 214 | LEU  | 2.8  |
| 1   | A     | 284 | GLU  | 2.8  |
| 1   | C     | 263 | ARG  | 2.8  |
| 1   | B     | 168 | PHE  | 2.8  |
| 1   | E     | 65  | PHE  | 2.8  |
| 1   | B     | 221 | ILE  | 2.8  |
| 1   | F     | 44  | ILE  | 2.8  |
| 1   | C     | 292 | SER  | 2.8  |
| 1   | B     | 279 | ALA  | 2.8  |
| 1   | B     | 216 | LEU  | 2.7  |
| 1   | D     | 31  | GLU  | 2.7  |
| 1   | F     | 281 | GLU  | 2.7  |
| 1   | C     | 12  | TYR  | 2.7  |
| 1   | B     | 217 | LYS  | 2.7  |
| 1   | F     | 278 | THR  | 2.7  |
| 1   | B     | 223 | ASP  | 2.7  |
| 1   | H     | 47  | ASP  | 2.7  |
| 1   | F     | 269 | GLU  | 2.7  |
| 1   | B     | 71  | ASP  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 294 | TYR  | 2.7  |
| 1   | H     | 274 | GLU  | 2.7  |
| 1   | D     | 291 | GLY  | 2.6  |
| 1   | E     | 61  | ILE  | 2.6  |
| 1   | H     | 350 | LYS  | 2.6  |
| 1   | B     | 51  | ARG  | 2.6  |
| 1   | D     | 27  | VAL  | 2.6  |
| 1   | A     | 224 | GLU  | 2.6  |
| 1   | A     | 264 | GLU  | 2.6  |
| 1   | E     | 64  | THR  | 2.6  |
| 1   | F     | 64  | THR  | 2.6  |
| 1   | C     | 283 | PRO  | 2.6  |
| 1   | F     | 48  | PHE  | 2.6  |
| 1   | G     | 3   | ILE  | 2.6  |
| 1   | G     | 6   | ILE  | 2.6  |
| 1   | G     | 216 | LEU  | 2.6  |
| 1   | H     | 52  | LEU  | 2.6  |
| 1   | H     | 213 | ASN  | 2.6  |
| 1   | H     | 49  | VAL  | 2.6  |
| 1   | B     | 292 | SER  | 2.6  |
| 1   | F     | 279 | ALA  | 2.6  |
| 1   | H     | 4   | ALA  | 2.6  |
| 1   | E     | 202 | LYS  | 2.6  |
| 1   | F     | 63  | ASP  | 2.6  |
| 1   | A     | 282 | ILE  | 2.6  |
| 1   | E     | 23  | ILE  | 2.6  |
| 1   | G     | 273 | PHE  | 2.6  |
| 1   | C     | 212 | GLU  | 2.6  |
| 1   | E     | 180 | LEU  | 2.6  |
| 1   | A     | 292 | SER  | 2.6  |
| 1   | B     | 287 | THR  | 2.6  |
| 1   | B     | 54  | LYS  | 2.6  |
| 1   | G     | 170 | ARG  | 2.6  |
| 1   | D     | 296 | THR  | 2.6  |
| 1   | A     | 281 | GLU  | 2.5  |
| 1   | C     | 274 | GLU  | 2.5  |
| 1   | F     | 273 | PHE  | 2.5  |
| 1   | E     | 183 | VAL  | 2.5  |
| 1   | B     | 11  | SER  | 2.5  |
| 1   | E     | 296 | THR  | 2.5  |
| 1   | A     | 12  | TYR  | 2.5  |
| 1   | H     | 74  | TYR  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 26  | ASP  | 2.5  |
| 1   | H     | 30  | ASP  | 2.5  |
| 1   | G     | 174 | GLU  | 2.5  |
| 1   | H     | 129 | LYS  | 2.5  |
| 1   | H     | 375 | LYS  | 2.5  |
| 1   | H     | 39  | GLU  | 2.5  |
| 1   | A     | 273 | PHE  | 2.5  |
| 1   | C     | 214 | LEU  | 2.5  |
| 1   | F     | 49  | VAL  | 2.5  |
| 1   | D     | 173 | ALA  | 2.5  |
| 1   | H     | 412 | VAL  | 2.5  |
| 1   | D     | 56  | ARG  | 2.5  |
| 1   | C     | 25  | GLU  | 2.4  |
| 1   | B     | 55  | ASP  | 2.4  |
| 1   | G     | 276 | TYR  | 2.4  |
| 1   | G     | 280 | VAL  | 2.4  |
| 1   | H     | 11  | SER  | 2.4  |
| 1   | D     | 222 | PRO  | 2.4  |
| 1   | C     | 3   | ILE  | 2.4  |
| 1   | B     | 48  | PHE  | 2.4  |
| 1   | C     | 278 | THR  | 2.4  |
| 1   | A     | 26  | ASP  | 2.4  |
| 1   | F     | 277 | ARG  | 2.4  |
| 1   | G     | 5   | VAL  | 2.4  |
| 1   | H     | 46  | VAL  | 2.4  |
| 1   | H     | 69  | VAL  | 2.4  |
| 1   | G     | 4   | ALA  | 2.4  |
| 1   | B     | 284 | GLU  | 2.4  |
| 1   | H     | 42  | GLN  | 2.4  |
| 1   | C     | 276 | TYR  | 2.4  |
| 1   | D     | 58  | LYS  | 2.4  |
| 1   | G     | 275 | LYS  | 2.4  |
| 1   | H     | 279 | ALA  | 2.4  |
| 1   | G     | 406 | GLU  | 2.4  |
| 1   | C     | 415 | GLY  | 2.3  |
| 1   | E     | 169 | ILE  | 2.3  |
| 1   | F     | 28  | ARG  | 2.3  |
| 1   | H     | 6   | ILE  | 2.3  |
| 1   | H     | 26  | ASP  | 2.3  |
| 1   | D     | 273 | PHE  | 2.3  |
| 1   | E     | 57  | PHE  | 2.3  |
| 1   | F     | 34  | PHE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 66  | GLU  | 2.3  |
| 1   | G     | 177 | SER  | 2.3  |
| 1   | B     | 321 | GLY  | 2.3  |
| 1   | F     | 61  | ILE  | 2.3  |
| 1   | E     | 70  | VAL  | 2.3  |
| 1   | A     | 24  | SER  | 2.3  |
| 1   | C     | 40  | GLU  | 2.3  |
| 1   | F     | 5   | VAL  | 2.3  |
| 1   | B     | 163 | ASN  | 2.3  |
| 1   | C     | 4   | ALA  | 2.3  |
| 1   | C     | 180 | LEU  | 2.3  |
| 1   | C     | 282 | ILE  | 2.3  |
| 1   | H     | 172 | ILE  | 2.3  |
| 1   | G     | 225 | ASP  | 2.3  |
| 1   | B     | 281 | GLU  | 2.3  |
| 1   | F     | 406 | GLU  | 2.3  |
| 1   | G     | 284 | GLU  | 2.3  |
| 1   | E     | 28  | ARG  | 2.3  |
| 1   | G     | 19  | GLY  | 2.2  |
| 1   | C     | 177 | SER  | 2.2  |
| 1   | F     | 54  | LYS  | 2.2  |
| 1   | H     | 23  | ILE  | 2.2  |
| 1   | H     | 169 | ILE  | 2.2  |
| 1   | G     | 204 | GLU  | 2.2  |
| 1   | D     | 213 | ASN  | 2.2  |
| 1   | D     | 215 | LYS  | 2.2  |
| 1   | F     | 6   | ILE  | 2.2  |
| 1   | D     | 30  | ASP  | 2.2  |
| 1   | E     | 30  | ASP  | 2.2  |
| 1   | C     | 174 | GLU  | 2.2  |
| 1   | H     | 15  | GLU  | 2.2  |
| 1   | F     | 263 | ARG  | 2.2  |
| 1   | D     | 283 | PRO  | 2.2  |
| 1   | E     | 35  | TYR  | 2.2  |
| 1   | D     | 410 | GLU  | 2.2  |
| 1   | F     | 56  | ARG  | 2.2  |
| 1   | G     | 219 | SER  | 2.2  |
| 1   | A     | 271 | GLU  | 2.2  |
| 1   | E     | 26  | ASP  | 2.2  |
| 1   | H     | 22  | ASP  | 2.2  |
| 1   | F     | 43  | LYS  | 2.2  |
| 1   | H     | 57  | PHE  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 394 | VAL  | 2.1  |
| 1   | D     | 5   | VAL  | 2.1  |
| 1   | H     | 124 | VAL  | 2.1  |
| 1   | G     | 262 | ALA  | 2.1  |
| 1   | A     | 19  | GLY  | 2.1  |
| 1   | A     | 204 | GLU  | 2.1  |
| 1   | F     | 410 | GLU  | 2.1  |
| 1   | E     | 47  | ASP  | 2.1  |
| 1   | F     | 22  | ASP  | 2.1  |
| 1   | E     | 211 | PHE  | 2.1  |
| 1   | H     | 68  | ALA  | 2.1  |
| 1   | B     | 261 | ARG  | 2.1  |
| 1   | C     | 55  | ASP  | 2.1  |
| 1   | C     | 0   | HIS  | 2.1  |
| 1   | D     | 167 | ASN  | 2.1  |
| 1   | G     | 180 | LEU  | 2.1  |
| 1   | D     | 28  | ARG  | 2.1  |
| 1   | D     | 39  | GLU  | 2.1  |
| 1   | D     | 181 | GLU  | 2.1  |
| 1   | F     | 3   | ILE  | 2.1  |
| 1   | D     | 12  | TYR  | 2.1  |
| 1   | A     | 215 | LYS  | 2.1  |
| 1   | E     | 58  | LYS  | 2.1  |
| 1   | A     | 177 | SER  | 2.1  |
| 1   | E     | 24  | SER  | 2.1  |
| 1   | D     | 163 | ASN  | 2.1  |
| 1   | A     | 2   | ARG  | 2.1  |
| 1   | E     | 174 | GLU  | 2.1  |
| 1   | G     | 296 | THR  | 2.1  |
| 1   | C     | 54  | LYS  | 2.1  |
| 1   | E     | 225 | ASP  | 2.1  |
| 1   | D     | 70  | VAL  | 2.0  |
| 1   | H     | 280 | VAL  | 2.0  |
| 1   | E     | 68  | ALA  | 2.0  |
| 1   | A     | 22  | ASP  | 2.0  |
| 1   | E     | 74  | TYR  | 2.0  |
| 1   | F     | 26  | ASP  | 2.0  |
| 1   | D     | 24  | SER  | 2.0  |
| 1   | B     | 45  | VAL  | 2.0  |
| 1   | B     | 49  | VAL  | 2.0  |
| 1   | F     | 46  | VAL  | 2.0  |
| 1   | H     | 176 | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 224 | GLU  | 2.0  |
| 1   | H     | 163 | ASN  | 2.0  |
| 1   | D     | 282 | ILE  | 2.0  |
| 1   | E     | 29  | ILE  | 2.0  |
| 1   | B     | 26  | ASP  | 2.0  |
| 1   | F     | 125 | ASP  | 2.0  |
| 1   | C     | 11  | SER  | 2.0  |
| 1   | C     | 295 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

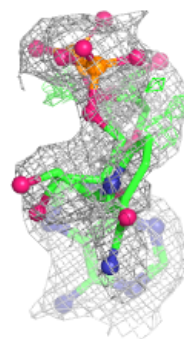
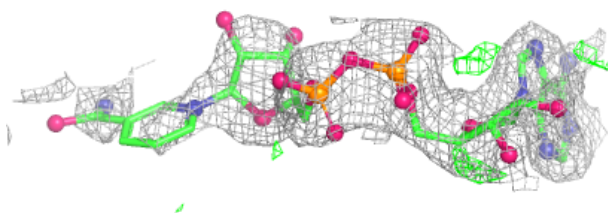
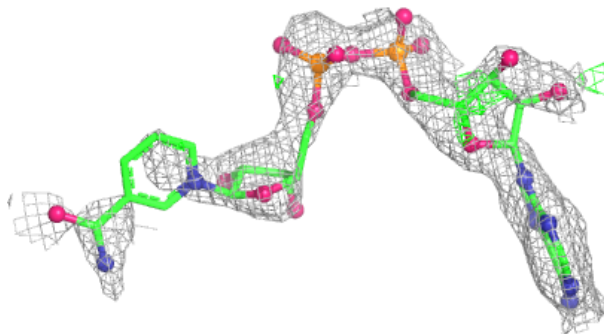
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 5   | SO4  | D     | 1416 | 5/5   | 0.62 | 0.19 | 41,42,45,49                | 0     |
| 5   | SO4  | B     | 1416 | 5/5   | 0.72 | 0.15 | 42,43,45,50                | 0     |
| 3   | MN   | G     | 1417 | 1/1   | 0.75 | 0.13 | 45,45,45,45                | 1     |
| 2   | NAD  | G     | 1416 | 44/44 | 0.77 | 0.21 | 10,16,18,18                | 44    |
| 2   | NAD  | C     | 1416 | 44/44 | 0.78 | 0.21 | 11,16,19,19                | 44    |
| 2   | NAD  | A     | 1416 | 44/44 | 0.82 | 0.20 | 11,16,18,19                | 44    |
| 4   | G6P  | C     | 1418 | 16/16 | 0.84 | 0.21 | 14,20,23,24                | 16    |
| 3   | MN   | A     | 1420 | 1/1   | 0.84 | 0.26 | 42,42,42,42                | 0     |
| 3   | MN   | A     | 1417 | 1/1   | 0.84 | 0.09 | 35,35,35,35                | 1     |
| 5   | SO4  | G     | 1418 | 5/5   | 0.84 | 0.10 | 54,54,55,57                | 0     |
| 4   | G6P  | A     | 1418 | 16/16 | 0.85 | 0.23 | 13,24,27,28                | 16    |
| 5   | SO4  | E     | 1416 | 5/5   | 0.86 | 0.10 | 40,40,41,43                | 0     |
| 3   | MN   | C     | 1417 | 1/1   | 0.87 | 0.10 | 35,35,35,35                | 1     |
| 3   | MN   | A     | 1419 | 1/1   | 0.94 | 0.07 | 35,35,35,35                | 1     |

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.

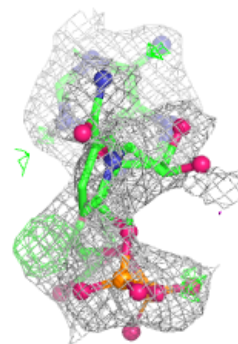
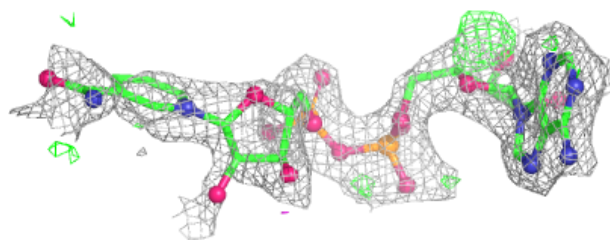
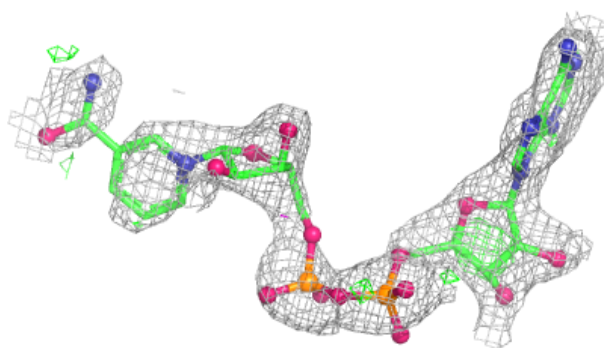
**Electron density around NAD G 1416:**

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

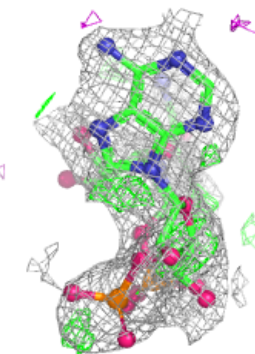
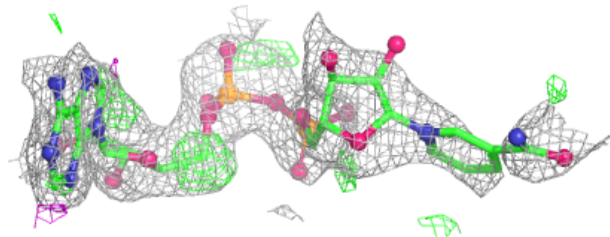
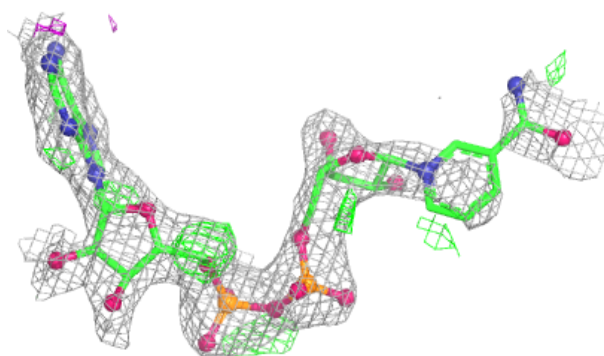


**Electron density around NAD C 1416:**

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

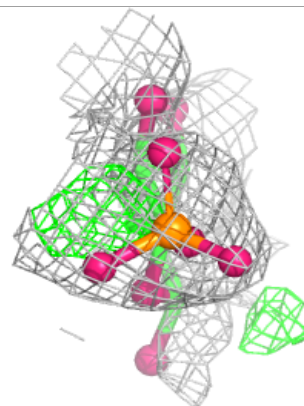
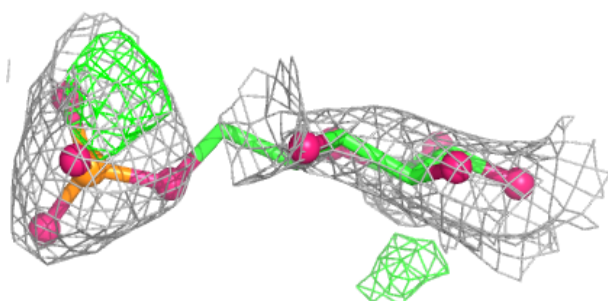
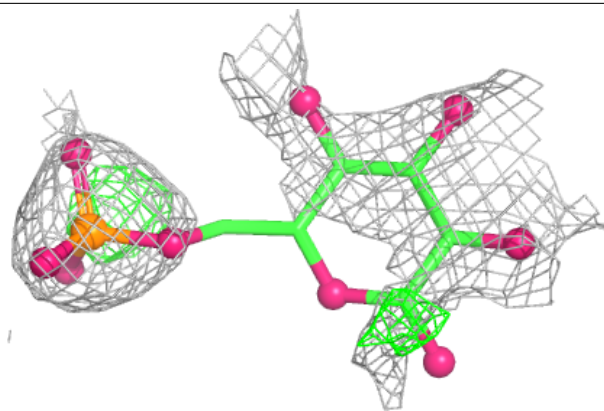
**Electron density around NAD A 1416:**

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

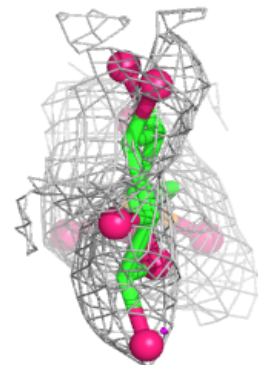
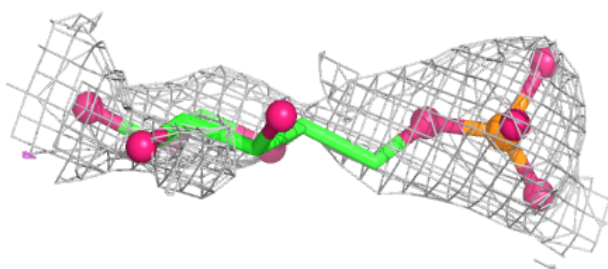
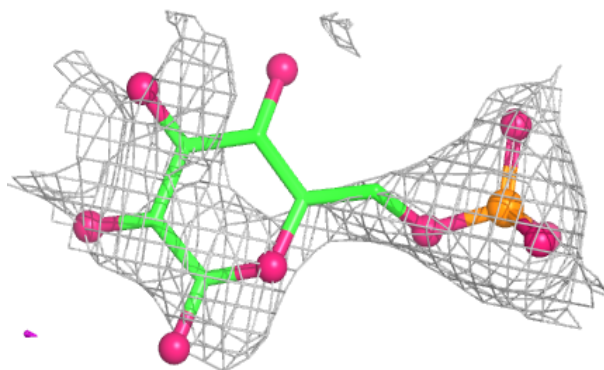


**Electron density around G6P C 1418:**

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

**Electron density around G6P A 1418:**

$2mF_o - DF_c$  (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.