# W O R L D W I D E
# wwPDB
## P R O T E I N   D A T A   B A N K

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

Jan 17, 2023 – 02:26 PM JST

| | | |
|---|---|---|
| PDB ID | : | 7WMZ |
| Title | : | Crystal structure of methylenetetrahydrofolate reductase MSMEG_6649 from Mycobacterium smegmatis with NADH |
| Authors | : | Lin, W.; Wang, W. |
| Deposited on | : | 2022-01-17 |
| Resolution | : | 1.92 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 | : | 2.31.3 |
| 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) | : | 2.31.3 |

# 1   Overall quality at a glance  ⓘ

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

The reported resolution of this entry is 1.92 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.
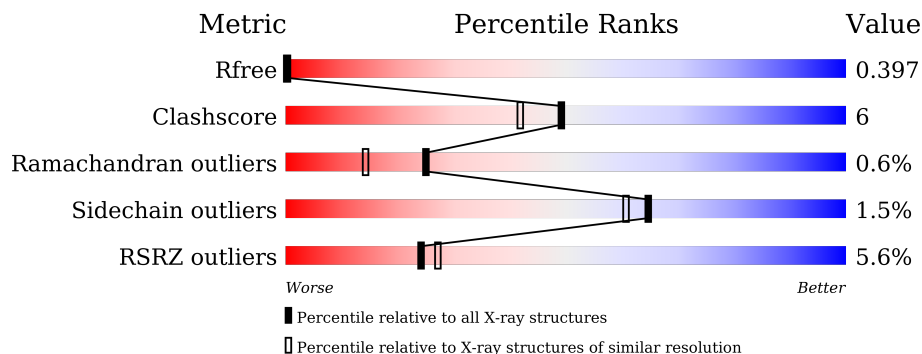


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 7937 (1.94-1.90) |
| Clashscore | 141614 | 8644 (1.94-1.90) |
| Ramachandran outliers | 138981 | 8530 (1.94-1.90) |
| Sidechain outliers | 138945 | 8530 (1.94-1.90) |
| RSRZ outliers | 127900 | 7793 (1.94-1.90) |

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 >=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 | 296 | 6% · 80% · 17% · · |
| 1 | B | 296 | 6% · 85% · 11% · · |
| 1 | C | 296 | 6% · 79% · 19% · · |
| 1 | D | 296 | 5% · 84% · 14% · |
| 1 | E | 296 | 4% · 90% · 8% · |
| 1 | F | 296 | 7% · 85% · 14% · |

# 2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14441 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 Methylenetetrahydrofolate reductase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | E | 290 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2263 | 1446 | 390 | 416 | 11 | | | |
| 1 | A | 290 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2259 | 1443 | 389 | 416 | 11 | | | |
| 1 | B | 288 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2239 | 1432 | 382 | 414 | 11 | | | |
| 1 | C | 292 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2260 | 1445 | 385 | 420 | 10 | | | |
| 1 | D | 290 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2258 | 1443 | 392 | 412 | 11 | | | |
| 1 | F | 292 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2267 | 1447 | 389 | 420 | 11 | | | |

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).
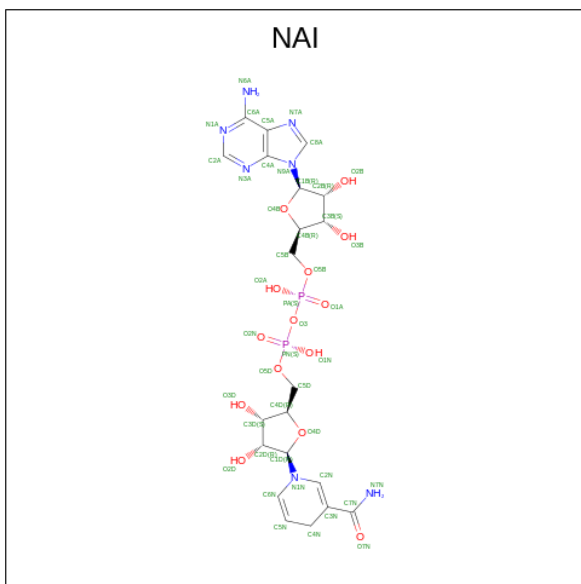
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | E | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |
| 2 | A | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |
| 2 | B | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |
| 2 | C | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |
| 2 | D | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |
| 2 | F | 1 | Total 44 | C 21 | N 7 | O 14 | P 2 | 0 | 0 |

- Molecule 3 is water.

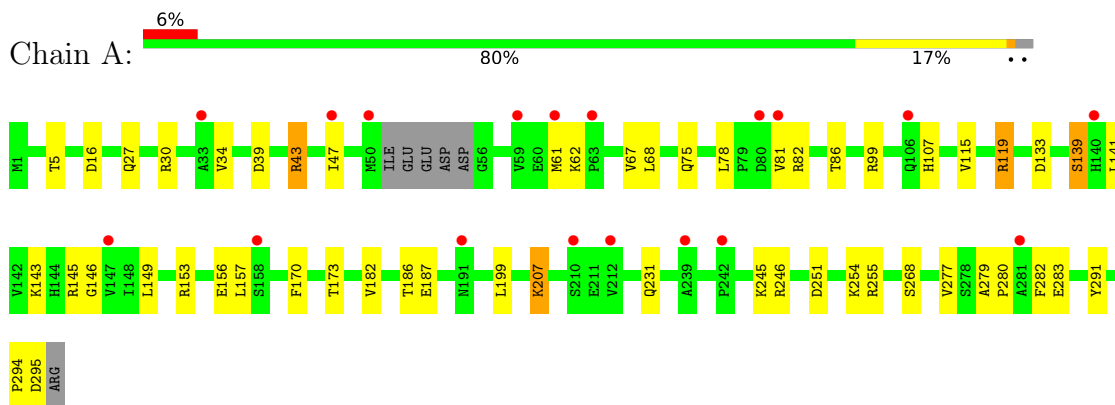| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | E | 115 | Total 115 | O 115 | 0 | 0 |
| 3 | A | 98 | Total 98 | O 98 | 0 | 0 |
| 3 | B | 114 | Total 114 | O 114 | 0 | 0 |
| 3 | C | 108 | Total 108 | O 108 | 0 | 0 |
| 3 | D | 96 | Total 96 | O 96 | 0 | 0 |
| 3 | F | 100 | Total 100 | O 100 | 0 | 0 |

# 3 Residue-property plots ⓘ

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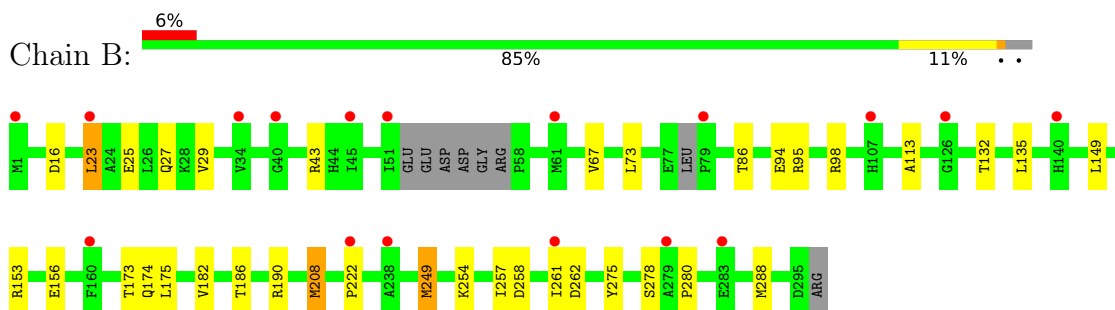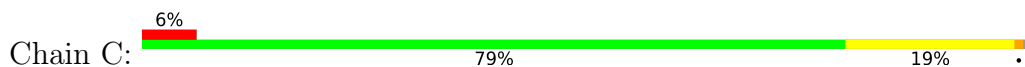
• Molecule 1: Methylenetetrahydrofolate reductase

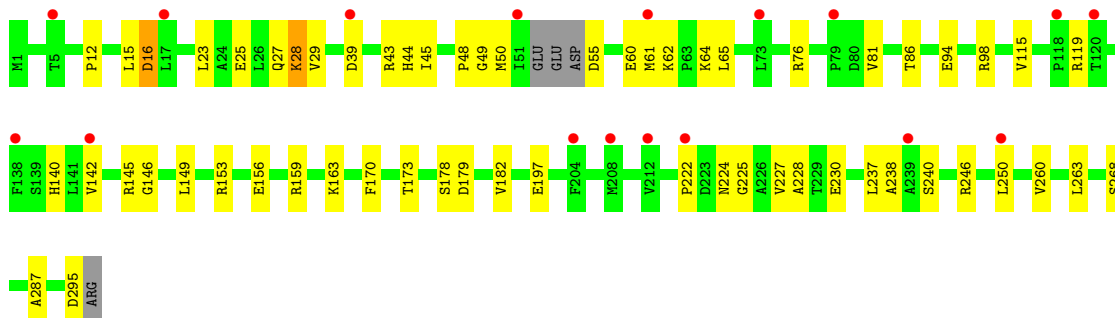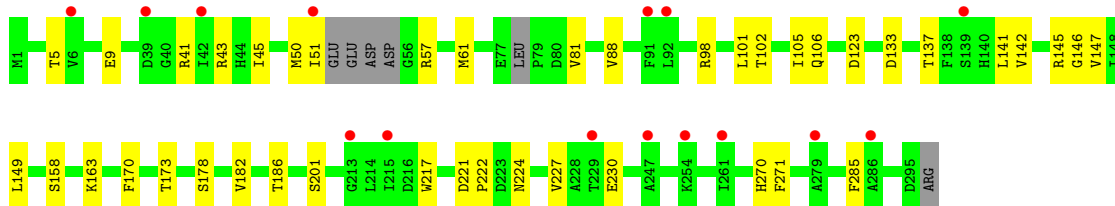Chain E:

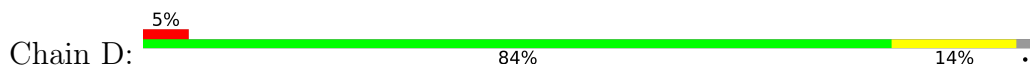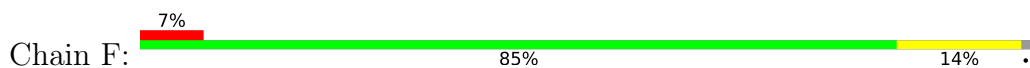• Molecule 1: Methylenetetrahydrofolate reductase

Chain A:

• Molecule 1: Methylenetetrahydrofolate reductase

Chain B:

• Molecule 1: Methylenetetrahydrofolate reductase

Chain C:

M1 T5 P12 L15 D16 L17 L23 A24 E25 L26 Q27 K28 V29 D39 R43 H44 I45 P48 G49 M50 I51 GLU GLU ASP D55 E60 M61 K62 P63 K64 L65 L73 R76 P79 D80 V81 T86 E94 R98 V115 P118 R119 T120

F138 S139 H140 L141 V142 R145 G146 L149 R153 E156 R159 K163 F170 T173 S178 D179 V182 E197 F204 M208 V212 P222 D223 N224 G225 A226 V227 A228 T229 E230 L237 A238 A239 S240 R246 L250 V260 L263 S268

A287 D295 ARG

• Molecule 1: Methylenetetrahydrofolate reductase

Chain D:

5%

84% 14% •

M1 T5 V6 E9 D39 G40 R41 I42 R43 H44 I45 M50 I51 GLU GLU ASP ASP G56 R57 M61 E77 LEU P79 D80 V81 V88 F91 L92 R98 L101 T102 I105 Q106 D123 D133 T137 F138 S139 H140 L141 V142 R145 G146 V147 I148

L149 S158 K163 F170 T173 S178 V182 T186 S201 G213 L214 I215 D216 W217 D221 P222 D223 N224 V227 A228 T229 E230 A247 K254 I261 H270 F271 A279 F285 A286 D295 ARG

• Molecule 1: Methylenetetrahydrofolate reductase

Chain F:

7%

85% 14% •

M1 N4 A22 L23 L26 V29 P48 I51 GLU GLU ASP D55 V59 E60 M61 K64 E77 T86 E94 R95 S96 L97 R98 T102 A103 M121 T122 E125 G128 T132 L135 S139 H140 K143 V147 P151 T152 R153

E156 L157 S158 R159 F170 I181 F184 E187 G203 I215 I219 Q232 R246 L252 R255 G259 V260 I261 D262 E272 V277 F282 E283 T284 M288 P294 D295 ARG

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | I 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 70.93Å 104.29Å 318.53Å<br>90.00° 94.08° 90.00° | Depositor |
| Resolution (Å) | 19.52 – 1.92<br>19.52 – 1.92 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.0 (19.52-1.92)<br>98.3 (19.52-1.92) | Depositor<br>EDS |
| $R_{merge}$ | 0.08 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.33 (at 1.92Å) | Xtriage |
| Refinement program | PHENIX 1.14_3260 | Depositor |
| R, $R_{free}$ | 0.355 , 0.403<br>0.355 , 0.397 | Depositor<br>DCC |
| $R_{free}$ test set | 8736 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 23.7 | Xtriage |
| Anisotropy | 1.026 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 31.8 | EDS |
| L-test for twinning[2] | $< |L| > = 0.51, < L^2 > = 0.35$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 14441 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1105e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

## 5.1  Standard geometry ⓘ

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

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 | 0.49 | 0/2307 | 0.55 | 0/3128 |
| 1 | B | 0.45 | 0/2285 | 0.56 | 0/3096 |
| 1 | C | 0.38 | 0/2308 | 0.53 | 0/3133 |
| 1 | D | 0.41 | 0/2305 | 0.57 | 0/3122 |
| 1 | E | 0.35 | 0/2309 | 0.51 | 0/3128 |
| 1 | F | 0.43 | 0/2314 | 0.55 | 0/3138 |
| All | All | 0.42 | 0/13828 | 0.54 | 0/18745 |

There are no bond length outliers.

There are no bond angle outliers.

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 | 2259 | 0 | 2262 | 35 | 0 |
| 1 | B | 2239 | 0 | 2242 | 27 | 0 |
| 1 | C | 2260 | 0 | 2248 | 34 | 0 |
| 1 | D | 2258 | 0 | 2267 | 26 | 0 |
| 1 | E | 2263 | 0 | 2276 | 15 | 0 |
| 1 | F | 2267 | 0 | 2263 | 25 | 0 |
| 2 | A | 44 | 0 | 27 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 44 | 0 | 27 | 0 | 0 |
| 2 | C | 44 | 0 | 27 | 0 | 0 |
| 2 | D | 44 | 0 | 27 | 1 | 0 |
| 2 | E | 44 | 0 | 27 | 0 | 0 |
| 2 | F | 44 | 0 | 27 | 0 | 0 |
| 3 | A | 98 | 0 | 0 | 5 | 0 |
| 3 | B | 114 | 0 | 0 | 3 | 0 |
| 3 | C | 108 | 0 | 0 | 4 | 0 |
| 3 | D | 96 | 0 | 0 | 0 | 0 |
| 3 | E | 115 | 0 | 0 | 3 | 0 |
| 3 | F | 100 | 0 | 0 | 3 | 0 |
| All | All | 14441 | 0 | 13720 | 162 | 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.

The worst 5 of 162 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:249:MET:CE | 1:B:288:MET:HE1 | 1.77 | 1.12 |
| 1:B:249:MET:HE2 | 1:B:288:MET:CE | 1.84 | 1.07 |
| 1:B:249:MET:CE | 1:B:288:MET:CE | 2.37 | 1.01 |
| 1:E:147:VAL:HG21 | 1:E:163:LYS:HD3 | 1.44 | 0.97 |
| 1:C:45:ILE:HG12 | 1:C:81:VAL:HG11 | 1.46 | 0.96 |

There are no symmetry-related clashes.

## 5.3    Torsion angles ⓘ

### 5.3.1    Protein backbone ⓘ

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 | 286/296 (97%) | 281 (98%) | 4 (1%) | 1 (0%) | 41 | 31 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | B | 282/296 (95%) | 270 (96%) | 10 (4%) | 2 (1%) | 22 | 11 |
| 1 | C | 288/296 (97%) | 275 (96%) | 9 (3%) | 4 (1%) | 11 | 3 |
| 1 | D | 284/296 (96%) | 277 (98%) | 5 (2%) | 2 (1%) | 22 | 11 |
| 1 | E | 284/296 (96%) | 271 (95%) | 13 (5%) | 0 | 100 | 100 |
| 1 | F | 288/296 (97%) | 284 (99%) | 3 (1%) | 1 (0%) | 41 | 31 |
| All | All | 1712/1776 (96%) | 1658 (97%) | 44 (3%) | 10 (1%) | 25 | 14 |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 222 | PRO |
| 1 | C | 60 | GLU |
| 1 | F | 61 | MET |
| 1 | B | 208 | MET |
| 1 | C | 61 | MET |

### 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 | 241/248 (97%) | 236 (98%) | 5 (2%) | 53 | 46 |
| 1 | B | 239/248 (96%) | 234 (98%) | 5 (2%) | 53 | 46 |
| 1 | C | 240/248 (97%) | 237 (99%) | 3 (1%) | 69 | 66 |
| 1 | D | 240/248 (97%) | 237 (99%) | 3 (1%) | 69 | 66 |
| 1 | E | 242/248 (98%) | 240 (99%) | 2 (1%) | 81 | 81 |
| 1 | F | 241/248 (97%) | 238 (99%) | 3 (1%) | 71 | 69 |
| All | All | 1443/1488 (97%) | 1422 (98%) | 21 (2%) | 65 | 61 |

5 of 21 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 295 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 158 | SER |
| 1 | F | 157 | LEU |
| 1 | F | 1 | MET |
| 1 | D | 123 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 248 | GLN |
| 1 | C | 140 | HIS |
| 1 | C | 231 | GLN |
| 1 | A | 75 | GLN |
| 1 | E | 183 | 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 2 | NAI | B | 301 | - | 42,48,48 | 1.30 | 4 (9%) | 47,73,73 | 0.83 | 2 (4%) |
| 2 | NAI | D | 301 | - | 42,48,48 | 1.34 | 3 (7%) | 47,73,73 | 0.98 | 3 (6%) |
| 2 | NAI | C | 301 | - | 42,48,48 | 1.35 | 4 (9%) | 47,73,73 | 0.77 | 1 (2%) |
| 2 | NAI | F | 301 | - | 42,48,48 | 1.37 | 4 (9%) | 47,73,73 | 0.76 | 2 (4%) |
| 2 | NAI | E | 301 | - | 42,48,48 | 1.36 | 4 (9%) | 47,73,73 | 0.76 | 3 (6%) |
| 2 | NAI | A | 301 | - | 42,48,48 | 1.35 | 4 (9%) | 47,73,73 | 0.76 | 2 (4%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | NAI | B | 301 | - | - | 4/25/72/72 | 0/5/5/5 |
| 2 | NAI | D | 301 | - | - | 7/25/72/72 | 0/5/5/5 |
| 2 | NAI | C | 301 | - | - | 6/25/72/72 | 0/5/5/5 |
| 2 | NAI | F | 301 | - | - | 8/25/72/72 | 0/5/5/5 |
| 2 | NAI | E | 301 | - | - | 5/25/72/72 | 0/5/5/5 |
| 2 | NAI | A | 301 | - | - | 7/25/72/72 | 0/5/5/5 |

The worst 5 of 23 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | F | 301 | NAI | C4N-C3N | -5.82 | 1.38 | 1.49 |
| 2 | D | 301 | NAI | C4N-C3N | -5.74 | 1.38 | 1.49 |
| 2 | E | 301 | NAI | C4N-C3N | -5.64 | 1.38 | 1.49 |
| 2 | A | 301 | NAI | C4N-C3N | -5.57 | 1.39 | 1.49 |
| 2 | C | 301 | NAI | C4N-C3N | -5.54 | 1.39 | 1.49 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|------------|---------|
| 2 | D | 301 | NAI | C3N-C2N-N1N | -4.25 | 117.03 | 123.10 |
| 2 | B | 301 | NAI | C3D-C2D-C1D | 2.61 | 106.38 | 101.43 |
| 2 | B | 301 | NAI | C3N-C2N-N1N | -2.59 | 119.40 | 123.10 |
| 2 | A | 301 | NAI | C3N-C2N-N1N | -2.59 | 119.40 | 123.10 |
| 2 | D | 301 | NAI | C3D-C2D-C1D | 2.51 | 106.19 | 101.43 |

There are no chirality outliers.
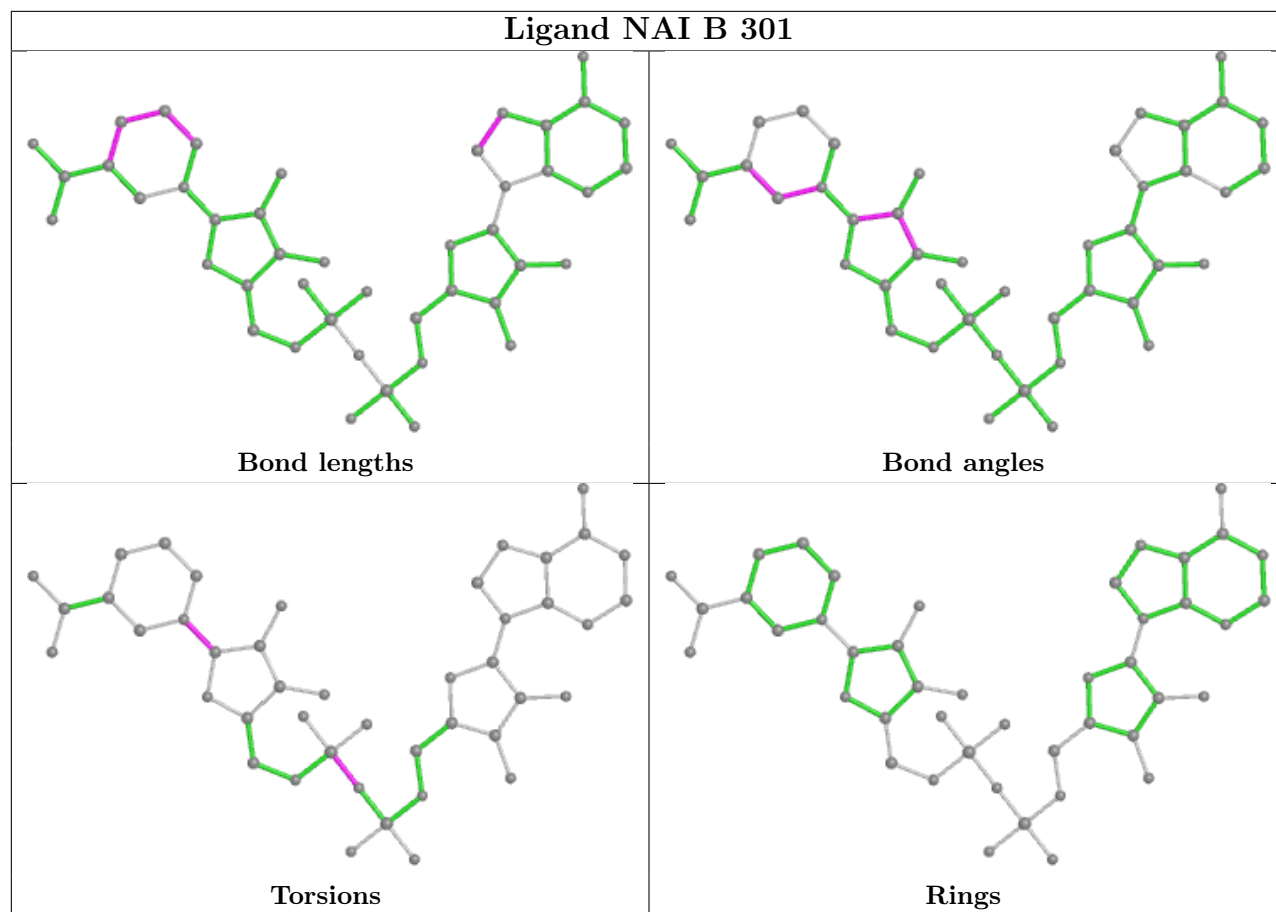
5 of 37 torsion outliers are listed below:

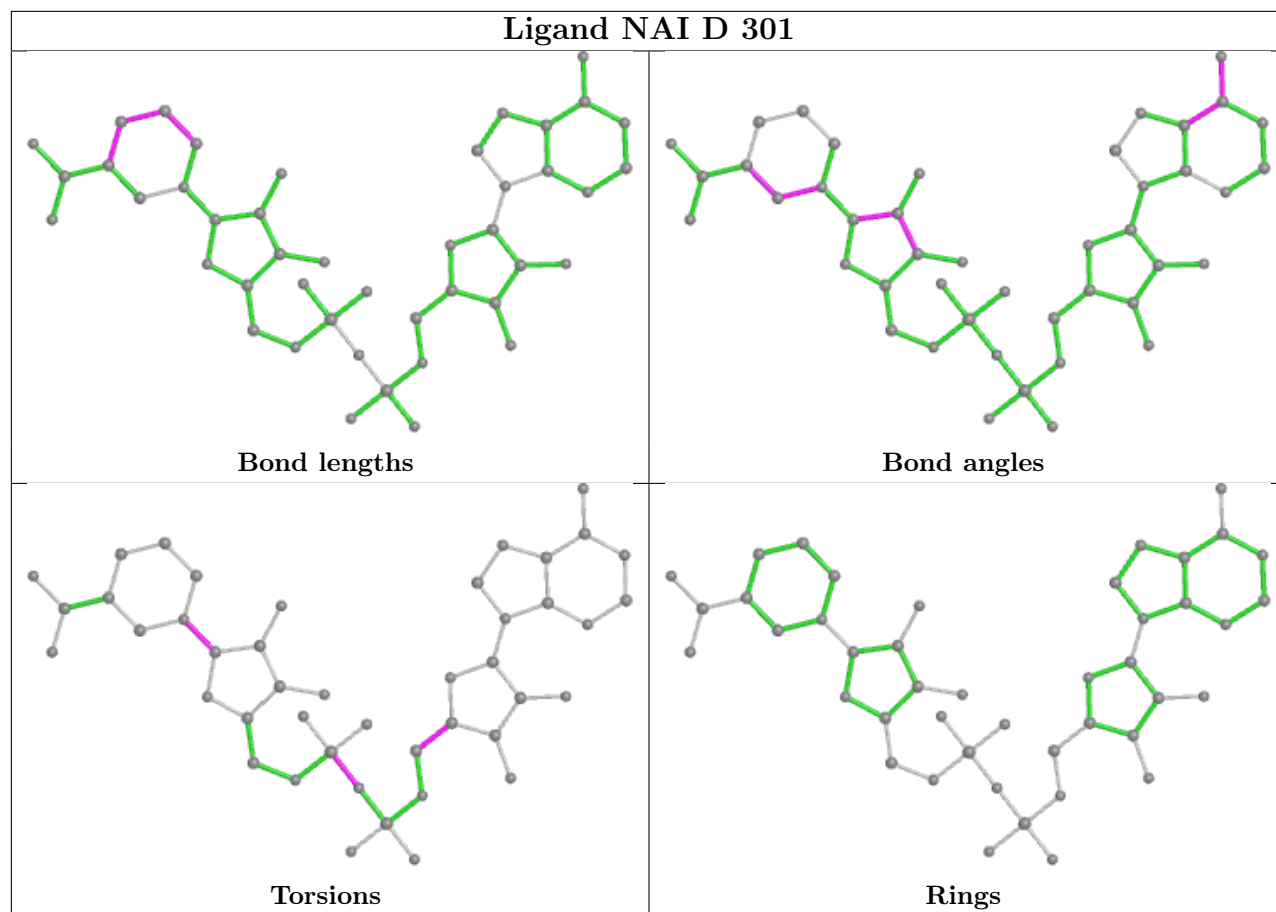| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | C | 301 | NAI | C5B-O5B-PA-O1A |
| 2 | F | 301 | NAI | C5B-O5B-PA-O1A |
| 2 | A | 301 | NAI | C3B-C4B-C5B-O5B |
| 2 | D | 301 | NAI | C3B-C4B-C5B-O5B |
| 2 | A | 301 | NAI | O4B-C4B-C5B-O5B |

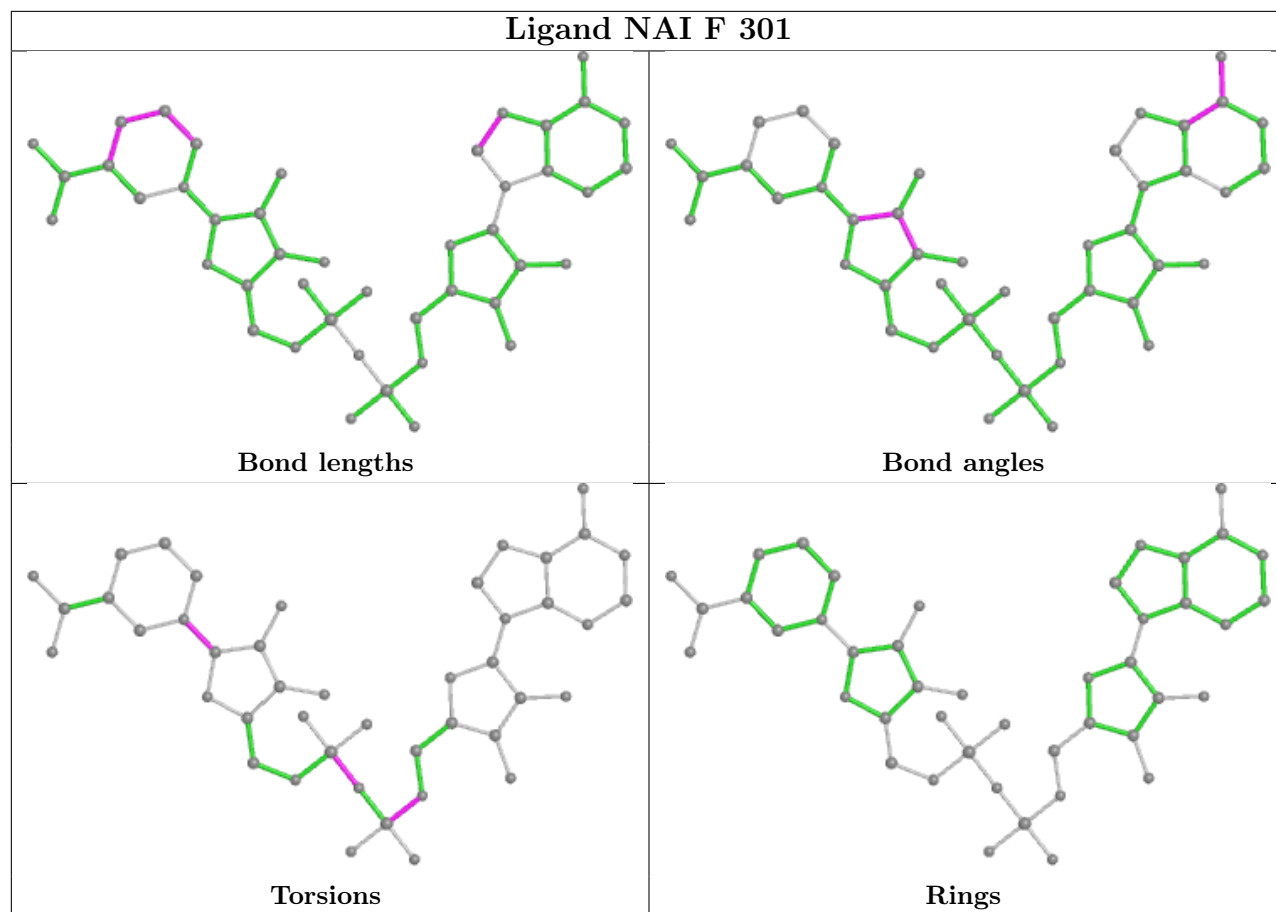There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | D | 301 | NAI | 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 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 NAI B 301



Bond lengths



Bond angles



Torsions



Rings

## Ligand NAI D 301


Bond lengths


Bond angles


Torsions


Rings

## Ligand NAI C 301


Bond lengths


Bond angles


Torsions


Rings

## Ligand NAI F 301



**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## Ligand NAI E 301



Bond lengths

Bond angles

Torsions

Rings

## Ligand NAI A 301



**Bond lengths**

**Bond angles**

**Torsions**

**Rings**
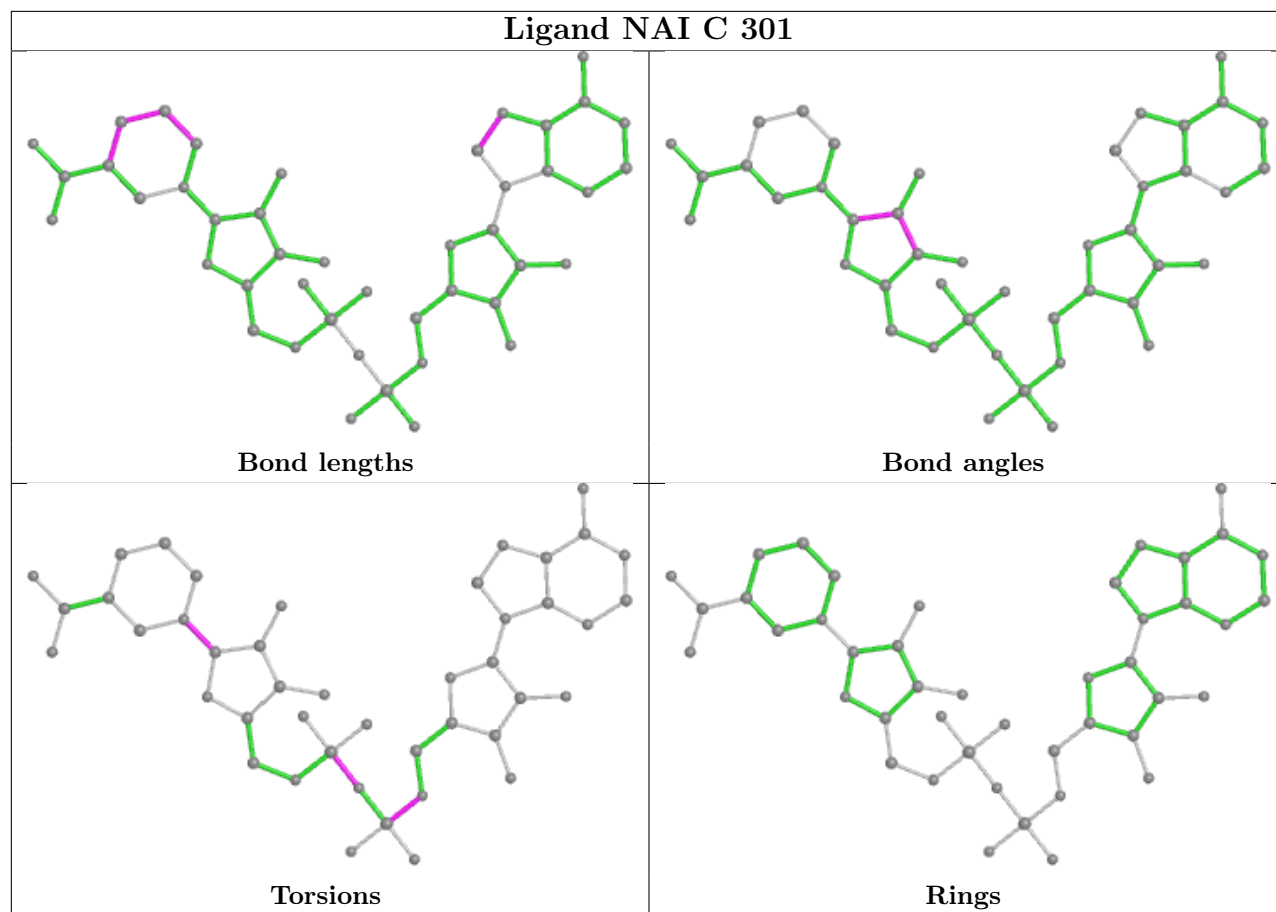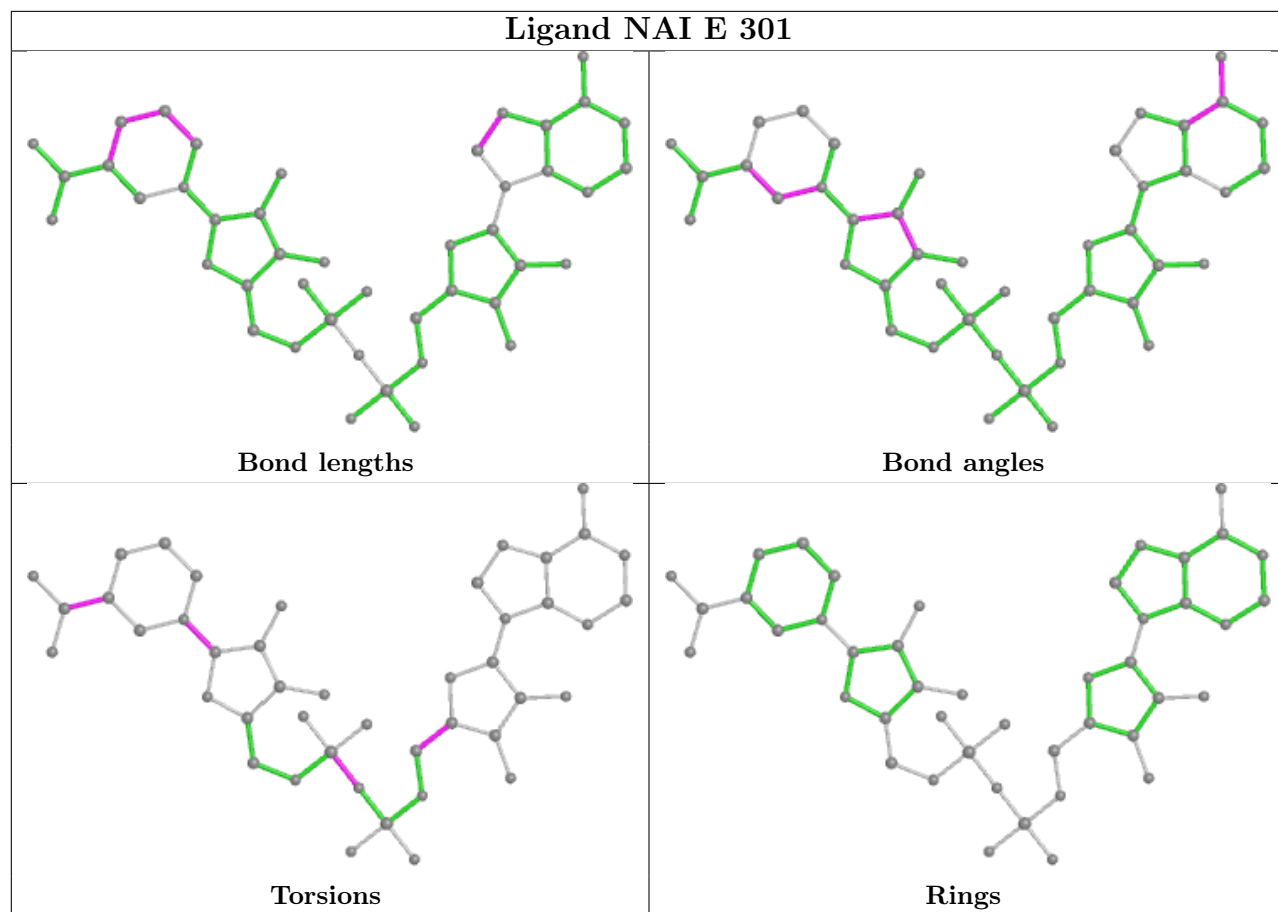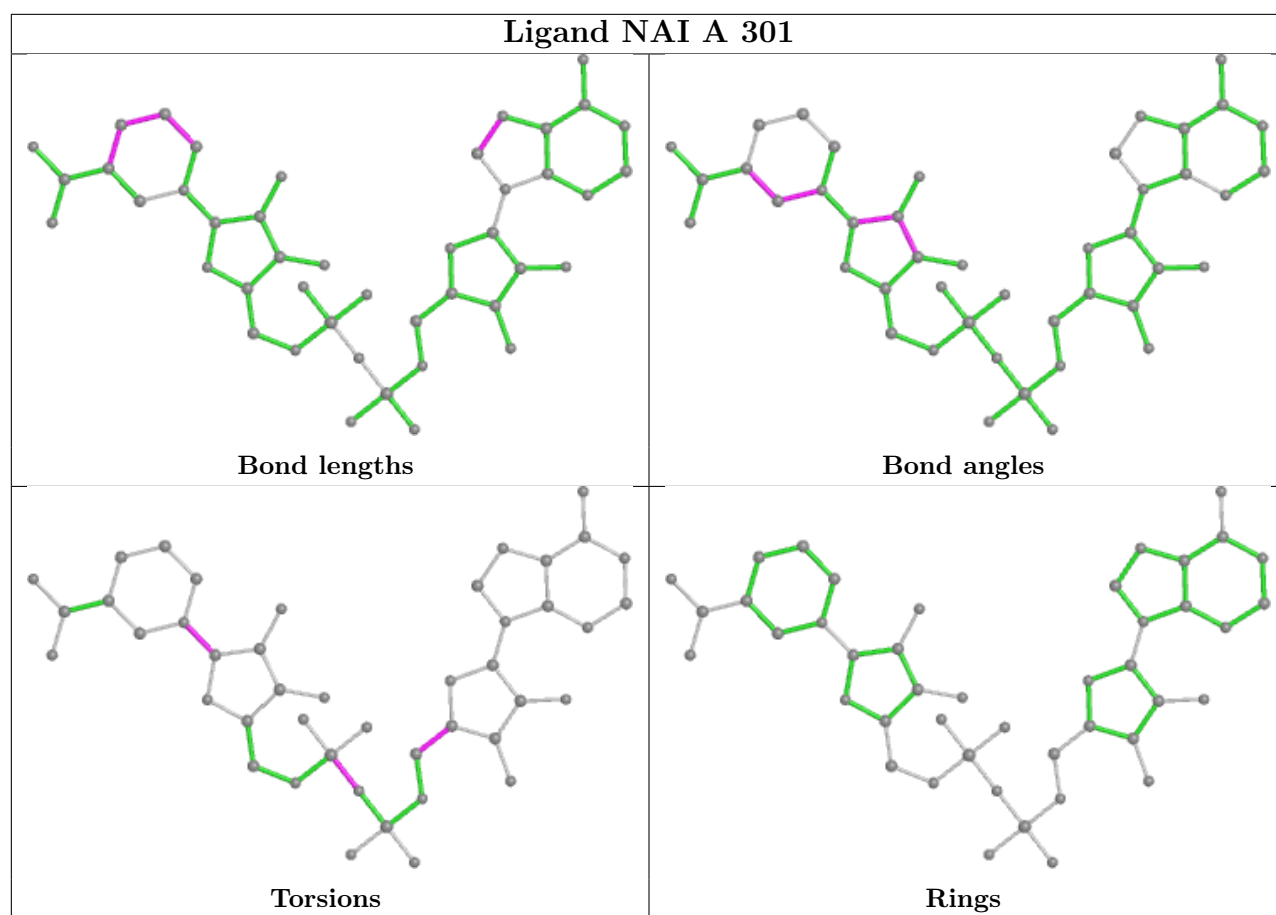
## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|-------|----------|--------|---------|----|----|----------|-------|
| 1 | A | 290/296 (97%) | 0.79 | 18 (6%) | 20 | 23 | 27, 35, 41, 47 | 0 |
| 1 | B | 288/296 (97%) | 0.83 | 17 (5%) | 22 | 25 | 26, 34, 39, 44 | 0 |
| 1 | C | 292/296 (98%) | 0.80 | 17 (5%) | 23 | 26 | 27, 36, 41, 45 | 0 |
| 1 | D | 290/296 (97%) | 0.81 | 15 (5%) | 27 | 30 | 27, 35, 41, 47 | 0 |
| 1 | E | 290/296 (97%) | 0.79 | 11 (3%) | 40 | 43 | 26, 35, 40, 44 | 0 |
| 1 | F | 292/296 (98%) | 0.79 | 20 (6%) | 17 | 19 | 26, 35, 40, 45 | 0 |
| All | All | 1742/1776 (98%) | 0.80 | 98 (5%) | 24 | 27 | 26, 35, 41, 47 | 0 |

The worst 5 of 98 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 140 | HIS | 4.6 |
| 1 | A | 33 | ALA | 4.5 |
| 1 | C | 51 | ILE | 3.8 |
| 1 | B | 34 | VAL | 3.5 |
| 1 | C | 239 | ALA | 3.5 |

## 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 monosaccharides in this entry.

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## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ 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 | NAI | D | 301 | 44/44 | 0.83 | 0.18 | 33,35,37,38 | 0 |
| 2 | NAI | E | 301 | 44/44 | 0.87 | 0.15 | 32,34,35,35 | 0 |
| 2 | NAI | B | 301 | 44/44 | 0.89 | 0.13 | 32,33,35,35 | 0 |
| 2 | NAI | C | 301 | 44/44 | 0.89 | 0.14 | 32,34,36,36 | 0 |
| 2 | NAI | A | 301 | 44/44 | 0.89 | 0.14 | 34,35,37,38 | 0 |
| 2 | NAI | F | 301 | 44/44 | 0.91 | 0.13 | 31,33,34,35 | 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 NAI D 301:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)
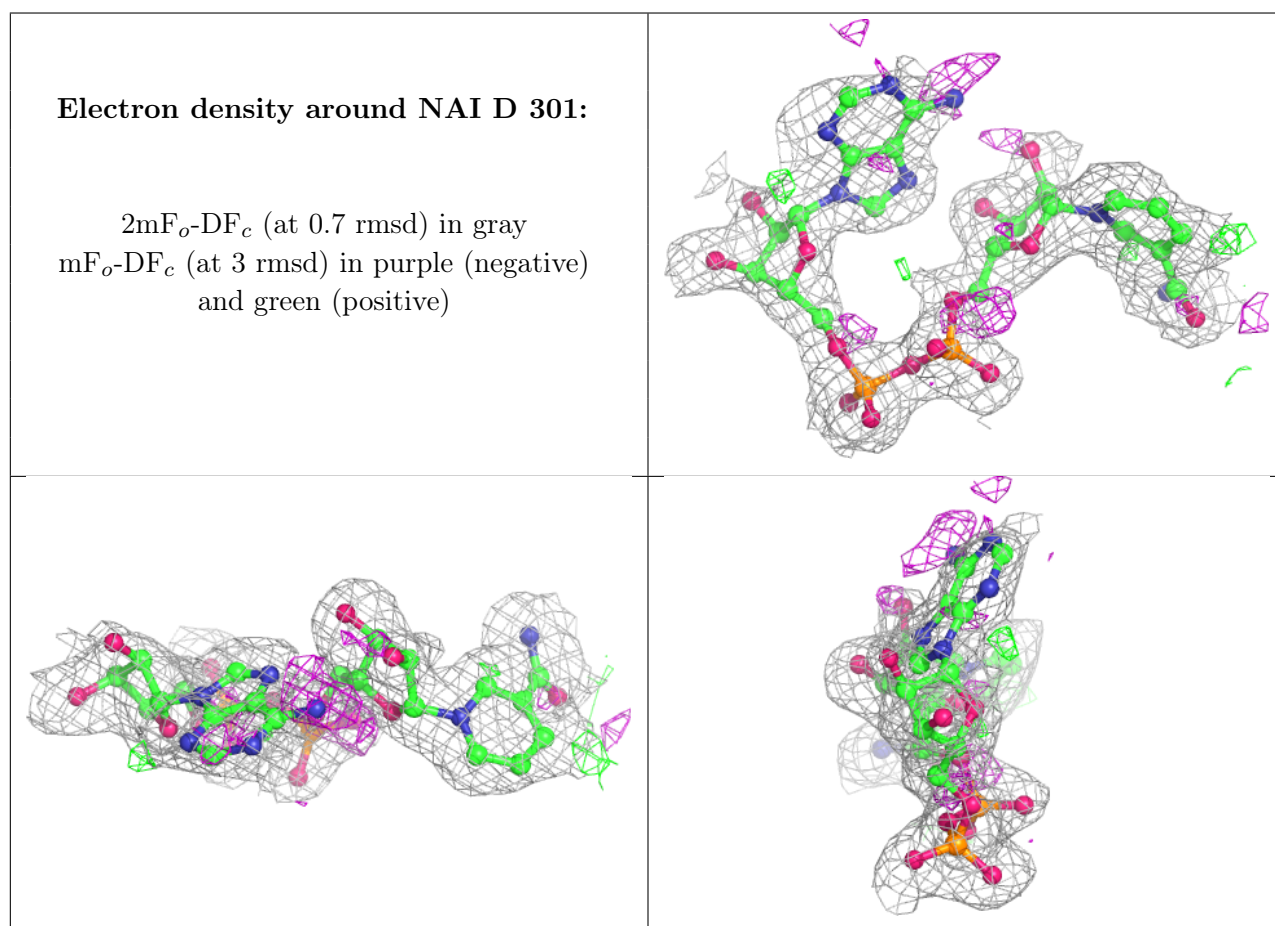
**Electron density around NAI E 301:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
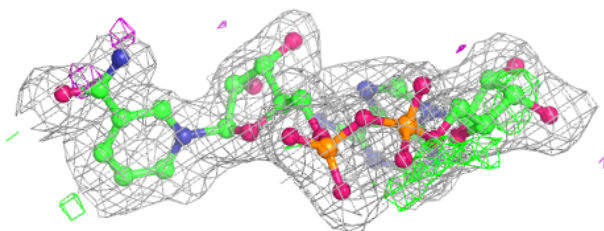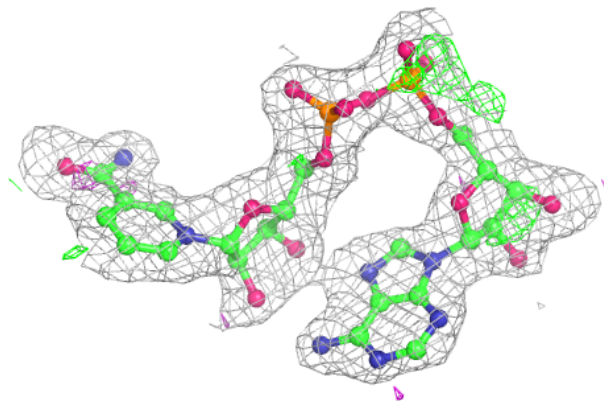$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
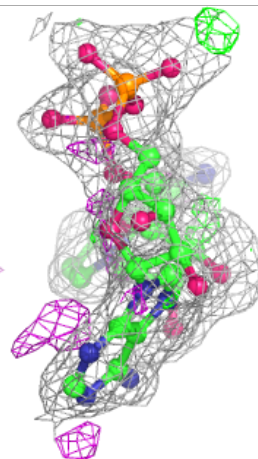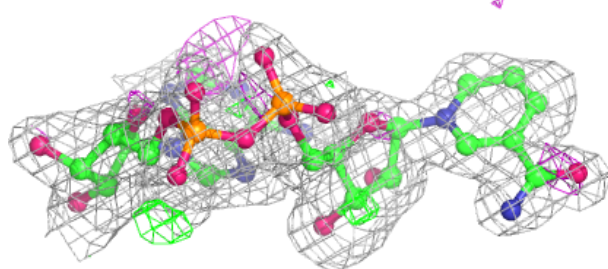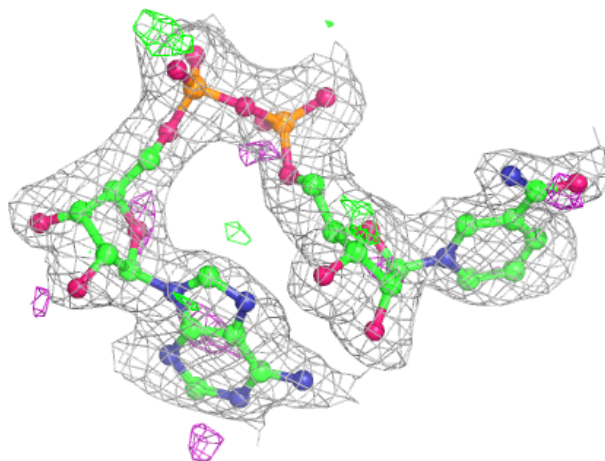
**Electron density around NAI B 301:**

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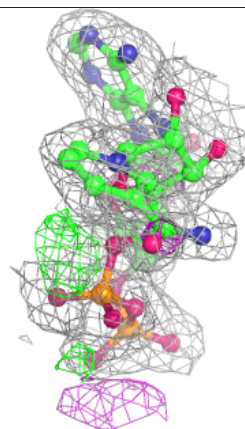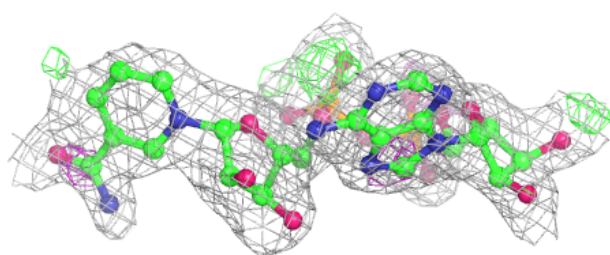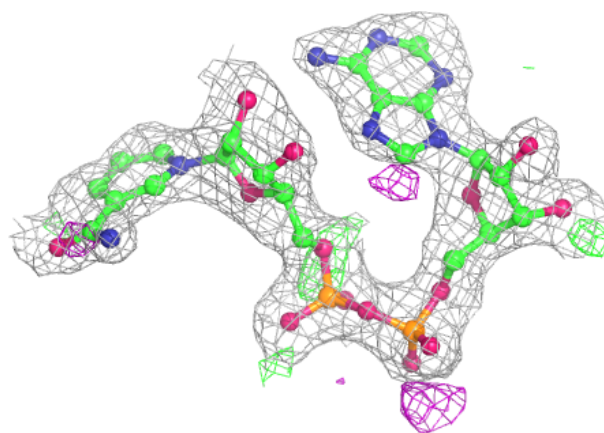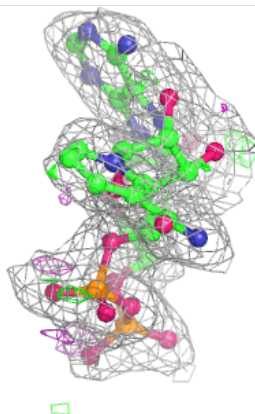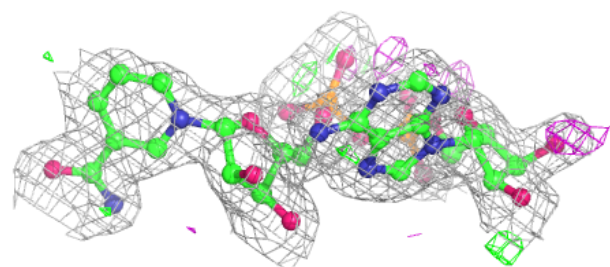and green (positive)
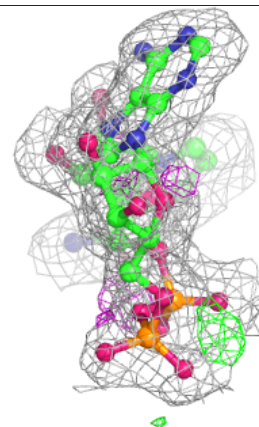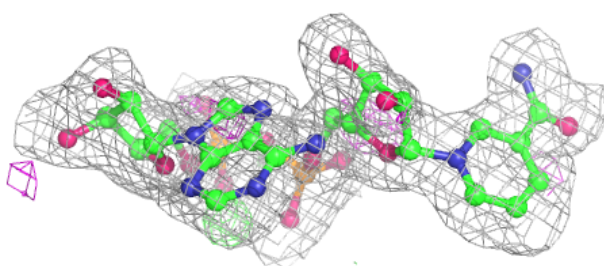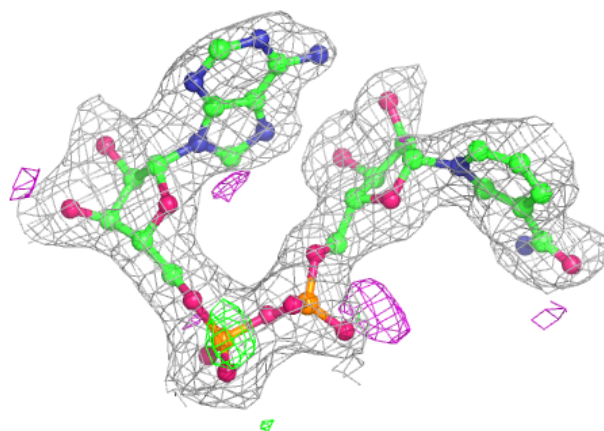


**Electron density around NAI C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
$mF_o-DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
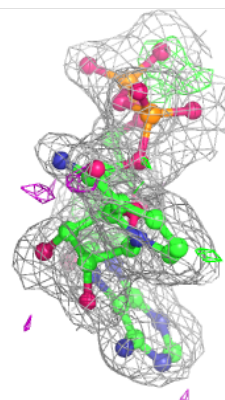
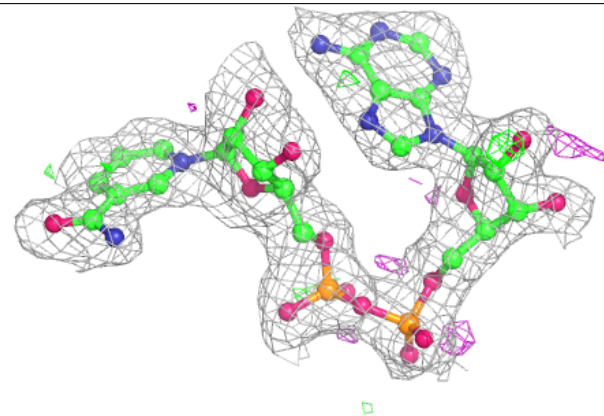**Electron density around NAI A 301:**

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



**Electron density around NAI F 301:**

$2mF_o$-$DF_c$ (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.