# Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 05:00 pm BST

| | | |
|---|---|---|
| PDB ID | : | 3PTZ |
| Title | : | Role of Packing Defects in the Evolution of Allostery and Induced Fit in Human UDP-Glucose Dehydrogenase. |
| Authors | : | Kadirvelraj, R.; Wood, Z.A. |
| Deposited on | : | 2010-12-03 |
| Resolution | : | 2.50 Å(reported) |

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

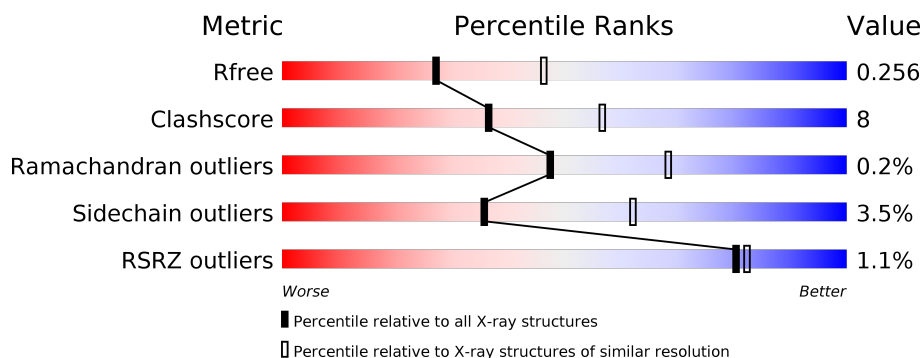| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

| Metric | Percentile Ranks | Value |
|--------|-----------------|-------|
| Rfree | | 0.256 |
| Clashscore | | 8 |
| Ramachandran outliers | | 0.2% |
| Sidechain outliers | | 3.5% |
| RSRZ outliers | | 1.1% |

*Worse* — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|----------------------------------------------------|
| $R_{free}$ | 130704 | 4661 (2.50-2.50) |
| Clashscore | 141614 | 5346 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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 | 494 | 79% · 13% · 7% |
| 1 | B | 494 | 81% · 11% · 7% |
| 1 | C | 494 | 2% / 77% · 14% · 7% |
| 1 | D | 494 | % / 75% · 16% · 7% |
| 1 | E | 494 | 77% · 15% · 7% |
| 1 | F | 494 | 3% / 73% · 18% · 7% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22753 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 UDP-glucose 6-dehydrogenase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 1 | A | 458 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3589 | 2271 | 619 | 679 | 20 | | | |
| 1 | B | 457 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3581 | 2266 | 618 | 678 | 19 | | | |
| 1 | C | 457 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3581 | 2266 | 618 | 678 | 19 | | | |
| 1 | D | 457 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3581 | 2266 | 618 | 678 | 19 | | | |
| 1 | E | 458 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3589 | 2271 | 619 | 679 | 20 | | | |
| 1 | F | 457 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3581 | 2266 | 618 | 678 | 19 | | | |

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
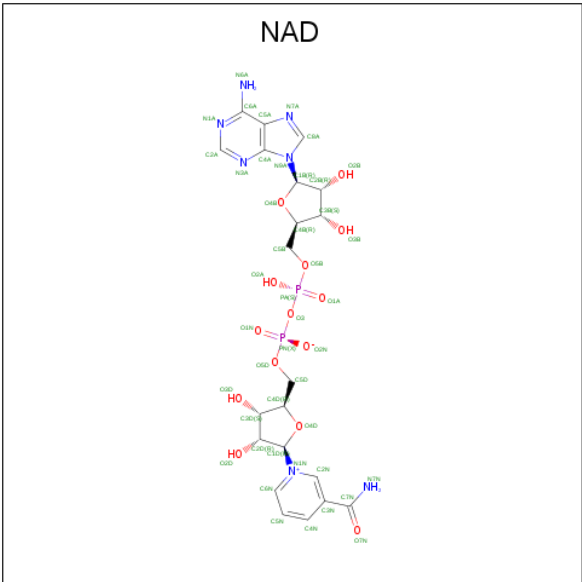
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: $C_{14}H_{22}N_2O_{16}P_2$).
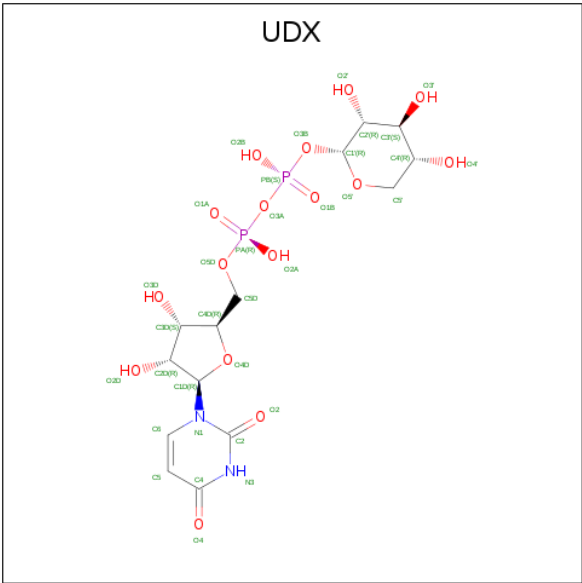


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |
| 3 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |

*Continued from previous page...*

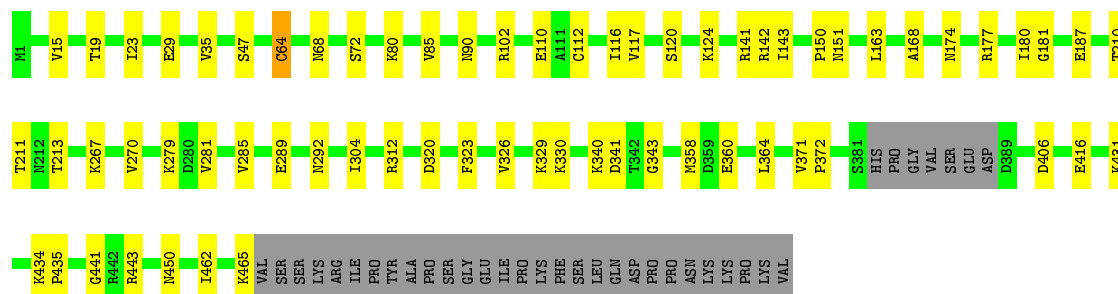| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|----|---------|---------|
| 3 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 34 | 14 | 2 | 16 | 2 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 4 | A | 164 | Total | O | 0 | 0 |
| | | | 164 | 164 | | |
| 4 | B | 141 | Total | O | 0 | 0 |
| | | | 141 | 141 | | |
| 4 | C | 121 | Total | O | 0 | 0 |
| | | | 121 | 121 | | |
| 4 | D | 87 | Total | O | 0 | 0 |
| | | | 87 | 87 | | |
| 4 | E | 161 | Total | O | 0 | 0 |
| | | | 161 | 161 | | |
| 4 | F | 109 | Total | O | 0 | 0 |
| | | | 109 | 109 | | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
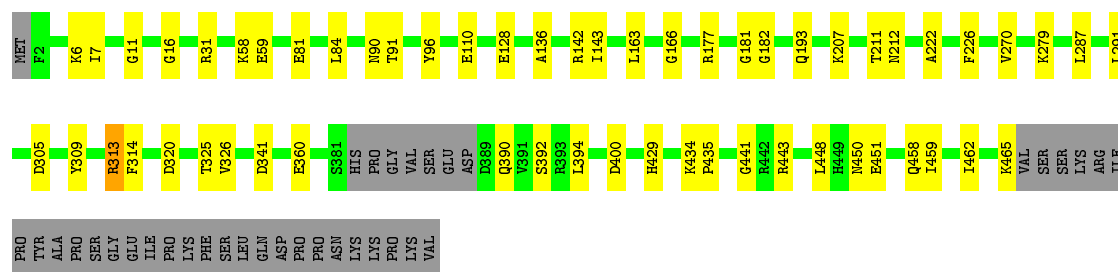
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain A:

79%          13%    7%

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain B:

81%          11%    7%

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain C:

2%

77%          14%  •  7%

GLU ASP D389 Q390 V391 S392 R393 L394 I397 D400 P401 A404 A408 H409 A436 F439 R443 H449 Q453 I462 G463 K464 K465 VAL SER SER LYS ARG ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO
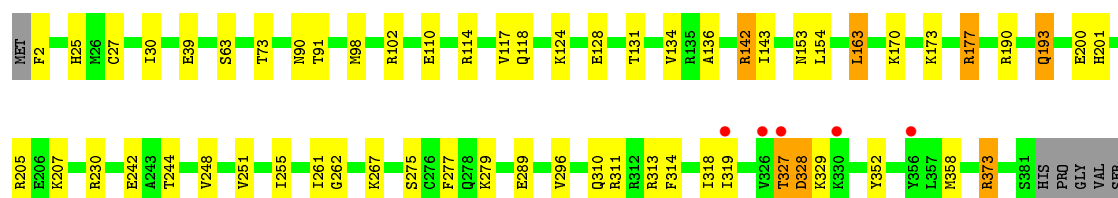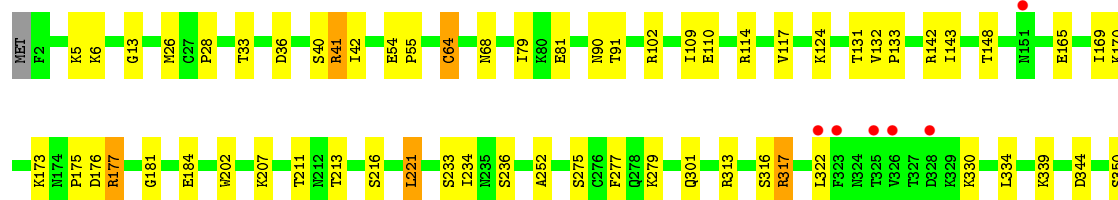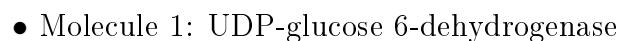
LYS VAL

• Molecule 1: UDP-glucose 6-dehydrogenase

Chain D:



MET F2 I10 V15 T19 P28 E29 I30 T33 V34 V37 I42 G66 K67 N68 L69 F70 F71 S72 T73 N74 D77 L84 N90 Y96 G97 M98 R102 C112 Q118 Y123 K124 I125 E128 K129 S130 P133 V134 R135 A136 R142

I143 N147 P150 N151 E161 F162 L163 L172 R177 G181 E187 R190 Q193 C196 Y199 W202 E206 T211 W214 K220 I234 N235 S236 D258 K267 V270 S275 C276 F277 Q278 K279 D320 T325 V326 K329 K330

I331 A332 I333 K355 A362 H363 L364 H365 I366 E374 V378 S381 HIS PRO GLY VAL SER GLU ASP D389 Q390 V391 E403 A408 D418 E422 E426 H429 K434 F439 D440 G441 E451 L452 Q453 T454 I455 I459 E460 T461 I462 K465 VAL SER

SER LYS ARG ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS VAL

• Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:



M1 G11 G17 H25 R31 N43 A44 W45 N46 S47 L50 K58 S63 C64 R65 D76 S88 Y96 G97 M98 G99 K100 E110 R114 Q118 N119 K124 K129 R141 R142 I143 L154 N159 P160 E161 F162 L163 K173 R177

I180 G181 E184 Q193 K207 I208 L209 T210 T211 N212 T213 K220 F226 D247 V248 E249 M257 N263 K264 K267 S275 K279 V296 Q301 D305 R312 D320 F323 N324 T325 V326 K340 D341 D344 K355 D359 E360

R373 S381 HIS PRO GLY VAL SER GLU ASP D389 R393 I397 D400 P401 H409 L423 K434 P435 H449 Q453 Q458 G463 K464 K465 VAL SER SER LYS ARG ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS

LYS PRO LYS VAL

• Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:



MET F2 K5 K6 G13 M26 C27 P28 T33 D36 S40 R41 I42 E54 P55 C64 N68 I79 K80 E81 N90 T91 R102 I109 E110 R114 V117 K124 T131 V132 P133 R142 I143 T148 N151 E165 I169 K170

K173 N174 P175 D176 R177 G181 E184 W202 K207 T211 N212 T213 S216 L221 S233 I234 N235 S236 A252 S275 C276 F277 Q278 K279 Q301 R313 S316 R317 L322 F323 N324 T325 V326 T327 D328 K329 K330 L334 K339 D344 S350

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 89.10Å 196.67Å 111.74Å<br>90.00° 111.88° 90.00° | Depositor |
| Resolution (Å) | 49.17 – 2.50<br>49.17 – 2.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.3 (49.17-2.50)<br>97.3 (49.17-2.50) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.07 | Depositor |
| $<I/\sigma(I)>$ [1] | 2.73 (at 2.51Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| R, $R_{free}$ | 0.189 , 0.258<br>0.190 , 0.256 | Depositor<br>DCC |
| $R_{free}$ test set | 6018 reflections (5.03%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 32.4 | Xtriage |
| Anisotropy | 0.042 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 40.3 | EDS |
| L-test for twinning[2] | $<|L|> = 0.49$, $<L^2> = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.018 for h,-k,-h-l | Xtriage |
| $F_o,F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 22753 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 31.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5  Model quality (i)

## 5.1  Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
UDX, NAD

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 | 0.93 | 1/3653 (0.0%) | 0.87 | 0/4941 |
| 1 | B | 0.89 | 1/3645 (0.0%) | 0.86 | 4/4931 (0.1%) |
| 1 | C | 0.84 | 0/3645 | 0.81 | 1/4931 (0.0%) |
| 1 | D | 0.84 | 1/3645 (0.0%) | 0.79 | 0/4931 |
| 1 | E | 0.88 | 0/3653 | 0.86 | 6/4941 (0.1%) |
| 1 | F | 0.84 | 0/3645 | 0.81 | 2/4931 (0.0%) |
| All | All | 0.87 | 3/21886 (0.0%) | 0.83 | 13/29606 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | B | 59 | GLU | CG-CD | 5.17 | 1.59 | 1.51 |
| 1 | A | 64 | CYS | CB-SG | -5.16 | 1.73 | 1.81 |
| 1 | D | 196 | CYS | CB-SG | -5.01 | 1.73 | 1.81 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|------------|----------|
| 1 | B | 313 | ARG | NE-CZ-NH1 | -7.50 | 116.55 | 120.30 |
| 1 | E | 312 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 1 | E | 209 | LEU | CA-CB-CG | 7.07 | 131.56 | 115.30 |
| 1 | F | 344 | ASP | CB-CG-OD1 | 6.20 | 123.88 | 118.30 |
| 1 | E | 1 | MET | CG-SD-CE | -5.89 | 90.77 | 100.20 |
| 1 | B | 31 | ARG | NE-CZ-NH2 | -5.85 | 117.38 | 120.30 |
| 1 | C | 311 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | E | 305 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 1 | F | 102 | ARG | NE-CZ-NH1 | -5.21 | 117.69 | 120.30 |
| 1 | E | 31 | ARG | NE-CZ-NH1 | 5.15 | 122.87 | 120.30 |
| 1 | B | 305 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | E | 344 | ASP | CB-CG-OD1 | 5.02 | 122.82 | 118.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | B | 448 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3589 | 0 | 3611 | 60 | 0 |
| 1 | B | 3581 | 0 | 3599 | 51 | 0 |
| 1 | C | 3581 | 0 | 3599 | 59 | 0 |
| 1 | D | 3581 | 0 | 3599 | 50 | 0 |
| 1 | E | 3589 | 0 | 3611 | 66 | 0 |
| 1 | F | 3581 | 0 | 3599 | 67 | 0 |
| 2 | A | 44 | 0 | 26 | 12 | 0 |
| 2 | B | 44 | 0 | 26 | 18 | 0 |
| 2 | C | 44 | 0 | 26 | 13 | 0 |
| 2 | D | 44 | 0 | 26 | 10 | 0 |
| 2 | E | 44 | 0 | 26 | 11 | 0 |
| 2 | F | 44 | 0 | 26 | 14 | 0 |
| 3 | A | 34 | 0 | 20 | 0 | 0 |
| 3 | B | 34 | 0 | 20 | 0 | 0 |
| 3 | C | 34 | 0 | 20 | 1 | 0 |
| 3 | D | 34 | 0 | 20 | 1 | 0 |
| 3 | E | 34 | 0 | 20 | 0 | 0 |
| 3 | F | 34 | 0 | 20 | 1 | 0 |
| 4 | A | 164 | 0 | 0 | 11 | 0 |
| 4 | B | 141 | 0 | 0 | 6 | 0 |
| 4 | C | 121 | 0 | 0 | 10 | 0 |
| 4 | D | 87 | 0 | 0 | 4 | 0 |
| 4 | E | 161 | 0 | 0 | 19 | 0 |
| 4 | F | 109 | 0 | 0 | 16 | 0 |
| All | All | 22753 | 0 | 21894 | 347 | 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 8.

All (347) 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:B:279:LYS:CE | 2:B:500:NAD:H6N | 1.63 | 1.28 |
| 1:A:279:LYS:HE3 | 2:A:500:NAD:C6N | 1.67 | 1.24 |
| 1:D:90:ASN:HB2 | 2:D:500:NAD:N7N | 1.51 | 1.24 |
| 1:C:90:ASN:HB2 | 2:C:500:NAD:N7N | 1.54 | 1.21 |
| 1:B:279:LYS:HE2 | 2:B:500:NAD:H6N | 1.23 | 1.14 |
| 4:A:778:HOH:O | 1:C:142:ARG:HD2 | 1.52 | 1.10 |
| 1:B:451:GLU:HB2 | 4:B:596:HOH:O | 1.50 | 1.09 |
| 1:B:279:LYS:NZ | 2:B:500:NAD:H6N | 1.67 | 1.09 |
| 1:D:90:ASN:HB2 | 2:D:500:NAD:H71N | 1.01 | 1.08 |
| 1:A:279:LYS:HE3 | 2:A:500:NAD:H6N | 1.28 | 1.06 |
| 1:F:356:TYR:HB3 | 4:F:553:HOH:O | 1.53 | 1.05 |
| 2:B:500:NAD:O1A | 2:B:500:NAD:N7N | 1.94 | 1.00 |
| 1:A:279:LYS:CE | 2:A:500:NAD:C6N | 2.39 | 0.99 |
| 1:A:279:LYS:HZ2 | 2:A:500:NAD:H1D | 1.25 | 0.99 |
| 1:C:90:ASN:HB2 | 2:C:500:NAD:H71N | 0.86 | 0.98 |
| 1:E:193:GLN:HG2 | 4:E:608:HOH:O | 1.59 | 0.98 |
| 1:B:279:LYS:HZ3 | 2:B:500:NAD:C6N | 1.81 | 0.94 |
| 1:F:421:LYS:HB3 | 4:F:542:HOH:O | 1.68 | 0.94 |
| 1:A:90:ASN:HB2 | 2:A:500:NAD:H71N | 1.31 | 0.93 |
| 1:D:90:ASN:CB | 2:D:500:NAD:H71N | 1.81 | 0.92 |
| 1:B:279:LYS:NZ | 2:B:500:NAD:H1D | 1.86 | 0.91 |
| 1:B:279:LYS:HE2 | 2:B:500:NAD:C6N | 1.99 | 0.91 |
| 1:C:90:ASN:CB | 2:C:500:NAD:H71N | 1.80 | 0.90 |
| 1:B:279:LYS:HZ3 | 2:B:500:NAD:H6N | 1.28 | 0.88 |
| 1:B:279:LYS:HZ1 | 2:B:500:NAD:H1D | 1.38 | 0.88 |
| 1:A:279:LYS:NZ | 2:A:500:NAD:H1D | 1.89 | 0.87 |
| 1:D:90:ASN:CB | 2:D:500:NAD:N7N | 2.36 | 0.86 |
| 1:F:389:ASP:HB2 | 4:F:670:HOH:O | 1.75 | 0.85 |
| 1:F:275:SER:O | 2:F:500:NAD:H5N | 1.77 | 0.84 |
| 1:C:279:LYS:HZ3 | 2:C:500:NAD:C6N | 1.92 | 0.82 |
| 1:F:90:ASN:HB2 | 2:F:500:NAD:H71N | 1.43 | 0.81 |
| 1:A:142:ARG:HD2 | 4:E:579:HOH:O | 1.80 | 0.81 |
| 1:A:292:ASN:HB3 | 4:F:520:HOH:O | 1.79 | 0.80 |
| 1:E:320:ASP:HB3 | 4:E:513:HOH:O | 1.81 | 0.80 |
| 1:F:330:LYS:HE2 | 1:F:406:ASP:O | 1.82 | 0.80 |
| 1:C:275:SER:O | 2:C:500:NAD:H5N | 1.85 | 0.76 |
| 1:B:326:VAL:CG2 | 1:B:360:GLU:HB3 | 2.16 | 0.76 |
| 1:C:200:GLU:OE1 | 1:C:205:ARG:HD3 | 1.86 | 0.76 |
| 1:C:373:ARG:HB3 | 1:C:397:ILE:HG21 | 1.68 | 0.75 |
| 1:B:193:GLN:HG3 | 4:B:565:HOH:O | 1.87 | 0.74 |

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:359:ASP:HB3 | 4:E:587:HOH:O | 1.88 | 0.74 |
| 1:E:279:LYS:HE2 | 2:E:500:NAD:C6N | 2.18 | 0.74 |
| 1:A:326:VAL:HG22 | 1:A:360:GLU:HB3 | 1.69 | 0.74 |
| 1:E:326:VAL:HG22 | 1:E:360:GLU:HB3 | 1.71 | 0.73 |
| 1:E:173:LYS:HD2 | 4:E:643:HOH:O | 1.87 | 0.73 |
| 1:F:427:ARG:CD | 4:F:558:HOH:O | 2.36 | 0.72 |
| 1:F:90:ASN:HB2 | 2:F:500:NAD:N7N | 2.06 | 0.71 |
| 1:A:110:GLU:HG3 | 1:A:143:ILE:HD11 | 1.73 | 0.70 |
| 1:F:313:ARG:O | 1:F:317:ARG:HB2 | 1.92 | 0.70 |
| 1:E:355:LYS:HE2 | 4:E:784:HOH:O | 1.92 | 0.69 |
| 1:E:76:ASP:HB3 | 1:E:119:ASN:OD1 | 1.92 | 0.69 |
| 1:C:27:CYS:HB3 | 1:C:30:ILE:HD12 | 1.75 | 0.69 |
| 1:D:33:THR:HG23 | 1:D:70:PHE:HB2 | 1.74 | 0.68 |
| 1:B:314:PHE:CD1 | 1:B:462:ILE:HD11 | 2.28 | 0.68 |
| 1:B:326:VAL:CG2 | 1:B:360:GLU:CB | 2.71 | 0.68 |
| 1:D:15:VAL:O | 1:D:19:THR:HG23 | 1.92 | 0.68 |
| 1:F:390:GLN:HG2 | 1:F:394:LEU:HD12 | 1.77 | 0.67 |
| 1:B:90:ASN:HB2 | 2:B:500:NAD:C2N | 2.25 | 0.67 |
| 1:C:110:GLU:HG3 | 1:C:143:ILE:HD11 | 1.77 | 0.66 |
| 1:D:275:SER:HB2 | 2:D:500:NAD:C5N | 2.26 | 0.66 |
| 1:D:355:LYS:HE3 | 4:D:529:HOH:O | 1.95 | 0.66 |
| 1:E:389:ASP:HB3 | 4:E:506:HOH:O | 1.95 | 0.66 |
| 1:E:184:GLU:HG2 | 4:E:605:HOH:O | 1.96 | 0.65 |
| 1:C:352:TYR:HB3 | 4:C:568:HOH:O | 1.96 | 0.65 |
| 1:D:19:THR:HG22 | 1:D:172:LEU:HD21 | 1.76 | 0.64 |
| 1:E:279:LYS:HZ3 | 2:E:500:NAD:C5N | 2.10 | 0.64 |
| 1:E:275:SER:HB2 | 2:E:500:NAD:C6N | 2.28 | 0.64 |
| 1:B:465:LYS:HE3 | 4:B:779:HOH:O | 1.99 | 0.62 |
| 1:E:279:LYS:NZ | 2:E:500:NAD:C6N | 2.63 | 0.62 |
| 1:E:275:SER:O | 2:E:500:NAD:H6N | 1.98 | 0.62 |
| 1:F:91:THR:H | 2:F:500:NAD:H2N | 1.64 | 0.62 |
| 1:B:390:GLN:HB3 | 1:B:394:LEU:HD12 | 1.82 | 0.62 |
| 1:A:90:ASN:CB | 2:A:500:NAD:H71N | 2.07 | 0.61 |
| 1:F:427:ARG:HD2 | 4:F:558:HOH:O | 1.95 | 0.61 |
| 1:A:102:ARG:HD2 | 4:A:665:HOH:O | 1.99 | 0.61 |
| 1:E:296:VAL:HG13 | 1:F:236:SER:HB2 | 1.82 | 0.61 |
| 1:A:90:ASN:HB2 | 2:A:500:NAD:N7N | 2.09 | 0.61 |
| 1:F:449:HIS:O | 1:F:453:GLN:HG3 | 2.01 | 0.60 |
| 1:A:80:LYS:HE2 | 4:A:609:HOH:O | 2.00 | 0.60 |
| 2:B:500:NAD:H51N | 2:B:500:NAD:H2N | 1.84 | 0.60 |
| 1:E:279:LYS:CE | 2:E:500:NAD:C6N | 2.79 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:58:LYS:HE2 | 4:E:626:HOH:O | 2.01 | 0.60 |
| 1:C:153:ASN:HA | 4:C:593:HOH:O | 2.02 | 0.60 |
| 1:B:279:LYS:NZ | 2:B:500:NAD:C6N | 2.46 | 0.59 |
| 1:D:422:GLU:HA | 4:D:707:HOH:O | 2.00 | 0.59 |
| 1:C:114:ARG:O | 1:C:117:VAL:HG12 | 2.02 | 0.59 |
| 1:F:90:ASN:HA | 2:F:500:NAD:H2D | 1.85 | 0.59 |
| 1:B:309:TYR:CZ | 1:B:313:ARG:HD3 | 2.38 | 0.59 |
| 1:C:163:LEU:C | 1:C:163:LEU:HD12 | 2.23 | 0.59 |
| 1:E:458:GLN:HG2 | 4:E:578:HOH:O | 2.02 | 0.58 |
| 1:C:296:VAL:HG13 | 1:D:236:SER:HB2 | 1.86 | 0.58 |
| 1:F:427:ARG:HD3 | 4:F:558:HOH:O | 2.00 | 0.58 |
| 1:A:326:VAL:HG22 | 1:A:360:GLU:CB | 2.33 | 0.58 |
| 1:B:458:GLN:NE2 | 1:F:142:ARG:HH12 | 2.02 | 0.58 |
| 1:D:325:THR:O | 1:D:329:LYS:HE3 | 2.04 | 0.57 |
| 1:F:301:GLN:NE2 | 4:F:507:HOH:O | 2.37 | 0.57 |
| 1:D:331:ILE:HD12 | 1:D:362:ALA:HB1 | 1.86 | 0.57 |
| 1:D:451:GLU:O | 1:D:455:ILE:HG13 | 2.05 | 0.57 |
| 1:A:187:GLU:HG2 | 4:A:563:HOH:O | 2.04 | 0.56 |
| 1:D:441:GLY:HA2 | 1:D:462:ILE:HD12 | 1.85 | 0.56 |
| 1:C:279:LYS:HD3 | 2:C:500:NAD:C5N | 2.35 | 0.56 |
| 1:C:279:LYS:NZ | 2:C:500:NAD:C6N | 2.67 | 0.56 |
| 1:F:450:ASN:O | 1:F:454:THR:HB | 2.05 | 0.56 |
| 1:D:10:ILE:HG21 | 1:D:112:CYS:SG | 2.46 | 0.55 |
| 1:B:326:VAL:HG23 | 1:B:360:GLU:CB | 2.36 | 0.55 |
| 1:E:279:LYS:NZ | 2:E:500:NAD:C5N | 2.68 | 0.55 |
| 1:B:110:GLU:HG2 | 1:B:143:ILE:HD11 | 1.88 | 0.55 |
| 1:F:6:LYS:NZ | 4:F:525:HOH:O | 2.39 | 0.55 |
| 1:D:74:ASN:ND2 | 1:D:77:ASP:HB2 | 2.22 | 0.55 |
| 1:C:131:THR:HG21 | 4:C:541:HOH:O | 2.07 | 0.55 |
| 1:D:199:TYR:HA | 1:D:202:TRP:CZ3 | 2.41 | 0.55 |
| 1:B:279:LYS:NZ | 2:B:500:NAD:C1D | 2.65 | 0.55 |
| 1:B:90:ASN:HB2 | 2:B:500:NAD:C3N | 2.38 | 0.54 |
| 1:F:79:ILE:O | 1:F:124:LYS:HE3 | 2.06 | 0.54 |
| 1:A:292:ASN:CB | 4:F:520:HOH:O | 2.47 | 0.54 |
| 1:A:326:VAL:HA | 1:A:329:LYS:HD2 | 1.89 | 0.54 |
| 1:B:279:LYS:HZ3 | 2:B:500:NAD:H1D | 1.68 | 0.54 |
| 1:E:279:LYS:HE2 | 2:E:500:NAD:H6N | 1.89 | 0.54 |
| 1:C:389:ASP:O | 1:C:392:SER:HB2 | 2.08 | 0.54 |
| 2:B:500:NAD:C2N | 2:B:500:NAD:H51N | 2.36 | 0.54 |
| 1:A:279:LYS:NZ | 2:A:500:NAD:C1D | 2.65 | 0.53 |
| 1:C:170:LYS:HG2 | 4:C:530:HOH:O | 2.08 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:226:PHE:CZ | 1:F:233:SER:HB3 | 2.44 | 0.53 |
| 1:D:34:VAL:O | 1:D:71:PHE:HA | 2.09 | 0.53 |
| 1:C:390:GLN:HG2 | 1:C:394:LEU:HD12 | 1.91 | 0.53 |
| 1:F:181:GLY:HA2 | 1:F:211:THR:O | 2.08 | 0.53 |
| 1:C:262:GLY:HA2 | 4:C:584:HOH:O | 2.08 | 0.53 |
| 1:C:244:THR:HG1 | 1:D:214:TRP:HE1 | 1.57 | 0.53 |
| 4:A:579:HOH:O | 1:E:409:HIS:HD2 | 1.91 | 0.53 |
| 1:F:317:ARG:NH2 | 1:F:461:THR:O | 2.41 | 0.53 |
| 1:A:181:GLY:HA2 | 1:A:211:THR:O | 2.09 | 0.53 |
| 1:B:279:LYS:HZ1 | 2:B:500:NAD:C1D | 2.17 | 0.53 |
| 1:C:90:ASN:HA | 2:C:500:NAD:H2D | 1.91 | 0.53 |
| 1:D:134:VAL:O | 1:D:135:ARG:HB2 | 2.09 | 0.52 |
| 1:A:141:ARG:NH2 | 1:A:213:THR:OG1 | 2.42 | 0.52 |
| 1:B:279:LYS:CE | 2:B:500:NAD:C6N | 2.57 | 0.52 |
| 1:C:242:GLU:OE1 | 1:C:313:ARG:NH1 | 2.42 | 0.52 |
| 1:F:334:LEU:HB3 | 1:F:420:PHE:CZ | 2.44 | 0.52 |
| 1:C:201:HIS:HD2 | 4:C:518:HOH:O | 1.92 | 0.52 |
| 1:A:180:ILE:O | 1:A:210:THR:HA | 2.09 | 0.52 |
| 1:C:90:ASN:HA | 2:C:500:NAD:H2N | 1.90 | 0.52 |
| 1:A:416:GLU:HG2 | 1:A:416:GLU:O | 2.08 | 0.52 |
| 1:B:443:ARG:HD3 | 1:B:462:ILE:O | 2.09 | 0.52 |
| 1:E:301:GLN:NE2 | 4:E:593:HOH:O | 2.43 | 0.52 |
| 1:B:326:VAL:HG23 | 1:B:360:GLU:HB3 | 1.88 | 0.52 |
| 1:C:449:HIS:O | 1:C:453:GLN:HG3 | 2.10 | 0.51 |
| 1:A:320:ASP:O | 1:A:323:PHE:N | 2.42 | 0.51 |
| 1:B:182:GLY:O | 1:B:212:ASN:HA | 2.10 | 0.51 |
| 1:D:429:HIS:CE1 | 1:D:434:LYS:HE3 | 2.45 | 0.51 |
| 1:B:326:VAL:HG22 | 1:B:360:GLU:HB3 | 1.92 | 0.51 |
| 1:D:130:SER:HB2 | 2:D:500:NAD:O3D | 2.10 | 0.51 |
| 1:F:169:ILE:HG12 | 4:F:499:HOH:O | 2.10 | 0.51 |
| 1:A:270:VAL:HG22 | 1:A:270:VAL:O | 2.10 | 0.51 |
| 1:E:160:PRO:HB3 | 1:E:220:LYS:HG2 | 1.92 | 0.51 |
| 1:A:29:GLU:HB3 | 4:A:587:HOH:O | 2.10 | 0.50 |
| 1:D:161:GLU:CG | 1:D:163:LEU:HD23 | 2.42 | 0.50 |
| 2:D:500:NAD:H4N | 4:D:764:HOH:O | 2.11 | 0.50 |
| 1:F:373:ARG:O | 1:F:377:VAL:HG23 | 2.11 | 0.50 |
| 1:C:39:GLU:HG3 | 1:C:73:THR:HG21 | 1.94 | 0.50 |
| 1:D:326:VAL:CG1 | 1:D:331:ILE:HD11 | 2.42 | 0.50 |
| 1:F:133:PRO:O | 1:F:221:LEU:HD11 | 2.11 | 0.50 |
| 1:C:110:GLU:CG | 1:C:143:ILE:HD11 | 2.42 | 0.50 |
| 1:E:163:LEU:HD12 | 1:E:163:LEU:C | 2.32 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:110:GLU:CG | 1:F:143:ILE:HD11 | 2.42 | 0.50 |
| 1:F:184:GLU:HG3 | 4:F:554:HOH:O | 2.10 | 0.50 |
| 1:B:326:VAL:CG2 | 1:B:360:GLU:HB2 | 2.39 | 0.50 |
| 1:B:441:GLY:HA2 | 1:B:462:ILE:HD13 | 1.94 | 0.50 |
| 1:C:230:ARG:NH1 | 1:C:261:ILE:O | 2.37 | 0.50 |
| 1:C:2:PHE:HB2 | 1:C:190:ARG:NH1 | 2.26 | 0.49 |
| 1:B:287:LEU:HD11 | 1:B:291:LEU:HD11 | 1.94 | 0.49 |
| 1:C:310:GLN:OE1 | 1:C:313:ARG:NH2 | 2.45 | 0.49 |
| 1:E:162:PHE:CD1 | 1:E:220:LYS:HE2 | 2.47 | 0.49 |
| 1:C:207:LYS:HE3 | 4:C:533:HOH:O | 2.12 | 0.49 |
| 1:E:400:ASP:HB2 | 1:E:401:PRO:CD | 2.43 | 0.49 |
| 1:B:166:GLY:HA2 | 1:B:341:ASP:O | 2.12 | 0.49 |
| 1:B:181:GLY:HA2 | 1:B:211:THR:O | 2.13 | 0.49 |
| 1:A:279:LYS:NZ | 2:A:500:NAD:N1N | 2.60 | 0.49 |
| 1:C:128:GLU:HG3 | 1:C:136:ALA:HB1 | 1.93 | 0.49 |
| 1:E:110:GLU:HB3 | 1:E:143:ILE:HD11 | 1.95 | 0.49 |
| 1:E:312:ARG:HH11 | 1:E:312:ARG:CG | 2.26 | 0.49 |
| 1:E:96:TYR:HA | 1:E:100:LYS:HB2 | 1.94 | 0.49 |
| 1:F:279:LYS:HD2 | 2:F:500:NAD:C5N | 2.43 | 0.49 |
| 1:E:373:ARG:HB2 | 1:E:397:ILE:HG21 | 1.95 | 0.49 |
| 1:F:400:ASP:OD1 | 1:F:403:GLU:HB2 | 2.13 | 0.49 |
| 1:E:124:LYS:HB2 | 1:E:154:LEU:CD2 | 2.43 | 0.48 |
| 1:F:275:SER:HB2 | 2:F:500:NAD:C5N | 2.43 | 0.48 |
| 1:B:314:PHE:CD1 | 1:B:462:ILE:CD1 | 2.96 | 0.48 |
| 1:F:91:THR:CG2 | 1:F:109:ILE:HD12 | 2.43 | 0.48 |
| 1:C:110:GLU:HG3 | 1:C:143:ILE:CD1 | 2.43 | 0.48 |
| 1:F:177:ARG:HD3 | 4:F:562:HOH:O | 2.13 | 0.48 |
| 1:C:318:ILE:HA | 1:C:439:PHE:CE1 | 2.48 | 0.48 |
| 1:D:123:TYR:O | 1:D:124:LYS:HG3 | 2.12 | 0.48 |
| 1:B:450:ASN:O | 1:B:451:GLU:C | 2.51 | 0.48 |
| 1:D:130:SER:HB2 | 2:D:500:NAD:C3D | 2.44 | 0.48 |
| 1:F:36:ASP:HB3 | 1:F:42:ILE:HD11 | 1.96 | 0.48 |
| 1:C:25:HIS:CE1 | 1:C:173:LYS:HZ1 | 2.32 | 0.48 |
| 1:E:325:THR:O | 1:E:325:THR:HG23 | 2.14 | 0.48 |
| 1:A:443:ARG:HD3 | 1:A:462:ILE:O | 2.13 | 0.48 |
| 1:F:91:THR:O | 1:F:279:LYS:NZ | 2.47 | 0.48 |
| 1:E:118:GLN:HB3 | 1:E:119:ASN:ND2 | 2.29 | 0.47 |
| 1:F:175:PRO:O | 1:F:207:LYS:HE2 | 2.14 | 0.47 |
| 1:D:150:PRO:O | 1:D:151:ASN:HB2 | 2.14 | 0.47 |
| 1:C:314:PHE:CD1 | 1:C:462:ILE:HD11 | 2.49 | 0.47 |
| 1:F:26:MET:HG3 | 1:F:202:TRP:CD2 | 2.49 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:350:SER:OG | 1:F:414:CYS:HB3 | 2.15 | 0.47 |
| 1:A:343:GLY:O | 1:A:371:VAL:HG22 | 2.14 | 0.47 |
| 1:C:190:ARG:HD3 | 4:C:521:HOH:O | 2.15 | 0.47 |
| 1:E:381:SER:C | 4:E:777:HOH:O | 2.53 | 0.47 |
| 1:C:329:LYS:HD3 | 1:C:409:HIS:ND1 | 2.29 | 0.47 |
| 1:A:281:VAL:HG11 | 1:A:304:ILE:HG12 | 1.96 | 0.47 |
| 1:A:431:LYS:HD2 | 4:A:646:HOH:O | 2.14 | 0.47 |
| 1:D:277:PHE:CE2 | 3:D:501:UDX:H5A1 | 2.49 | 0.47 |
| 1:E:326:VAL:HG22 | 1:E:360:GLU:CB | 2.42 | 0.47 |
| 1:E:434:LYS:HA | 1:E:435:PRO:C | 2.33 | 0.47 |
| 1:F:169:ILE:HG22 | 1:F:173:LYS:HD2 | 1.97 | 0.47 |
| 1:A:187:GLU:CG | 4:A:563:HOH:O | 2.63 | 0.46 |
| 1:C:248:VAL:HG12 | 1:C:463:GLY:HA3 | 1.96 | 0.46 |
| 1:E:401:PRO:HG2 | 1:E:423:LEU:HD21 | 1.95 | 0.46 |
| 1:E:181:GLY:HA2 | 1:E:211:THR:O | 2.15 | 0.46 |
| 1:B:458:GLN:HE21 | 1:F:142:ARG:HH12 | 1.63 | 0.46 |
| 1:B:6:LYS:HD2 | 4:B:601:HOH:O | 2.16 | 0.46 |
| 1:C:318:ILE:HG12 | 1:C:439:PHE:CD1 | 2.51 | 0.46 |
| 1:D:90:ASN:HB2 | 2:D:500:NAD:H72N | 1.64 | 0.46 |
| 1:E:114:ARG:NH2 | 4:E:541:HOH:O | 2.36 | 0.46 |
| 1:A:441:GLY:HA2 | 1:A:462:ILE:HG13 | 1.98 | 0.46 |
| 1:D:128:GLU:HG3 | 1:D:136:ALA:HB1 | 1.96 | 0.46 |
| 1:E:45:TRP:O | 1:E:65:ARG:NH1 | 2.49 | 0.46 |
| 1:F:452:LEU:O | 1:F:457:PHE:HB2 | 2.16 | 0.46 |
| 1:D:333:ILE:HB | 1:D:366:ILE:HG12 | 1.97 | 0.46 |
| 1:E:393:ARG:HD2 | 4:E:695:HOH:O | 2.15 | 0.46 |
| 1:E:449:HIS:O | 1:E:453:GLN:HG3 | 2.16 | 0.46 |
| 1:D:181:GLY:HA2 | 1:D:211:THR:O | 2.16 | 0.45 |
| 1:D:84:LEU:HD12 | 1:D:125:ILE:O | 2.16 | 0.45 |
| 1:A:120:SER:HB3 | 1:A:124:LYS:HE2 | 1.98 | 0.45 |
| 1:B:222:ALA:O | 1:B:226:PHE:HD1 | 1.99 | 0.45 |
| 1:E:275:SER:O | 2:E:500:NAD:C6N | 2.64 | 0.45 |
| 1:E:279:LYS:HE3 | 2:E:500:NAD:O2D | 2.16 | 0.45 |
| 1:B:325:THR:HB | 4:F:523:HOH:O | 2.16 | 0.45 |
| 1:D:439:PHE:CE1 | 1:D:460:GLU:HG3 | 2.51 | 0.45 |
| 1:E:114:ARG:NE | 4:E:541:HOH:O | 2.36 | 0.45 |
| 1:F:131:THR:H | 2:F:500:NAD:H4D | 1.81 | 0.45 |
| 1:A:163:LEU:HD13 | 1:A:168:ALA:HB2 | 1.99 | 0.45 |
| 1:C:102:ARG:NH1 | 1:C:289:GLU:OE2 | 2.43 | 0.45 |
| 1:D:374:GLU:O | 1:D:378:VAL:HG23 | 2.17 | 0.45 |
| 1:A:142:ARG:HD3 | 1:E:323:PHE:HE2 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:279:LYS:NZ | 2:A:500:NAD:C6N | 2.79 | 0.45 |
| 1:B:207:LYS:HE3 | 4:B:556:HOH:O | 2.17 | 0.45 |
| 1:A:142:ARG:HD3 | 1:E:323:PHE:CE2 | 2.53 | 0.44 |
| 1:C:279:LYS:NZ | 2:C:500:NAD:C5N | 2.81 | 0.44 |
| 1:D:206:GLU:H | 1:D:206:GLU:CD | 2.19 | 0.44 |
| 1:E:110:GLU:CD | 4:E:570:HOH:O | 2.54 | 0.44 |
| 1:A:330:LYS:NZ | 1:A:406:ASP:O | 2.41 | 0.44 |
| 1:A:326:VAL:CG2 | 1:A:360:GLU:HB2 | 2.47 | 0.44 |
| 1:E:50:LEU:HD11 | 1:E:58:LYS:HA | 2.00 | 0.44 |
| 1:B:11:GLY:O | 1:B:16:GLY:HA3 | 2.18 | 0.44 |
| 1:B:429:HIS:CE1 | 1:B:434:LYS:HE3 | 2.52 | 0.44 |
| 1:E:340:LYS:O | 1:E:341:ASP:HB2 | 2.18 | 0.44 |
| 1:F:234:ILE:HD11 | 1:F:252:ALA:HB2 | 2.00 | 0.44 |
| 1:A:434:LYS:HA | 1:A:435:PRO:C | 2.39 | 0.44 |
| 1:F:13:GLY:HA2 | 1:F:41:ARG:NH2 | 2.33 | 0.44 |
| 1:A:90:ASN:HD22 | 2:A:500:NAD:H72N | 1.66 | 0.44 |
| 2:E:500:NAD:H3D | 4:E:535:HOH:O | 2.17 | 0.44 |
| 1:F:28:PRO:HA | 1:F:68:ASN:ND2 | 2.33 | 0.44 |
| 1:F:455:ILE:O | 1:F:455:ILE:CG2 | 2.66 | 0.44 |
| 1:B:163:LEU:HD12 | 1:B:163:LEU:C | 2.38 | 0.43 |
| 1:A:281:VAL:O | 1:A:285:VAL:HG23 | 2.18 | 0.43 |
| 1:A:326:VAL:CG2 | 1:A:360:GLU:CB | 2.95 | 0.43 |
| 1:E:263:ASN:OD1 | 1:E:264:LYS:HD3 | 2.17 | 0.43 |
| 1:C:251:VAL:O | 1:C:255:ILE:HG13 | 2.18 | 0.43 |
| 1:B:58:LYS:HD2 | 4:B:573:HOH:O | 2.18 | 0.43 |
| 1:F:170:LYS:HG2 | 4:F:571:HOH:O | 2.19 | 0.43 |
| 1:F:64:CYS:HB2 | 1:F:68:ASN:OD1 | 2.17 | 0.43 |
| 1:C:443:ARG:HD3 | 1:C:462:ILE:O | 2.18 | 0.43 |
| 1:D:453:GLN:HG3 | 1:D:459:ILE:HD11 | 2.00 | 0.43 |
| 1:F:165:GLU:O | 1:F:339:LYS:NZ | 2.50 | 0.43 |
| 1:A:292:ASN:CA | 4:F:520:HOH:O | 2.66 | 0.43 |
| 1:D:143:ILE:O | 1:D:147:ASN:ND2 | 2.37 | 0.43 |
| 1:C:134:VAL:HB | 4:C:610:HOH:O | 2.18 | 0.43 |
| 1:A:150:PRO:O | 1:A:151:ASN:HB2 | 2.19 | 0.42 |
| 1:A:312:ARG:NH2 | 1:C:98:MET:SD | 2.92 | 0.42 |
| 1:B:270:VAL:O | 1:B:270:VAL:HG22 | 2.18 | 0.42 |
| 1:C:193:GLN:HG3 | 4:C:553:HOH:O | 2.18 | 0.42 |
| 1:F:90:ASN:HD22 | 2:F:500:NAD:H72N | 1.65 | 0.42 |
| 1:F:91:THR:HG21 | 1:F:109:ILE:HD12 | 2.01 | 0.42 |
| 1:A:340:LYS:O | 1:A:341:ASP:HB2 | 2.19 | 0.42 |
| 1:D:234:ILE:HA | 1:D:234:ILE:HD12 | 1.85 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:54:GLU:O | 1:F:55:PRO:C | 2.58 | 0.42 |
| 1:F:213:THR:O | 1:F:216:SER:HB3 | 2.19 | 0.42 |
| 1:B:7:ILE:HG12 | 1:B:84:LEU:HD23 | 2.00 | 0.42 |
| 1:D:364:LEU:HA | 1:D:364:LEU:HD23 | 1.75 | 0.42 |
| 1:E:207:LYS:HD3 | 4:E:607:HOH:O | 2.19 | 0.42 |
| 1:E:43:ASN:O | 1:E:47:SER:HB3 | 2.20 | 0.42 |
| 1:E:129:LYS:HG3 | 1:E:159:ASN:O | 2.20 | 0.42 |
| 1:F:427:ARG:HA | 1:F:430:LYS:HD2 | 2.02 | 0.42 |
| 1:A:371:VAL:HA | 1:A:372:PRO:HD3 | 1.90 | 0.42 |
| 1:E:247:ASP:HA | 1:E:463:GLY:O | 2.20 | 0.42 |
| 1:A:15:VAL:O | 1:A:19:THR:OG1 | 2.29 | 0.42 |
| 1:F:90:ASN:CB | 2:F:500:NAD:H71N | 2.23 | 0.42 |
| 1:C:358:MET:HB3 | 1:C:390:GLN:NE2 | 2.35 | 0.42 |
| 1:A:358:MET:HG3 | 1:A:364:LEU:HD11 | 2.01 | 0.42 |
| 1:C:177:ARG:CZ | 1:D:258:ASP:HB2 | 2.49 | 0.42 |
| 1:D:30:ILE:O | 1:D:68:ASN:HB2 | 2.20 | 0.42 |
| 1:F:277:PHE:CE2 | 3:F:501:UDX:H5A1 | 2.55 | 0.42 |
| 1:F:91:THR:N | 2:F:500:NAD:H2N | 2.33 | 0.42 |
| 1:A:465:LYS:HB2 | 4:A:582:HOH:O | 2.20 | 0.41 |
| 1:B:128:GLU:HG3 | 1:B:136:ALA:HB1 | 2.02 | 0.41 |
| 1:C:124:LYS:HB2 | 1:C:154:LEU:HD23 | 2.01 | 0.41 |
| 1:D:161:GLU:O | 1:D:220:LYS:CE | 2.68 | 0.41 |
| 1:D:330:LYS:HG2 | 1:D:408:ALA:HA | 2.01 | 0.41 |
| 1:E:257:MET:O | 1:F:176:ASP:HB3 | 2.20 | 0.41 |
| 1:E:312:ARG:HH11 | 1:E:312:ARG:HG3 | 1.84 | 0.41 |
| 1:F:434:LYS:HA | 1:F:435:PRO:C | 2.39 | 0.41 |
| 1:A:289:GLU:HG2 | 4:A:783:HOH:O | 2.19 | 0.41 |
| 1:B:434:LYS:HA | 1:B:435:PRO:C | 2.40 | 0.41 |
| 1:C:329:LYS:HB3 | 1:C:409:HIS:CD2 | 2.55 | 0.41 |
| 1:E:141:ARG:NH2 | 1:E:213:THR:OG1 | 2.54 | 0.41 |
| 1:F:110:GLU:HG3 | 1:F:143:ILE:HD11 | 2.01 | 0.41 |
| 1:A:35:VAL:HA | 1:A:72:SER:O | 2.20 | 0.41 |
| 1:F:90:ASN:ND2 | 2:F:500:NAD:N7N | 2.67 | 0.41 |
| 1:C:91:THR:H | 2:C:500:NAD:C2N | 2.33 | 0.41 |
| 1:D:270:VAL:HG22 | 1:D:270:VAL:O | 2.20 | 0.41 |
| 1:E:124:LYS:HB2 | 1:E:154:LEU:HD23 | 2.02 | 0.41 |
| 1:F:114:ARG:HG3 | 1:F:143:ILE:HD13 | 2.02 | 0.41 |
| 1:F:279:LYS:HD2 | 2:F:500:NAD:C6N | 2.51 | 0.41 |
| 1:A:85:VAL:HG11 | 1:A:116:ILE:CD1 | 2.50 | 0.41 |
| 1:C:279:LYS:HD3 | 2:C:500:NAD:H5N | 2.03 | 0.41 |
| 1:C:277:PHE:CE2 | 3:C:501:UDX:H5A1 | 2.56 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:418:ASP:HB3 | 4:D:531:HOH:O | 2.20 | 0.41 |
| 1:F:322:LEU:HD23 | 1:F:437:PHE:CD1 | 2.55 | 0.41 |
| 1:E:320:ASP:CB | 4:E:513:HOH:O | 2.51 | 0.41 |
| 1:A:19:THR:O | 1:A:23:ILE:HG13 | 2.21 | 0.41 |
| 1:A:64:CYS:HB2 | 1:A:68:ASN:OD1 | 2.21 | 0.41 |
| 1:E:279:LYS:HZ3 | 1:E:279:LYS:HG3 | 1.63 | 0.41 |
| 1:A:112:CYS:O | 1:A:116:ILE:HG13 | 2.21 | 0.41 |
| 1:B:91:THR:OG1 | 1:B:279:LYS:NZ | 2.54 | 0.41 |
| 1:E:17:GLY:HA3 | 1:E:45:TRP:CZ2 | 2.56 | 0.41 |
| 1:E:180:ILE:O | 1:E:210:THR:HA | 2.20 | 0.41 |
| 1:E:249:GLU:OE2 | 1:E:267:LYS:HE2 | 2.20 | 0.40 |
| 1:D:28:PRO:HA | 1:D:68:ASN:ND2 | 2.35 | 0.40 |
| 1:A:29:GLU:CB | 4:A:587:HOH:O | 2.69 | 0.40 |
| 1:A:326:VAL:HA | 1:A:329:LYS:CD | 2.52 | 0.40 |
| 1:C:400:ASP:HB2 | 1:C:401:PRO:CD | 2.51 | 0.40 |
| 1:C:91:THR:H | 2:C:500:NAD:H2N | 1.86 | 0.40 |
| 1:E:11:GLY:HA3 | 1:E:88:SER:O | 2.21 | 0.40 |
| 1:D:42:ILE:HA | 1:D:42:ILE:HD13 | 1.93 | 0.40 |
| 1:F:279:LYS:HE2 | 2:F:500:NAD:C6N | 2.51 | 0.40 |
| 1:D:37:VAL:HG13 | 2:D:500:NAD:C2A | 2.51 | 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 | 454/494 (92%) | 428 (94%) | 26 (6%) | 0 | 100 | 100 |
| 1 | B | 453/494 (92%) | 434 (96%) | 19 (4%) | 0 | 100 | 100 |
| 1 | C | 453/494 (92%) | 428 (94%) | 23 (5%) | 2 (0%) | 34 | 54 |
| 1 | D | 453/494 (92%) | 426 (94%) | 25 (6%) | 2 (0%) | 34 | 54 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|-----|-----|
| 1 | E | 454/494 (92%) | 435 (96%) | 19 (4%) | 0 | 100 | 100 |
| 1 | F | 453/494 (92%) | 423 (93%) | 29 (6%) | 1 (0%) | 47 | 68 |
| All | All | 2720/2964 (92%) | 2574 (95%) | 141 (5%) | 5 (0%) | 47 | 68 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 327 | THR |
| 1 | C | 328 | ASP |
| 1 | D | 118 | GLN |
| 1 | D | 133 | PRO |
| 1 | F | 448 | LEU |

### 5.3.2   Protein sidechains (i)

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 | 393/426 (92%) | 387 (98%) | 6 (2%) | 65 | 85 |
| 1 | B | 392/426 (92%) | 384 (98%) | 8 (2%) | 55 | 79 |
| 1 | C | 392/426 (92%) | 379 (97%) | 13 (3%) | 38 | 64 |
| 1 | D | 392/426 (92%) | 370 (94%) | 22 (6%) | 21 | 40 |
| 1 | E | 393/426 (92%) | 384 (98%) | 9 (2%) | 50 | 76 |
| 1 | F | 392/426 (92%) | 368 (94%) | 24 (6%) | 18 | 36 |
| All | All | 2354/2556 (92%) | 2272 (96%) | 82 (4%) | 36 | 62 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 47 | SER |
| 1 | A | 117 | VAL |
| 1 | A | 174 | ASN |
| 1 | A | 177 | ARG |
| 1 | A | 267 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 450 | ASN |
| 1 | B | 81 | GLU |
| 1 | B | 96 | TYR |
| 1 | B | 142 | ARG |
| 1 | B | 177 | ARG |
| 1 | B | 320 | ASP |
| 1 | B | 392 | SER |
| 1 | B | 400 | ASP |
| 1 | B | 459 | ILE |
| 1 | C | 63 | SER |
| 1 | C | 118 | GLN |
| 1 | C | 142 | ARG |
| 1 | C | 163 | LEU |
| 1 | C | 177 | ARG |
| 1 | C | 193 | GLN |
| 1 | C | 267 | LYS |
| 1 | C | 319 | ILE |
| 1 | C | 327 | THR |
| 1 | C | 328 | ASP |
| 1 | C | 373 | ARG |
| 1 | C | 391 | VAL |
| 1 | C | 465 | LYS |
| 1 | D | 33 | THR |
| 1 | D | 72 | SER |
| 1 | D | 90 | ASN |
| 1 | D | 96 | TYR |
| 1 | D | 102 | ARG |
| 1 | D | 135 | ARG |
| 1 | D | 142 | ARG |
| 1 | D | 177 | ARG |
| 1 | D | 187 | GLU |
| 1 | D | 190 | ARG |
| 1 | D | 193 | GLN |
| 1 | D | 267 | LYS |
| 1 | D | 279 | LYS |
| 1 | D | 320 | ASP |
| 1 | D | 326 | VAL |
| 1 | D | 374 | GLU |
| 1 | D | 391 | VAL |
| 1 | D | 403 | GLU |
| 1 | D | 422 | GLU |
| 1 | D | 426 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
| --- | --- | --- | --- |
| 1 | D | 459 | ILE |
| 1 | D | 462 | ILE |
| 1 | E | 25 | HIS |
| 1 | E | 63 | SER |
| 1 | E | 118 | GLN |
| 1 | E | 142 | ARG |
| 1 | E | 177 | ARG |
| 1 | E | 279 | LYS |
| 1 | E | 312 | ARG |
| 1 | E | 326 | VAL |
| 1 | E | 373 | ARG |
| 1 | F | 5 | LYS |
| 1 | F | 33 | THR |
| 1 | F | 40 | SER |
| 1 | F | 41 | ARG |
| 1 | F | 64 | CYS |
| 1 | F | 81 | GLU |
| 1 | F | 117 | VAL |
| 1 | F | 132 | VAL |
| 1 | F | 148 | THR |
| 1 | F | 177 | ARG |
| 1 | F | 221 | LEU |
| 1 | F | 316 | SER |
| 1 | F | 317 | ARG |
| 1 | F | 355 | LYS |
| 1 | F | 365 | HIS |
| 1 | F | 392 | SER |
| 1 | F | 400 | ASP |
| 1 | F | 421 | LYS |
| 1 | F | 422 | GLU |
| 1 | F | 431 | LYS |
| 1 | F | 444 | VAL |
| 1 | F | 454 | THR |
| 1 | F | 459 | ILE |
| 1 | F | 465 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
| --- | --- | --- | --- |
| 1 | A | 363 | HIS |
| 1 | A | 453 | GLN |
| 1 | B | 324 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 429 | HIS |
| 1 | B | 458 | GLN |
| 1 | C | 301 | GLN |
| 1 | E | 278 | GLN |
| 1 | E | 301 | GLN |
| 1 | E | 302 | GLN |
| 1 | E | 409 | HIS |
| 1 | F | 229 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|----------|--------|------|----------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 3 | UDX | F | 501 | - | 29,36,36 | 1.28 | 3 (10%) | 38,55,55 | 1.62 | 6 (15%) |
| 2 | NAD | F | 500 | - | 42,48,48 | 2.57 | 8 (19%) | 50,73,73 | 2.35 | 15 (30%) |
| 3 | UDX | A | 501 | - | 29,36,36 | 1.74 | 6 (20%) | 38,55,55 | 1.69 | 8 (21%) |
| 3 | UDX | D | 501 | - | 29,36,36 | 1.37 | 2 (6%) | 38,55,55 | 1.70 | 7 (18%) |
| 2 | NAD | D | 500 | - | 42,48,48 | 2.42 | 8 (19%) | 50,73,73 | 1.99 | 11 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 3 | UDX | B | 501 | - | 29,36,36 | 1.59 | 5 (17%) | 38,55,55 | 1.33 | 4 (10%) |
| 2 | NAD | B | 500 | - | 42,48,48 | 3.18 | 9 (21%) | 50,73,73 | 3.14 | 18 (36%) |
| 2 | NAD | E | 500 | - | 42,48,48 | 3.02 | 8 (19%) | 50,73,73 | 2.19 | 12 (24%) |
| 3 | UDX | E | 501 | - | 29,36,36 | 1.75 | 4 (13%) | 38,55,55 | 1.51 | 7 (18%) |
| 2 | NAD | C | 500 | - | 42,48,48 | 2.37 | 9 (21%) | 50,73,73 | 2.00 | 16 (32%) |
| 3 | UDX | C | 501 | - | 29,36,36 | 1.49 | 4 (13%) | 38,55,55 | 1.23 | 5 (13%) |
| 2 | NAD | A | 500 | - | 42,48,48 | 2.58 | 8 (19%) | 50,73,73 | 2.70 | 16 (32%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | UDX | F | 501 | - | - | 2/19/54/54 | 0/3/3/3 |
| 2 | NAD | F | 500 | - | - | 11/26/62/62 | 0/5/5/5 |
| 3 | UDX | A | 501 | - | - | 5/19/54/54 | 0/3/3/3 |
| 3 | UDX | D | 501 | - | - | 1/19/54/54 | 0/3/3/3 |
| 2 | NAD | D | 500 | - | - | 5/26/62/62 | 0/5/5/5 |
| 3 | UDX | B | 501 | - | - | 2/19/54/54 | 0/3/3/3 |
| 2 | NAD | B | 500 | - | - | 10/26/62/62 | 0/5/5/5 |
| 2 | NAD | E | 500 | - | - | 7/26/62/62 | 0/5/5/5 |
| 3 | UDX | E | 501 | - | - | 4/19/54/54 | 0/3/3/3 |
| 2 | NAD | C | 500 | - | - | 8/26/62/62 | 0/5/5/5 |
| 3 | UDX | C | 501 | - | - | 4/19/54/54 | 0/3/3/3 |
| 2 | NAD | A | 500 | - | - | 7/26/62/62 | 0/5/5/5 |

All (74) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | E | 500 | NAD | O4D-C1D | 12.27 | 1.58 | 1.41 |
| 2 | B | 500 | NAD | C2N-N1N | 10.66 | 1.47 | 1.35 |
| 2 | E | 500 | NAD | C4N-C3N | 10.43 | 1.57 | 1.39 |
| 2 | B | 500 | NAD | C4N-C3N | 10.34 | 1.57 | 1.39 |
| 2 | A | 500 | NAD | C4N-C3N | 9.60 | 1.55 | 1.39 |
| 2 | C | 500 | NAD | C4N-C3N | 9.04 | 1.54 | 1.39 |
| 2 | D | 500 | NAD | C4N-C3N | 8.90 | 1.54 | 1.39 |
| 2 | F | 500 | NAD | C4N-C3N | 8.88 | 1.54 | 1.39 |

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | A | 500 | NAD | C2N-N1N | 8.30 | 1.45 | 1.35 |
| 2 | D | 500 | NAD | C2N-N1N | 8.21 | 1.45 | 1.35 |
| 2 | F | 500 | NAD | C2N-N1N | 8.02 | 1.44 | 1.35 |
| 2 | E | 500 | NAD | C2N-N1N | 7.84 | 1.44 | 1.35 |
| 2 | B | 500 | NAD | C3N-C7N | 7.76 | 1.62 | 1.50 |
| 2 | F | 500 | NAD | O4D-C1D | 7.04 | 1.50 | 1.41 |
| 2 | C | 500 | NAD | C2N-N1N | 6.99 | 1.43 | 1.35 |
| 2 | B | 500 | NAD | O4D-C1D | 6.98 | 1.50 | 1.41 |
| 2 | A | 500 | NAD | O4D-C1D | 5.60 | 1.48 | 1.41 |
| 3 | A | 501 | UDX | C6-N1 | 5.40 | 1.42 | 1.35 |
| 2 | D | 500 | NAD | O4D-C1D | 5.37 | 1.48 | 1.41 |
| 3 | E | 501 | UDX | C6-N1 | 4.99 | 1.42 | 1.35 |
| 2 | C | 500 | NAD | C3N-C7N | 4.72 | 1.57 | 1.50 |
| 2 | B | 500 | NAD | C2N-C3N | 4.71 | 1.46 | 1.39 |
| 3 | E | 501 | UDX | C4-N3 | 4.69 | 1.41 | 1.33 |
| 2 | F | 500 | NAD | C3N-C7N | 4.38 | 1.57 | 1.50 |
| 3 | D | 501 | UDX | C4-N3 | 4.25 | 1.40 | 1.33 |
| 2 | C | 500 | NAD | O4D-C1D | 4.09 | 1.46 | 1.41 |
| 3 | F | 501 | UDX | O4D-C1D | 4.02 | 1.46 | 1.41 |
| 3 | B | 501 | UDX | O4D-C4D | 3.93 | 1.53 | 1.45 |
| 3 | C | 501 | UDX | C4-N3 | 3.90 | 1.39 | 1.33 |
| 2 | F | 500 | NAD | C2N-C3N | 3.87 | 1.45 | 1.39 |
| 2 | E | 500 | NAD | C6N-N1N | 3.84 | 1.44 | 1.35 |
| 2 | A | 500 | NAD | C6N-N1N | 3.81 | 1.44 | 1.35 |
| 2 | B | 500 | NAD | C6N-N1N | 3.77 | 1.44 | 1.35 |
| 2 | D | 500 | NAD | C3N-C7N | 3.57 | 1.55 | 1.50 |
| 3 | C | 501 | UDX | O4D-C1D | 3.57 | 1.46 | 1.41 |
| 2 | A | 500 | NAD | C3N-C7N | 3.56 | 1.55 | 1.50 |
| 3 | A | 501 | UDX | C4-N3 | 3.54 | 1.39 | 1.33 |
| 3 | A | 501 | UDX | O4D-C1D | 3.47 | 1.45 | 1.41 |
| 2 | B | 500 | NAD | O4D-C4D | 3.45 | 1.52 | 1.45 |
| 2 | A | 500 | NAD | C2N-C3N | 3.42 | 1.44 | 1.39 |
| 2 | D | 500 | NAD | PN-O1N | 3.42 | 1.63 | 1.50 |
| 3 | B | 501 | UDX | O4D-C1D | 3.37 | 1.45 | 1.41 |
| 3 | B | 501 | UDX | C6-N1 | 3.35 | 1.40 | 1.35 |
| 2 | C | 500 | NAD | O2D-C2D | 3.33 | 1.50 | 1.43 |
| 2 | C | 500 | NAD | C2N-C3N | 3.25 | 1.44 | 1.39 |
| 3 | E | 501 | UDX | O4D-C1D | 3.25 | 1.45 | 1.41 |
| 3 | E | 501 | UDX | O5'-C5' | 3.22 | 1.48 | 1.43 |
| 3 | C | 501 | UDX | C6-N1 | 3.20 | 1.39 | 1.35 |
| 2 | F | 500 | NAD | PN-O1N | 3.17 | 1.62 | 1.50 |
| 2 | C | 500 | NAD | C2D-C3D | 3.05 | 1.61 | 1.53 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | F | 500 | NAD | C2D-C3D | 3.02 | 1.61 | 1.53 |
| 2 | B | 500 | NAD | C2D-C1D | 2.97 | 1.58 | 1.53 |
| 2 | A | 500 | NAD | O4B-C1B | 2.91 | 1.45 | 1.41 |
| 2 | D | 500 | NAD | O4B-C1B | 2.89 | 1.45 | 1.41 |
| 3 | F | 501 | UDX | C6-N1 | 2.82 | 1.39 | 1.35 |
| 2 | C | 500 | NAD | PN-O1N | 2.79 | 1.60 | 1.50 |
| 3 | A | 501 | UDX | C4'-C3' | 2.65 | 1.56 | 1.52 |
| 2 | E | 500 | NAD | C3N-C7N | 2.61 | 1.54 | 1.50 |
| 3 | C | 501 | UDX | O5'-C5' | 2.61 | 1.47 | 1.43 |
| 2 | B | 500 | NAD | PN-O1N | 2.54 | 1.59 | 1.50 |
| 3 | A | 501 | UDX | O4D-C4D | 2.54 | 1.50 | 1.45 |
| 3 | B | 501 | UDX | O5'-C5' | -2.50 | 1.39 | 1.43 |
| 2 | D | 500 | NAD | C6N-N1N | 2.49 | 1.41 | 1.35 |
| 2 | D | 500 | NAD | C2N-C3N | 2.48 | 1.42 | 1.39 |
| 3 | A | 501 | UDX | O5'-C1' | 2.48 | 1.47 | 1.41 |
| 3 | D | 501 | UDX | C6-N1 | 2.40 | 1.38 | 1.35 |
| 2 | C | 500 | NAD | O4B-C1B | 2.29 | 1.44 | 1.41 |
| 2 | E | 500 | NAD | C2B-C1B | -2.25 | 1.50 | 1.53 |
| 3 | F | 501 | UDX | O2D-C2D | 2.24 | 1.48 | 1.43 |
| 3 | B | 501 | UDX | C4-N3 | 2.24 | 1.36 | 1.33 |
| 2 | A | 500 | NAD | C2B-C1B | -2.24 | 1.50 | 1.53 |
| 2 | E | 500 | NAD | C6N-C5N | 2.13 | 1.43 | 1.38 |
| 2 | E | 500 | NAD | C2N-C3N | 2.05 | 1.42 | 1.39 |
| 2 | F | 500 | NAD | C6N-N1N | 2.01 | 1.40 | 1.35 |

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | B | 500 | NAD | C6N-N1N-C2N | -10.72 | 112.20 | 121.97 |
| 2 | B | 500 | NAD | O4D-C1D-C2D | -8.59 | 94.38 | 106.93 |
| 2 | E | 500 | NAD | C6N-N1N-C2N | -8.37 | 114.34 | 121.97 |
| 2 | A | 500 | NAD | C6N-N1N-C2N | -7.81 | 114.86 | 121.97 |
| 2 | F | 500 | NAD | C5N-C4N-C3N | -7.16 | 111.88 | 120.34 |
| 2 | E | 500 | NAD | C5N-C4N-C3N | -6.77 | 112.33 | 120.34 |
| 3 | F | 501 | UDX | O5'-C1'-O3B | -6.73 | 102.57 | 111.36 |
| 2 | B | 500 | NAD | C5D-C4D-C3D | -6.65 | 90.27 | 115.18 |
| 3 | D | 501 | UDX | O5'-C1'-O3B | -6.48 | 102.90 | 111.36 |
| 2 | F | 500 | NAD | C6N-N1N-C2N | -6.40 | 116.14 | 121.97 |
| 2 | C | 500 | NAD | C5N-C4N-C3N | -6.22 | 112.98 | 120.34 |
| 2 | A | 500 | NAD | C2N-N1N-C1D | 6.12 | 132.76 | 119.14 |
| 2 | B | 500 | NAD | C2N-N1N-C1D | 5.89 | 132.25 | 119.14 |
| 2 | A | 500 | NAD | C5N-C4N-C3N | -5.79 | 113.49 | 120.34 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 2 | D | 500 | NAD | C5N-C4N-C3N | -5.73 | 113.57 | 120.34 |
| 2 | A | 500 | NAD | C5D-C4D-C3D | -5.51 | 94.54 | 115.18 |
| 2 | D | 500 | NAD | C6N-N1N-C2N | -5.13 | 117.30 | 121.97 |
| 2 | B | 500 | NAD | C5N-C4N-C3N | -5.06 | 114.35 | 120.34 |
| 2 | B | 500 | NAD | N3A-C2A-N1A | -4.86 | 121.08 | 128.68 |
| 2 | A | 500 | NAD | C2N-C3N-C4N | 4.74 | 123.64 | 118.26 |
| 2 | F | 500 | NAD | C2N-N1N-C1D | 4.74 | 129.70 | 119.14 |
| 2 | A | 500 | NAD | O4D-C1D-C2D | -4.61 | 100.19 | 106.93 |
| 2 | B | 500 | NAD | C5N-C6N-N1N | 4.61 | 127.01 | 120.40 |
| 2 | C | 500 | NAD | N3A-C2A-N1A | -4.54 | 121.58 | 128.68 |
| 2 | A | 500 | NAD | C3D-C2D-C1D | 4.53 | 107.80 | 100.98 |
| 2 | F | 500 | NAD | N3A-C2A-N1A | -4.52 | 121.62 | 128.68 |
| 2 | F | 500 | NAD | C6N-C5N-C4N | 4.51 | 125.99 | 119.44 |
| 2 | A | 500 | NAD | C5N-C6N-N1N | 4.49 | 126.84 | 120.40 |
| 2 | D | 500 | NAD | N3A-C2A-N1A | -4.47 | 121.70 | 128.68 |
| 2 | E | 500 | NAD | O4D-C1D-C2D | -4.45 | 100.42 | 106.93 |
| 3 | A | 501 | UDX | C5'-O5'-C1' | 4.44 | 121.35 | 112.38 |
| 2 | A | 500 | NAD | O3D-C3D-C4D | -4.39 | 98.36 | 111.05 |
| 2 | F | 500 | NAD | C5D-C4D-C3D | -4.32 | 99.01 | 115.18 |
| 2 | B | 500 | NAD | C3D-C2D-C1D | 4.21 | 107.32 | 100.98 |
| 2 | B | 500 | NAD | O4D-C4D-C5D | 4.19 | 123.16 | 109.37 |
| 2 | B | 500 | NAD | C5B-C4B-C3B | -4.17 | 99.55 | 115.18 |
| 2 | D | 500 | NAD | O4D-C1D-C2D | -4.14 | 100.88 | 106.93 |
| 2 | A | 500 | NAD | O4B-C1B-C2B | -4.03 | 101.03 | 106.93 |
| 3 | B | 501 | UDX | PA-O3A-PB | -4.03 | 118.99 | 132.83 |
| 2 | C | 500 | NAD | C2N-N1N-C1D | 3.95 | 127.94 | 119.14 |
| 2 | C | 500 | NAD | C6N-C5N-C4N | 3.95 | 125.18 | 119.44 |
| 3 | E | 501 | UDX | O3A-PB-O3B | 3.88 | 110.30 | 102.48 |
| 2 | E | 500 | NAD | C2N-C3N-C4N | 3.86 | 122.63 | 118.26 |
| 2 | B | 500 | NAD | O7N-C7N-C3N | 3.83 | 124.22 | 119.63 |
| 3 | E | 501 | UDX | O5'-C1'-C2' | -3.72 | 104.33 | 110.04 |
| 2 | D | 500 | NAD | C6N-C5N-C4N | 3.65 | 124.74 | 119.44 |
| 2 | A | 500 | NAD | N3A-C2A-N1A | -3.64 | 122.98 | 128.68 |
| 2 | C | 500 | NAD | C4N-C3N-C7N | -3.63 | 111.32 | 121.04 |
| 3 | E | 501 | UDX | O5'-C5'-C4' | -3.59 | 105.22 | 110.77 |
| 2 | C | 500 | NAD | O4B-C1B-C2B | -3.57 | 101.71 | 106.93 |
| 2 | D | 500 | NAD | PN-O3-PA | -3.54 | 120.68 | 132.83 |
| 2 | F | 500 | NAD | C4N-C3N-C7N | -3.54 | 111.57 | 121.04 |
| 2 | B | 500 | NAD | O7N-C7N-N7N | -3.51 | 117.59 | 122.58 |
| 2 | F | 500 | NAD | O4D-C1D-C2D | -3.41 | 101.94 | 106.93 |
| 2 | E | 500 | NAD | N3A-C2A-N1A | -3.39 | 123.38 | 128.68 |
| 2 | E | 500 | NAD | C5N-C6N-N1N | 3.36 | 125.22 | 120.40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 2 | C | 500 | NAD | C5D-C4D-C3D | -3.36 | 102.61 | 115.18 |
| 2 | B | 500 | NAD | C3N-C2N-N1N | 3.34 | 123.69 | 120.43 |
| 3 | A | 501 | UDX | O4D-C1D-C2D | -3.33 | 102.05 | 106.93 |
| 3 | D | 501 | UDX | O5'-C5'-C4' | -3.32 | 105.64 | 110.77 |
| 3 | A | 501 | UDX | O4'-C4'-C5' | -3.28 | 102.44 | 109.15 |
| 2 | E | 500 | NAD | O4B-C1B-C2B | -3.28 | 102.14 | 106.93 |
| 3 | C | 501 | UDX | O5'-C1'-O3B | -3.26 | 107.11 | 111.36 |
| 2 | A | 500 | NAD | PN-O3-PA | -3.20 | 121.85 | 132.83 |
| 2 | A | 500 | NAD | C4N-C3N-C7N | -3.16 | 112.59 | 121.04 |
| 3 | B | 501 | UDX | O5'-C1'-O3B | -3.11 | 107.30 | 111.36 |
| 3 | D | 501 | UDX | O3D-C3D-C4D | -3.07 | 102.16 | 111.05 |
| 3 | A | 501 | UDX | O5'-C1'-C2' | 3.07 | 114.76 | 110.04 |
| 3 | B | 501 | UDX | O3A-PB-O3B | 3.06 | 108.65 | 102.48 |
| 2 | F | 500 | NAD | O4D-C4D-C5D | 3.05 | 119.40 | 109.37 |
| 3 | B | 501 | UDX | O5'-C5'-C4' | 2.98 | 115.36 | 110.77 |
| 2 | D | 500 | NAD | C2N-N1N-C1D | 2.97 | 125.75 | 119.14 |
| 3 | A | 501 | UDX | O5'-C5'-C4' | -2.97 | 106.19 | 110.77 |
| 2 | C | 500 | NAD | C2N-C3N-C7N | 2.94 | 128.01 | 119.46 |
| 3 | A | 501 | UDX | PA-O3A-PB | -2.78 | 123.28 | 132.83 |
| 3 | A | 501 | UDX | O3A-PB-O3B | 2.77 | 108.07 | 102.48 |
| 2 | B | 500 | NAD | O3D-C3D-C4D | -2.76 | 103.06 | 111.05 |
| 2 | E | 500 | NAD | C6N-C5N-C4N | 2.69 | 123.34 | 119.44 |
| 2 | F | 500 | NAD | C2N-C3N-C7N | 2.65 | 127.17 | 119.46 |
| 2 | F | 500 | NAD | C2N-C3N-C4N | 2.64 | 121.25 | 118.26 |
| 2 | D | 500 | NAD | O4B-C1B-C2B | -2.64 | 103.07 | 106.93 |
| 2 | F | 500 | NAD | C3D-C2D-C1D | 2.63 | 104.94 | 100.98 |
| 2 | B | 500 | NAD | C6N-C5N-C4N | 2.61 | 123.24 | 119.44 |
| 2 | C | 500 | NAD | C3D-C2D-C1D | 2.49 | 104.73 | 100.98 |
| 2 | C | 500 | NAD | C6N-N1N-C2N | -2.48 | 119.72 | 121.97 |
| 3 | F | 501 | UDX | O3D-C3D-C4D | -2.46 | 103.94 | 111.05 |
| 3 | D | 501 | UDX | O5'-C1'-C2' | 2.45 | 113.80 | 110.04 |
| 3 | E | 501 | UDX | PA-O3A-PB | -2.41 | 124.57 | 132.83 |
| 3 | C | 501 | UDX | C5'-C4'-C3' | 2.40 | 112.61 | 109.67 |
| 2 | E | 500 | NAD | C5B-C4B-C3B | -2.39 | 106.22 | 115.18 |
| 2 | B | 500 | NAD | C1B-N9A-C4A | -2.39 | 122.44 | 126.64 |
| 3 | F | 501 | UDX | O3B-PB-O1B | 2.39 | 118.42 | 109.47 |
| 3 | C | 501 | UDX | O4'-C4'-C3' | -2.38 | 105.36 | 110.14 |
| 2 | A | 500 | NAD | O2D-C2D-C3D | -2.30 | 104.40 | 111.82 |
| 3 | C | 501 | UDX | O5'-C1'-C2' | 2.28 | 113.54 | 110.04 |
| 2 | D | 500 | NAD | C2N-C3N-C4N | 2.27 | 120.83 | 118.26 |
| 2 | F | 500 | NAD | O3D-C3D-C2D | 2.25 | 119.08 | 111.82 |
| 3 | E | 501 | UDX | O4D-C1D-C2D | -2.23 | 103.66 | 106.93 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | D | 500 | NAD | C4A-C5A-N7A | -2.21 | 107.09 | 109.40 |
| 2 | C | 500 | NAD | O2A-PA-O1A | -2.21 | 101.31 | 112.24 |
| 3 | F | 501 | UDX | O3B-C1'-C2' | 2.21 | 112.42 | 108.38 |
| 2 | A | 500 | NAD | PN-O5D-C5D | -2.20 | 108.76 | 121.68 |
| 2 | C | 500 | NAD | PN-O3-PA | -2.20 | 125.27 | 132.83 |
| 3 | E | 501 | UDX | C5'-O5'-C1' | 2.20 | 116.82 | 112.38 |
| 3 | F | 501 | UDX | PA-O3A-PB | -2.18 | 125.35 | 132.83 |
| 2 | E | 500 | NAD | C2N-N1N-C1D | 2.18 | 123.98 | 119.14 |
| 3 | C | 501 | UDX | O3A-PB-O3B | 2.17 | 106.85 | 102.48 |
| 3 | D | 501 | UDX | C4'-C3'-C2' | -2.16 | 107.16 | 110.89 |
| 3 | E | 501 | UDX | O3B-C1'-C2' | 2.15 | 112.32 | 108.38 |
| 2 | C | 500 | NAD | C2N-C3N-C4N | 2.13 | 120.67 | 118.26 |
| 2 | E | 500 | NAD | C4A-C5A-N7A | -2.12 | 107.19 | 109.40 |
| 2 | C | 500 | NAD | O2D-C2D-C3D | 2.12 | 118.67 | 111.82 |
| 3 | D | 501 | UDX | O4'-C4'-C3' | 2.11 | 114.36 | 110.14 |
| 2 | D | 500 | NAD | C3D-C2D-C1D | -2.10 | 97.82 | 100.98 |
| 2 | E | 500 | NAD | C1B-N9A-C4A | -2.10 | 122.96 | 126.64 |
| 2 | B | 500 | NAD | O2N-PN-O5D | 2.09 | 117.47 | 107.75 |
| 2 | F | 500 | NAD | O3D-C3D-C4D | -2.09 | 105.00 | 111.05 |
| 2 | F | 500 | NAD | C5N-C6N-N1N | 2.07 | 123.38 | 120.40 |
| 2 | A | 500 | NAD | O4D-C4D-C5D | 2.06 | 116.16 | 109.37 |
| 3 | D | 501 | UDX | O3A-PB-O3B | 2.05 | 106.62 | 102.48 |
| 2 | B | 500 | NAD | O5D-C5D-C4D | 2.05 | 116.05 | 108.99 |
| 3 | A | 501 | UDX | C5D-C4D-C3D | -2.03 | 107.58 | 115.18 |
| 2 | C | 500 | NAD | C4A-C5A-N7A | -2.03 | 107.29 | 109.40 |
| 3 | F | 501 | UDX | C6-N1-C2 | -2.02 | 118.00 | 121.20 |
| 2 | C | 500 | NAD | O4D-C4D-C5D | 2.01 | 115.98 | 109.37 |

There are no chirality outliers.

All (66) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | F | 500 | NAD | C5D-O5D-PN-O1N |
| 2 | F | 500 | NAD | C5D-O5D-PN-O2N |
| 2 | F | 500 | NAD | C2D-C1D-N1N-C2N |
| 2 | F | 500 | NAD | C2D-C1D-N1N-C6N |
| 3 | A | 501 | UDX | PA-O3A-PB-O3B |
| 3 | A | 501 | UDX | C2D-C1D-N1-C6 |
| 2 | D | 500 | NAD | O4D-C1D-N1N-C2N |
| 2 | D | 500 | NAD | O4D-C1D-N1N-C6N |
| 2 | D | 500 | NAD | C2D-C1D-N1N-C2N |
| 2 | D | 500 | NAD | C2D-C1D-N1N-C6N |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | B | 500 | NAD | O4D-C1D-N1N-C2N |
| 2 | B | 500 | NAD | O4D-C1D-N1N-C6N |
| 2 | B | 500 | NAD | C2D-C1D-N1N-C2N |
| 2 | B | 500 | NAD | C2D-C1D-N1N-C6N |
| 2 | E | 500 | NAD | C5D-O5D-PN-O3 |
| 2 | E | 500 | NAD | O4D-C1D-N1N-C2N |
| 3 | E | 501 | UDX | C2D-C1D-N1-C6 |
| 2 | C | 500 | NAD | C5D-O5D-PN-O1N |
| 2 | C | 500 | NAD | O4D-C4D-C5D-O5D |
| 2 | C | 500 | NAD | O4D-C1D-N1N-C6N |
| 2 | C | 500 | NAD | C2D-C1D-N1N-C6N |
| 2 | A | 500 | NAD | O4D-C1D-N1N-C2N |
| 2 | A | 500 | NAD | O4D-C1D-N1N-C6N |
| 2 | A | 500 | NAD | C2D-C1D-N1N-C6N |
| 2 | F | 500 | NAD | O4D-C4D-C5D-O5D |
| 2 | B | 500 | NAD | O4D-C4D-C5D-O5D |
| 2 | F | 500 | NAD | C3D-C4D-C5D-O5D |
| 2 | B | 500 | NAD | C3B-C4B-C5B-O5B |
| 3 | A | 501 | UDX | C1'-O3B-PB-O3A |
| 2 | E | 500 | NAD | O4D-C4D-C5D-O5D |
| 3 | D | 501 | UDX | C1'-O3B-PB-O3A |
| 3 | B | 501 | UDX | C1'-O3B-PB-O3A |
| 3 | C | 501 | UDX | C1'-O3B-PB-O3A |
| 2 | B | 500 | NAD | O4B-C4B-C5B-O5B |
| 2 | E | 500 | NAD | C3D-C4D-C5D-O5D |
| 3 | F | 501 | UDX | C1'-O3B-PB-O3A |
| 3 | E | 501 | UDX | C1'-O3B-PB-O3A |
| 2 | F | 500 | NAD | PN-O3-PA-O5B |
| 3 | E | 501 | UDX | PA-O3A-PB-O3B |
| 3 | C | 501 | UDX | PA-O3A-PB-O3B |
| 2 | A | 500 | NAD | PN-O3-PA-O5B |
| 2 | A | 500 | NAD | O4D-C4D-C5D-O5D |
| 2 | F | 500 | NAD | C5D-O5D-PN-O3 |
| 2 | C | 500 | NAD | C5D-O5D-PN-O3 |
| 3 | A | 501 | UDX | PB-O3A-PA-O2A |
| 2 | B | 500 | NAD | C5D-O5D-PN-O1N |
| 2 | B | 500 | NAD | C5D-O5D-PN-O2N |
| 2 | E | 500 | NAD | C5D-O5D-PN-O1N |
| 2 | E | 500 | NAD | C5D-O5D-PN-O2N |
| 2 | C | 500 | NAD | C5D-O5D-PN-O2N |
| 2 | F | 500 | NAD | O4B-C4B-C5B-O5B |
| 2 | F | 500 | NAD | PA-O3-PN-O2N |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | B | 500 | NAD | C3D-C4D-C5D-O5D |
| 3 | A | 501 | UDX | PB-O3A-PA-O1A |
| 3 | B | 501 | UDX | PB-O3A-PA-O1A |
| 3 | E | 501 | UDX | PB-O3A-PA-O1A |
| 3 | C | 501 | UDX | PB-O3A-PA-O1A |
| 2 | C | 500 | NAD | C2D-C1D-N1N-C2N |
| 2 | A | 500 | NAD | C2D-C1D-N1N-C2N |
| 2 | D | 500 | NAD | O4B-C4B-C5B-O5B |
| 2 | C | 500 | NAD | O4B-C4B-C5B-O5B |
| 2 | A | 500 | NAD | O4B-C4B-C5B-O5B |
| 2 | F | 500 | NAD | PA-O3-PN-O1N |
| 3 | F | 501 | UDX | C5D-O5D-PA-O1A |
| 3 | C | 501 | UDX | C5D-O5D-PA-O1A |
| 2 | E | 500 | NAD | O4B-C4B-C5B-O5B |

There are no ring outliers.

9 monomers are involved in 81 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | F | 501 | UDX | 1 | 0 |
| 2 | F | 500 | NAD | 14 | 0 |
| 3 | D | 501 | UDX | 1 | 0 |
| 2 | D | 500 | NAD | 10 | 0 |
| 2 | B | 500 | NAD | 18 | 0 |
| 2 | E | 500 | NAD | 11 | 0 |
| 2 | C | 500 | NAD | 13 | 0 |
| 3 | C | 501 | UDX | 1 | 0 |
| 2 | A | 500 | NAD | 12 | 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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand UDX F 501**


Bond lengths


Bond angles


Torsions


Rings

**Ligand NAD F 500**


Bond lengths


Bond angles


Torsions


Rings

## Ligand UDX A 501


Bond lengths


Bond angles


Torsions


Rings

## Ligand UDX D 501


Bond lengths


Bond angles


Torsions


Rings

## Ligand NAD D 500



Bond lengths



Bond angles



Torsions



Rings

## Ligand UDX B 501



Bond lengths



Bond angles



Torsions



Rings

## Ligand NAD B 500



Bond lengths



Bond angles



Torsions



Rings

**Ligand NAD E 500**



Bond lengths



Bond angles



Torsions



Rings

**Ligand UDX E 501**



Bond lengths



Bond angles



Torsions



Rings

**Ligand NAD C 500**


Bond lengths


Bond angles


Torsions


Rings

**Ligand UDX C 501**


Bond lengths


Bond angles


Torsions


Rings

**Ligand NAD A 500**



Bond lengths

Bond angles

Torsions

Rings

## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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$^{th}$ 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$^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|-------------|-------|
| 1 | A | 458/494 (92%) | -0.51 | 0 | 100 | 100 | 14, 23, 39, 53 | 0 |
| 1 | B | 457/494 (92%) | -0.45 | 0 | 100 | 100 | 14, 27, 41, 51 | 0 |
| 1 | C | 457/494 (92%) | -0.23 | 9 (1%) | 65 | 68 | 19, 30, 58, 68 | 0 |
| 1 | D | 457/494 (92%) | -0.27 | 4 (0%) | 84 | 86 | 20, 38, 53, 66 | 0 |
| 1 | E | 458/494 (92%) | -0.39 | 2 (0%) | 92 | 93 | 15, 26, 43, 60 | 0 |
| 1 | F | 457/494 (92%) | -0.03 | 14 (3%) | 49 | 52 | 18, 32, 54, 62 | 0 |
| All | All | 2744/2964 (92%) | -0.31 | 29 (1%) | 80 | 82 | 14, 29, 52, 68 | 0 |

All (29) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 98 | MET | 3.7 |
| 1 | C | 389 | ASP | 3.5 |
| 1 | F | 447 | GLY | 3.4 |
| 1 | D | 96 | TYR | 3.3 |
| 1 | F | 410 | ALA | 3.2 |
| 1 | C | 327 | THR | 3.0 |
| 1 | E | 98 | MET | 2.9 |
| 1 | F | 326 | VAL | 2.7 |
| 1 | C | 436 | ALA | 2.7 |
| 1 | F | 323 | PHE | 2.6 |
| 1 | C | 356 | TYR | 2.6 |
| 1 | D | 66 | GLY | 2.3 |
| 1 | C | 408 | ALA | 2.2 |
| 1 | F | 436 | ALA | 2.2 |
| 1 | F | 325 | THR | 2.2 |
| 1 | F | 322 | LEU | 2.2 |
| 1 | F | 433 | LEU | 2.2 |
| 1 | F | 409 | HIS | 2.2 |
| 1 | F | 437 | PHE | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 425 | TYR | 2.1 |
| 1 | C | 319 | ILE | 2.1 |
| 1 | E | 96 | TYR | 2.1 |
| 1 | F | 364 | LEU | 2.1 |
| 1 | C | 330 | LYS | 2.1 |
| 1 | F | 151 | ASN | 2.1 |
| 1 | F | 328 | ASP | 2.1 |
| 1 | D | 77 | ASP | 2.0 |
| 1 | C | 326 | VAL | 2.0 |
| 1 | C | 404 | ALA | 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 carbohydrates 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, $95^{th}$ 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$^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------------------|-------|
| 2 | NAD | D | 500 | 44/44 | 0.95 | 0.17 | 33,40,77,79 | 0 |
| 2 | NAD | C | 500 | 44/44 | 0.95 | 0.18 | 23,32,69,71 | 0 |
| 2 | NAD | E | 500 | 44/44 | 0.96 | 0.16 | 19,29,73,78 | 0 |
| 2 | NAD | F | 500 | 44/44 | 0.96 | 0.17 | 23,32,70,72 | 0 |
| 2 | NAD | B | 500 | 44/44 | 0.97 | 0.16 | 18,28,58,60 | 0 |
| 2 | NAD | A | 500 | 44/44 | 0.97 | 0.15 | 14,21,66,68 | 0 |
| 3 | UDX | F | 501 | 34/34 | 0.98 | 0.15 | 17,23,26,29 | 0 |
| 3 | UDX | B | 501 | 34/34 | 0.98 | 0.11 | 11,16,19,22 | 0 |
| 3 | UDX | C | 501 | 34/34 | 0.98 | 0.11 | 18,23,27,31 | 0 |
| 3 | UDX | D | 501 | 34/34 | 0.98 | 0.12 | 20,28,32,37 | 0 |
| 3 | UDX | E | 501 | 34/34 | 0.99 | 0.14 | 11,16,18,19 | 0 |
| 3 | UDX | A | 501 | 34/34 | 0.99 | 0.11 | 6,11,15,17 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
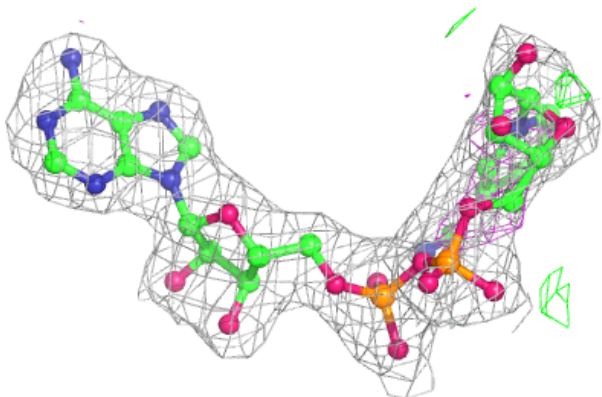
**Electron density around NAD D 500:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
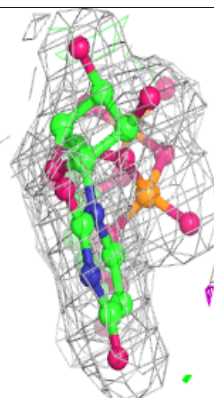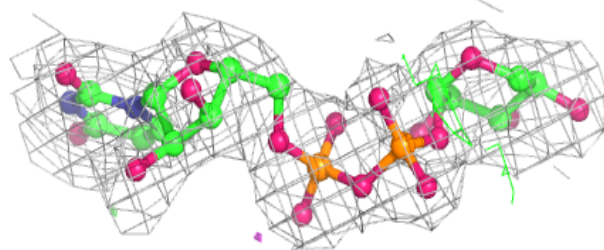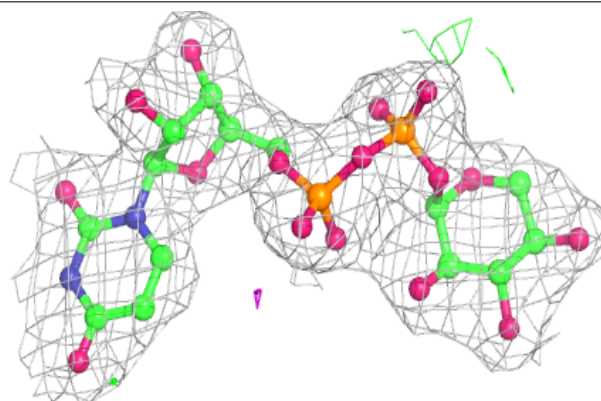$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
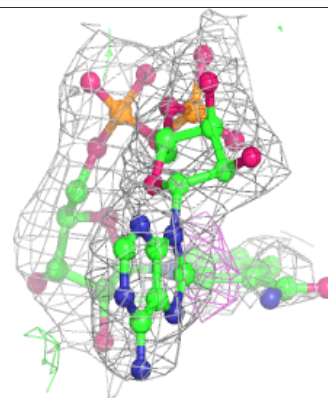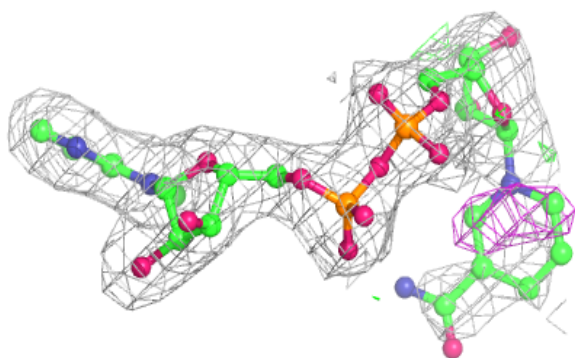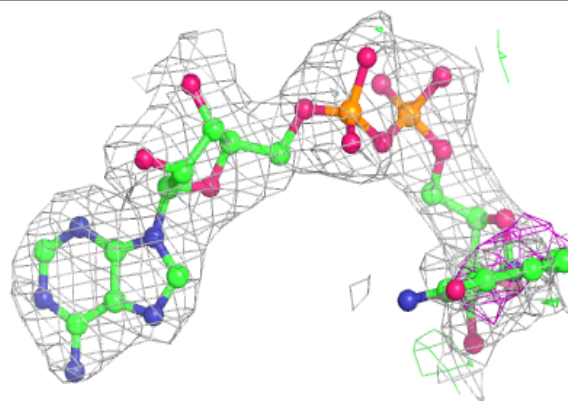
**Electron density around NAD C 500:**

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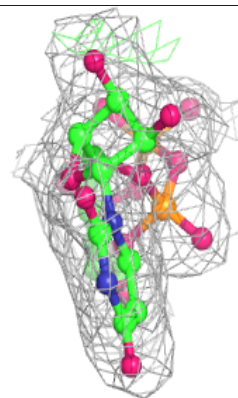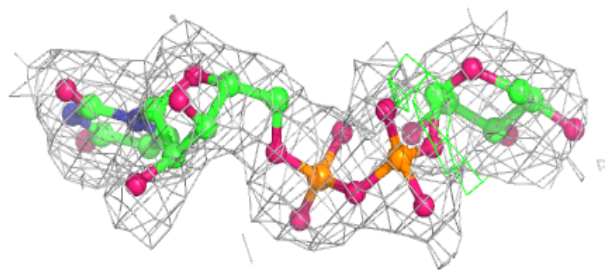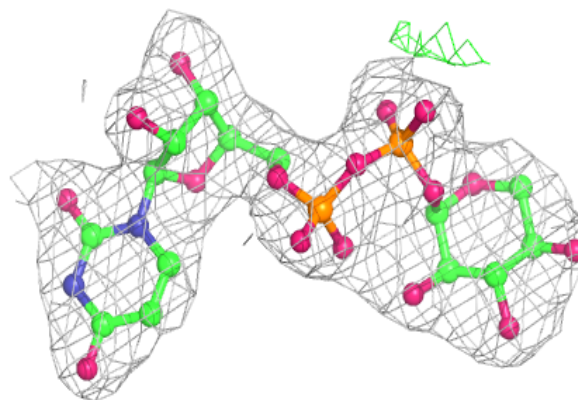$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
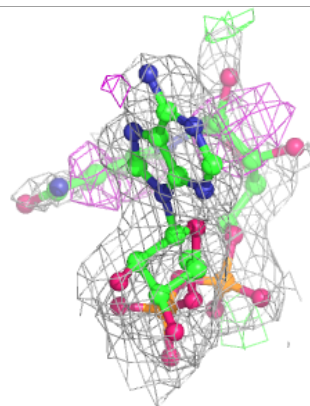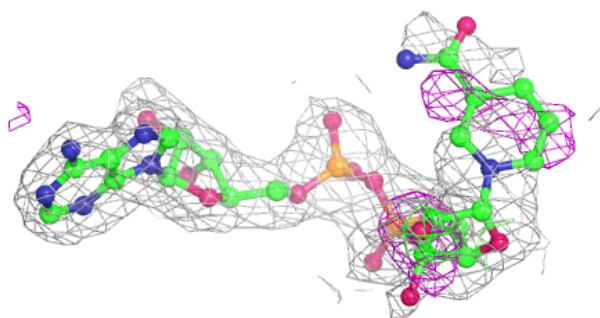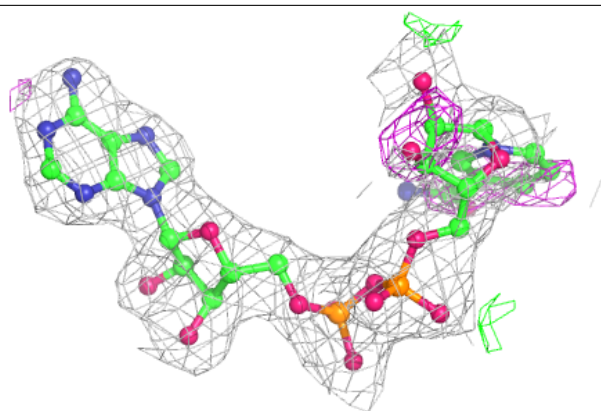


**Electron density around NAD E 500:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
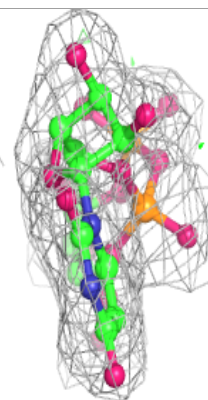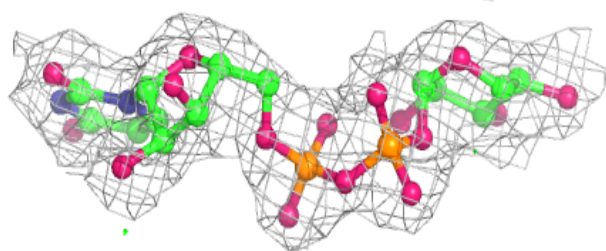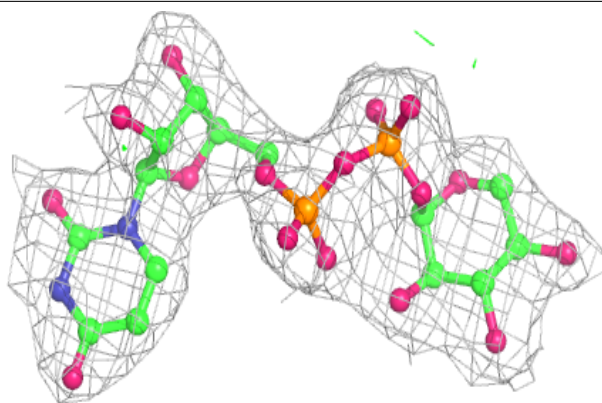and green (positive)
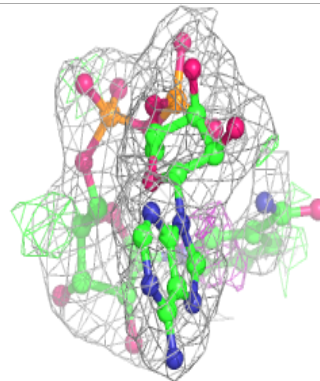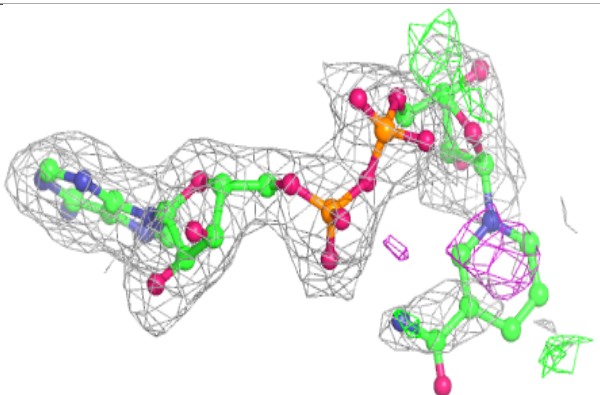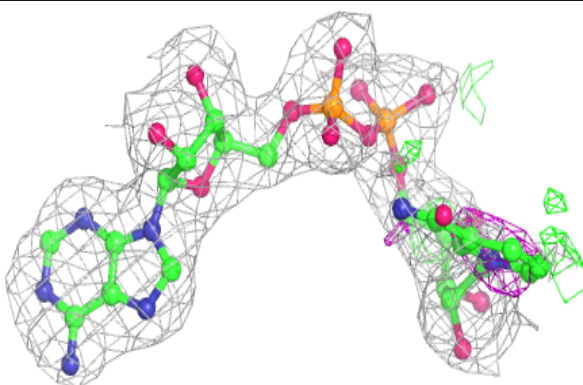
**Electron density around NAD F 500:**

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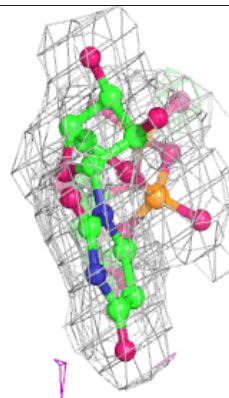and green (positive)
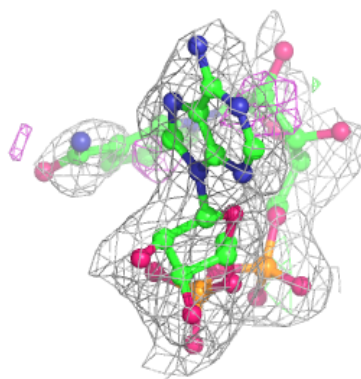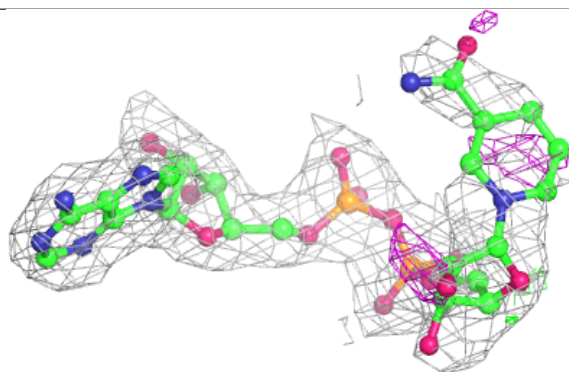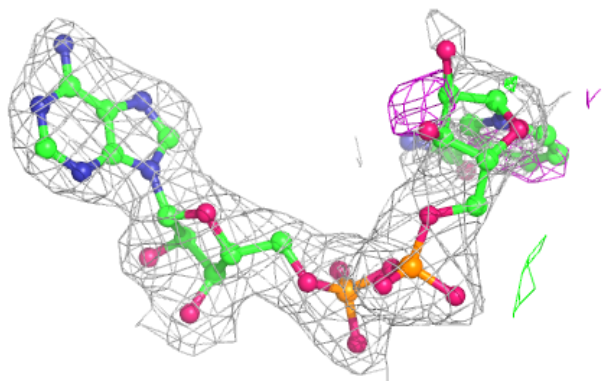


**Electron density around NAD B 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
$mF_o-DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
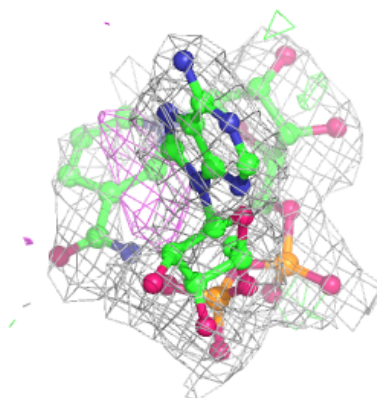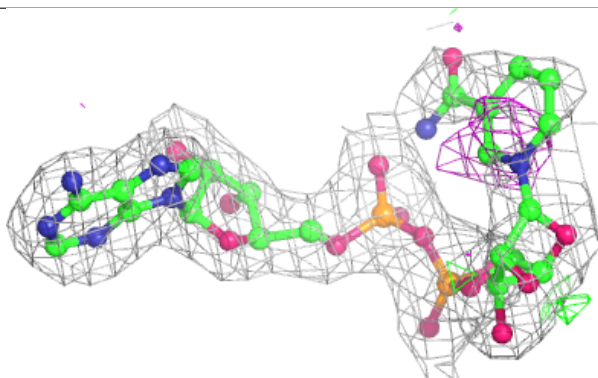
**Electron density around NAD A 500:**

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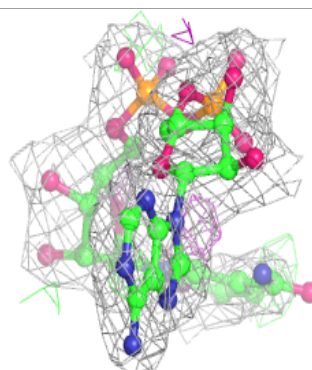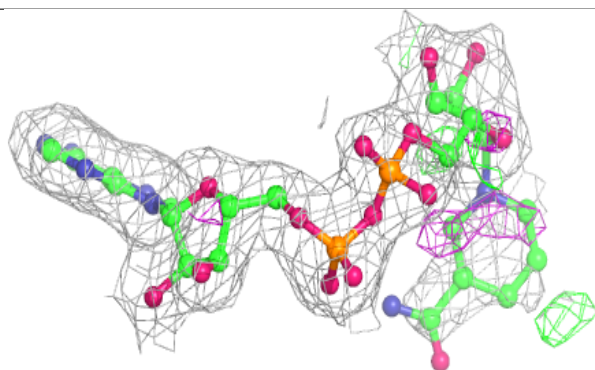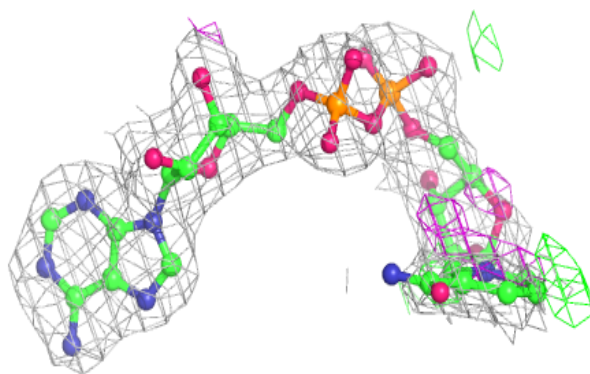


**Electron density around UDX F 501:**

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

**Electron density around UDX B 501:**

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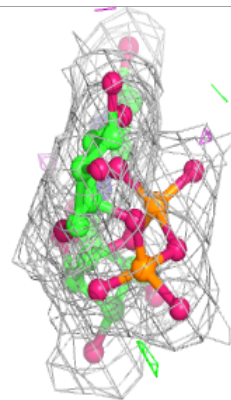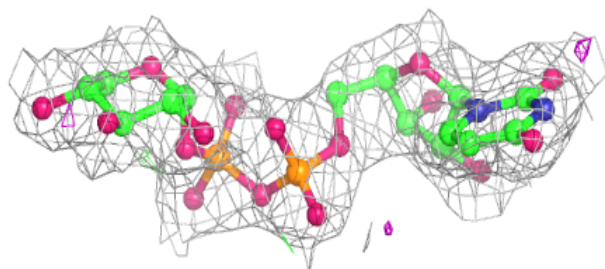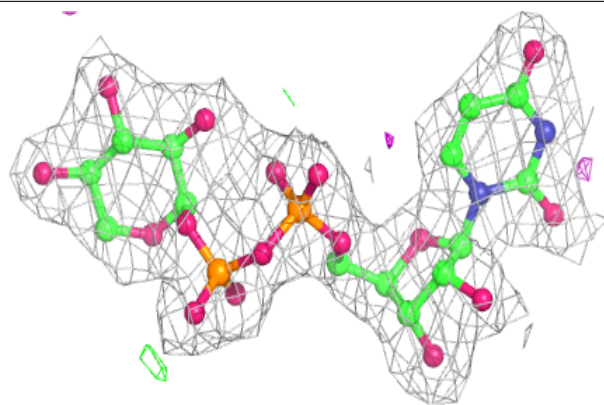


**Electron density around UDX C 501:**

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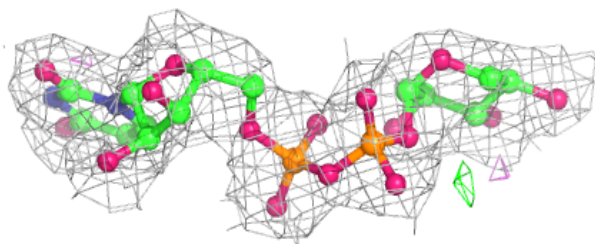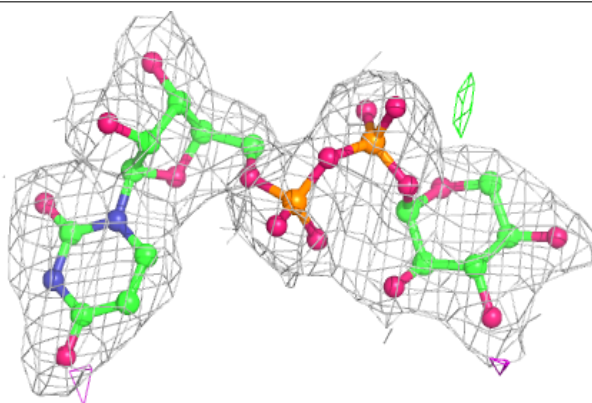$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UDX D 501:**

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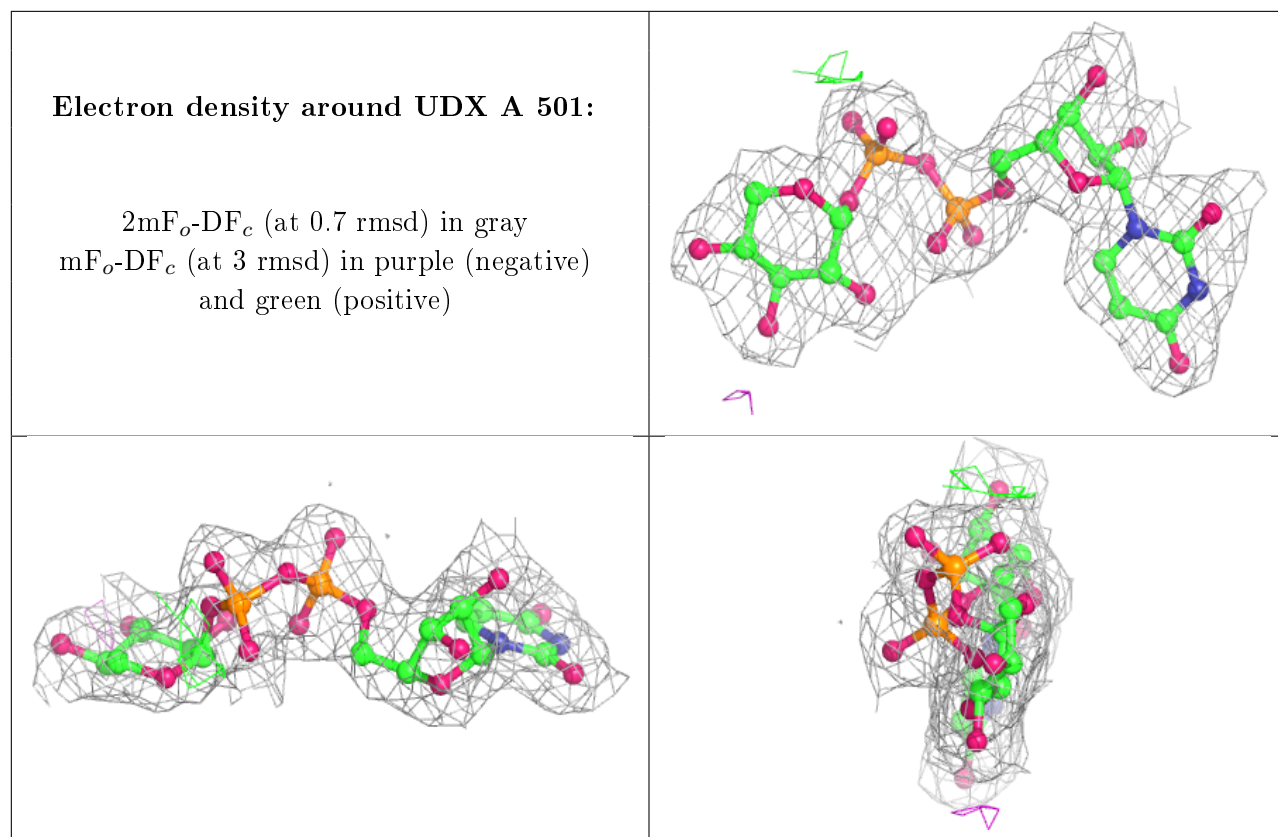$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around UDX E 501:**

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

**Electron density around UDX A 501:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.