# WORLDWIDE wwPDB PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 07:04 pm GMT

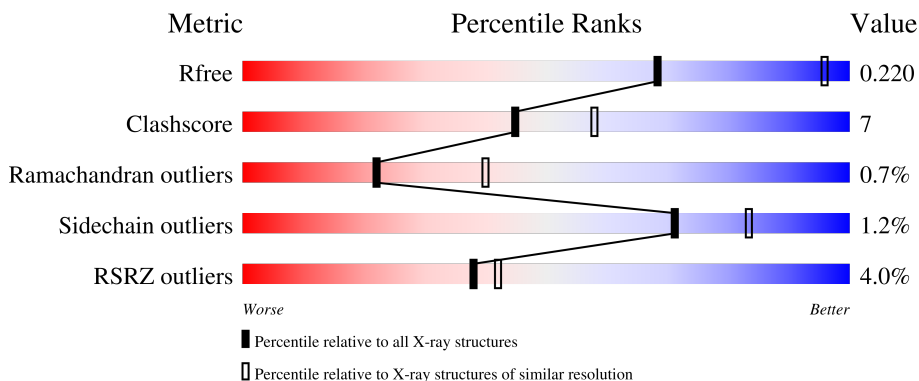| | | |
|---|---|---|
| PDB ID | : | 4UN9 |
| Title | : | THE CRYSTAL STRUCTURE OF I-DMOI IN COMPLEX WITH ITS TARGET DNA AT 8H INCUBATION IN 5MM MN (STATE 3) |
| Authors | : | Molina, R.; Stella, S.; Redondo, P.; Gomez, H.; Marcaida, M.J.; Orozco, M.; Prieto, J.; Montoya, G. |
| Deposited on | : | 2014-05-26 |
| Resolution | : | 2.73 Å(reported) |

# 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 2.73 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.
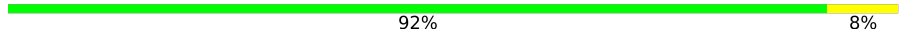
| Metric | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.220 |
| Clashscore | | 7 |
| Ramachandran outliers | | 0.7% |
| Sidechain outliers | | 1.2% |
| RSRZ outliers | | 4.0% |

*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 | 1271 (2.76-2.72) |
| Clashscore | 141614 | 1322 (2.76-2.72) |
| Ramachandran outliers | 138981 | 1297 (2.76-2.72) |
| Sidechain outliers | 138945 | 1298 (2.76-2.72) |
| RSRZ outliers | 127900 | 1243 (2.76-2.72) |

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 | 199 | 3% / 72% / 20% · 8% |
| 1 | D | 199 | 8% / 78% / 18% · · |
| 2 | B | 25 | 68% / 32% |
| 2 | E | 25 | 64% / 32% · |
| 2 | H | 25 | 68% / 32% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | C | 25 | 92%　　　　8% |
| 3 | F | 25 | 4%　84%　　16% |
| 3 | I | 25 | 8%　72%　　28% |
| 4 | G | 199 | 2%　72%　　17%　·　11% |

# 2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7792 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 HOMING ENDONUCLEASE I-DMOI.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 1 | A | 184 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 1541 | 994 | 281 | 263 | 3 | | | |
| 1 | D | 191 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1578 | 1017 | 287 | 271 | 3 | | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 1 | ALA | - | expression tag | UNP P21505 |
| A | 189 | ALA | - | expression tag | UNP P21505 |
| A | 190 | ALA | - | expression tag | UNP P21505 |
| A | 191 | ALA | - | expression tag | UNP P21505 |
| A | 192 | LEU | - | expression tag | UNP P21505 |
| A | 193 | GLU | - | expression tag | UNP P21505 |
| A | 194 | HIS | - | expression tag | UNP P21505 |
| A | 195 | HIS | - | expression tag | UNP P21505 |
| A | 196 | HIS | - | expression tag | UNP P21505 |
| A | 197 | HIS | - | expression tag | UNP P21505 |
| A | 198 | HIS | - | expression tag | UNP P21505 |
| A | 199 | HIS | - | expression tag | UNP P21505 |
| D | 1 | ALA | - | expression tag | UNP P21505 |
| D | 189 | ALA | - | expression tag | UNP P21505 |
| D | 190 | ALA | - | expression tag | UNP P21505 |
| D | 191 | ALA | - | expression tag | UNP P21505 |
| D | 192 | LEU | - | expression tag | UNP P21505 |
| D | 193 | GLU | - | expression tag | UNP P21505 |
| D | 194 | HIS | - | expression tag | UNP P21505 |
| D | 195 | HIS | - | expression tag | UNP P21505 |
| D | 196 | HIS | - | expression tag | UNP P21505 |
| D | 197 | HIS | - | expression tag | UNP P21505 |
| D | 198 | HIS | - | expression tag | UNP P21505 |
| D | 199 | HIS | - | expression tag | UNP P21505 |

- Molecule 2 is a DNA chain called 25MER.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 2 | B | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 511 | 242 | 94 | 151 | 24 | | | |
| 2 | E | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 511 | 242 | 94 | 151 | 24 | | | |
| 2 | H | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 511 | 242 | 94 | 151 | 24 | | | |

- Molecule 3 is a DNA chain called 25MER.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 3 | C | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 508 | 240 | 99 | 145 | 24 | | | |
| 3 | F | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 508 | 240 | 99 | 145 | 24 | | | |
| 3 | I | 25 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 508 | 240 | 99 | 145 | 24 | | | |

- Molecule 4 is a protein called HOMING ENDONUCLEASE I-DMOI.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 4 | G | 177 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 1502 | 972 | 272 | 255 | 3 | | | |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| G | 1 | ALA | - | expression tag | UNP P21505 |
| G | 6 | GLU | ASN | conflict | UNP P21505 |
| G | 189 | ALA | - | expression tag | UNP P21505 |
| G | 190 | ALA | - | expression tag | UNP P21505 |
| G | 191 | ALA | - | expression tag | UNP P21505 |
| G | 192 | LEU | - | expression tag | UNP P21505 |
| G | 193 | GLU | - | expression tag | UNP P21505 |
| G | 194 | HIS | - | expression tag | UNP P21505 |
| G | 195 | HIS | - | expression tag | UNP P21505 |
| G | 196 | HIS | - | expression tag | UNP P21505 |
| G | 197 | HIS | - | expression tag | UNP P21505 |
| G | 198 | HIS | - | expression tag | UNP P21505 |
| G | 199 | HIS | - | expression tag | UNP P21505 |

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 5 | A | 3 | Total 3 | Mn 3 | 0 | 0 |
| 5 | D | 3 | Total 3 | Mn 3 | 0 | 0 |
| 5 | G | 4 | Total 4 | Mn 4 | 0 | 0 |

- Molecule 6 is water.

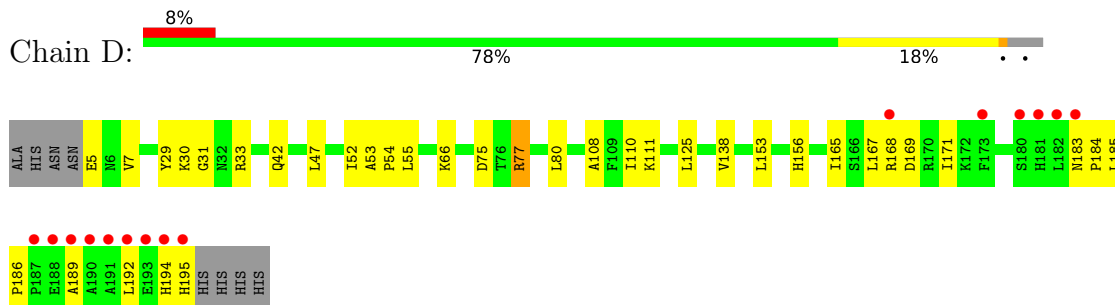| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 6 | A | 30 | Total 30 | O 30 | 0 | 0 |
| 6 | B | 6 | Total 6 | O 6 | 0 | 0 |
| 6 | C | 4 | Total 4 | O 4 | 0 | 0 |
| 6 | D | 25 | Total 25 | O 25 | 0 | 0 |
| 6 | E | 5 | Total 5 | O 5 | 0 | 0 |
| 6 | F | 2 | Total 2 | O 2 | 0 | 0 |
| 6 | G | 23 | Total 23 | O 23 | 0 | 0 |
| 6 | H | 6 | Total 6 | O 6 | 0 | 0 |
| 6 | I | 3 | Total 3 | O 3 | 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: HOMING ENDONUCLEASE I-DMOI
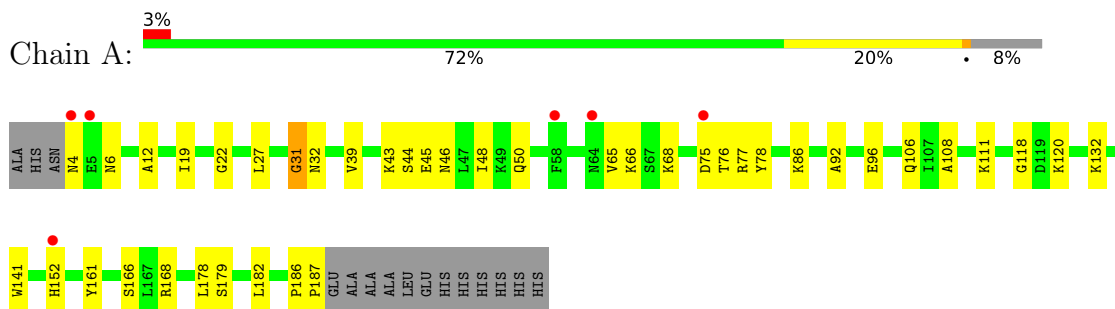
Chain A:

- Molecule 1: HOMING ENDONUCLEASE I-DMOI

Chain D:

- Molecule 2: 25MER

Chain B:

- Molecule 2: 25MER

Chain E:

- Molecule 2: 25MER

Chain H:

G1 T5 G6 G15 C19 G20 G21 C24 G25

• Molecule 3: 25MER

Chain C:

92%  8%

C1 C6 G7 C25

• Molecule 3: 25MER

Chain F:

4%

84%  16%

C1 G2 C3 A9 G18 C25

• Molecule 3: 25MER

Chain I:

8%

72%  28%

C1 G2 C3 C6 G7 G8 G18 G19 C20 G23 G24 C25
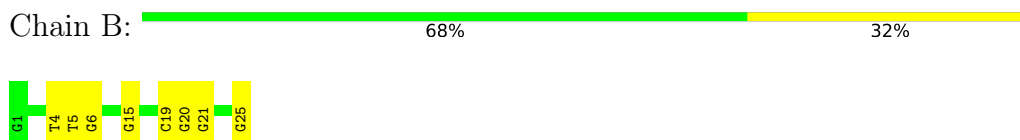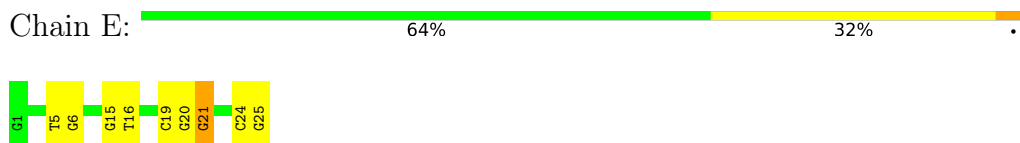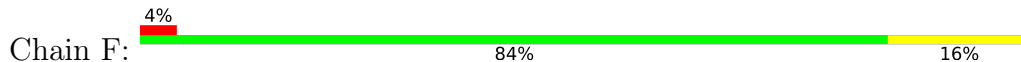
• Molecule 4: HOMING ENDONUCLEASE I-DMOI

Chain G:

2%

72%  17% • 11%

ALA HIS ASN ASN E5 I19 G22 K30 G31 N32 R33 V39 Q42 L47 I48 I60 V65 K66 S67 K68 D75 K86 L95 E96 R97 L100 Q106 F109 V115 K120 T121 L122 K123 K132 W141 G146 L153 D154 D155 H156

V160 Y161 V162 L163 L167 R170 V174 H181 LEU ASN PRO LEU PRO PRO GLU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS
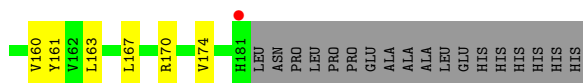
# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 107.03Å 70.66Å 107.26Å<br>90.00° 119.58° 90.00° | Depositor |
| Resolution (Å) | 42.86 – 2.73<br>42.86 – 2.73 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.6 (42.86-2.73)<br>99.3 (42.86-2.73) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.25 (at 2.73Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, $R_{free}$ | 0.178 , 0.220<br>0.182 , 0.220 | Depositor<br>DCC |
| $R_{free}$ test set | 1838 reflections (4.98%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 55.7 | Xtriage |
| Anisotropy | 0.456 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.41 , 63.9 | EDS |
| L-test for twinning[2] | $< |L| > = 0.48, < L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | 0.020 for -h-l,k,h<br>0.020 for l,k,-h-l<br>0.019 for h,-k,-h-l<br>0.024 for -h-l,-k,l<br>0.020 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 7792 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 46.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 ⓘ

## 5.1 Standard geometry ⓘ

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

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 | 0.51 | 0/1577 | 0.65 | 1/2123 (0.0%) |
| 1 | D | 0.50 | 0/1612 | 0.68 | 2/2171 (0.1%) |
| 2 | B | 1.00 | 0/572 | 1.06 | 1/882 (0.1%) |
| 2 | E | 1.00 | 0/572 | 1.06 | 1/882 (0.1%) |
| 2 | H | 1.07 | 1/572 (0.2%) | 1.03 | 0/882 |
| 3 | C | 0.92 | 0/570 | 1.01 | 0/877 |
| 3 | F | 0.99 | 0/570 | 1.00 | 2/877 (0.2%) |
| 3 | I | 0.93 | 0/570 | 1.03 | 2/877 (0.2%) |
| 4 | G | 0.50 | 0/1542 | 0.64 | 1/2068 (0.0%) |
| All | All | 0.75 | 1/8157 (0.0%) | 0.85 | 10/11639 (0.1%) |

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

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

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | H | 15 | DG | P-O5' | 5.08 | 1.64 | 1.59 |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 27 | LEU | CA-CB-CG | 7.14 | 131.73 | 115.30 |
| 1 | D | 77 | ARG | CG-CD-NE | -6.92 | 97.28 | 111.80 |
| 1 | D | 77 | ARG | CB-CG-CD | 6.29 | 127.97 | 111.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|------------|----------|
| 3 | F | 9 | DA | O4'-C1'-N9 | 5.95 | 112.16 | 108.00 |
| 4 | G | 31 | GLY | N-CA-C | -5.53 | 99.28 | 113.10 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 31 | GLY | Peptide |

## 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 | 1541 | 0 | 1613 | 25 | 0 |
| 1 | D | 1578 | 0 | 1645 | 21 | 0 |
| 2 | B | 511 | 0 | 282 | 6 | 0 |
| 2 | E | 511 | 0 | 282 | 7 | 0 |
| 2 | H | 511 | 0 | 282 | 6 | 0 |
| 3 | C | 508 | 0 | 279 | 3 | 0 |
| 3 | F | 508 | 0 | 279 | 1 | 0 |
| 3 | I | 508 | 0 | 279 | 5 | 0 |
| 4 | G | 1502 | 0 | 1596 | 24 | 0 |
| 5 | A | 3 | 0 | 0 | 0 | 0 |
| 5 | D | 3 | 0 | 0 | 0 | 0 |
| 5 | G | 4 | 0 | 0 | 0 | 0 |
| 6 | A | 30 | 0 | 0 | 4 | 0 |
| 6 | B | 6 | 0 | 0 | 0 | 0 |
| 6 | C | 4 | 0 | 0 | 0 | 0 |
| 6 | D | 25 | 0 | 0 | 1 | 0 |
| 6 | E | 5 | 0 | 0 | 0 | 0 |
| 6 | F | 2 | 0 | 0 | 0 | 0 |
| 6 | G | 23 | 0 | 0 | 0 | 0 |
| 6 | H | 6 | 0 | 0 | 0 | 0 |
| 6 | I | 3 | 0 | 0 | 0 | 0 |
| All | All | 7792 | 0 | 6537 | 90 | 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 7.

The worst 5 of 90 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:D:33:ARG:NH1 | 2:E:21:DG:O6 | 2.15 | 0.79 |
| 3:F:2:DG:H2" | 3:F:3:DC:H5" | 1.66 | 0.76 |
| 1:D:111:LYS:HD3 | 1:D:186:PRO:HD3 | 1.69 | 0.74 |
| 3:I:6:DC:H2" | 3:I:7:DG:H5' | 1.70 | 0.74 |
| 1:A:77:ARG:HH11 | 1:A:77:ARG:HG3 | 1.53 | 0.73 |

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 | 185/199 (93%) | 172 (93%) | 11 (6%) | 2 (1%) | 14 | 26 |
| 1 | D | 190/199 (96%) | 182 (96%) | 7 (4%) | 1 (0%) | 29 | 48 |
| 4 | G | 181/199 (91%) | 172 (95%) | 8 (4%) | 1 (1%) | 25 | 44 |
| All | All | 556/597 (93%) | 526 (95%) | 26 (5%) | 4 (1%) | 22 | 40 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 168 | ARG |
| 1 | A | 44 | SER |
| 1 | A | 75 | ASP |
| 4 | G | 122 | LEU |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 170/178 (96%) | 168 (99%) | 2 (1%) | 71 | 83 |
| 1 | D | 172/178 (97%) | 170 (99%) | 2 (1%) | 71 | 83 |
| 4 | G | 165/178 (93%) | 162 (98%) | 3 (2%) | 59 | 75 |
| All | All | 507/534 (95%) | 500 (99%) | 7 (1%) | 71 | 80 |

5 of 7 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 75 | ASP |
| 4 | G | 48 | ILE |
| 4 | G | 66[B] | LYS |
| 4 | G | 66[A] | LYS |
| 1 | D | 66 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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(Å$^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|-------------|-------|
| 1 | A | 184/199 (92%) | 0.40 | 6 (3%) | 46 | 52 | 27, 41, 61, 88 | 0 |
| 1 | D | 191/199 (95%) | 0.85 | 15 (7%) | 12 | 14 | 23, 42, 95, 131 | 0 |
| 2 | B | 25/25 (100%) | -0.08 | 0 | 100 | 100 | 36, 52, 60, 62 | 0 |
| 2 | E | 25/25 (100%) | 0.13 | 0 | 100 | 100 | 31, 48, 66, 70 | 0 |
| 2 | H | 25/25 (100%) | 0.37 | 0 | 100 | 100 | 36, 47, 57, 61 | 0 |
| 3 | C | 25/25 (100%) | 0.05 | 0 | 100 | 100 | 34, 49, 68, 70 | 0 |
| 3 | F | 25/25 (100%) | 0.35 | 1 (4%) | 38 | 42 | 35, 44, 80, 87 | 0 |
| 3 | I | 25/25 (100%) | 0.74 | 2 (8%) | 12 | 14 | 35, 48, 77, 85 | 0 |
| 4 | G | 177/199 (88%) | 0.40 | 4 (2%) | 60 | 67 | 24, 39, 59, 103 | 0 |
| All | All | 702/747 (93%) | 0.49 | 28 (3%) | 38 | 42 | 23, 42, 70, 131 | 0 |

The worst 5 of 28 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 191 | ALA | 13.6 |
| 1 | D | 195 | HIS | 12.8 |
| 1 | D | 194 | HIS | 10.0 |
| 1 | D | 192 | LEU | 8.8 |
| 1 | D | 189 | ALA | 7.8 |

## 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.

## 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($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------------------------|-------|
| 5 | MN | G | 1184 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 1 |
| 5 | MN | G | 1185 | 1/1 | 0.97 | 0.11 | 79,79,79,79 | 0 |
| 5 | MN | D | 1198 | 1/1 | 0.98 | 0.16 | 36,36,36,36 | 0 |
| 5 | MN | G | 1182 | 1/1 | 0.98 | 0.15 | 37,37,37,37 | 0 |
| 5 | MN | D | 1199 | 1/1 | 0.99 | 0.15 | 32,32,32,32 | 1 |
| 5 | MN | A | 1189 | 1/1 | 0.99 | 0.13 | 35,35,35,35 | 0 |
| 5 | MN | G | 1183 | 1/1 | 0.99 | 0.13 | 39,39,39,39 | 0 |
| 5 | MN | A | 1190 | 1/1 | 0.99 | 0.11 | 36,36,36,36 | 1 |
| 5 | MN | A | 1188 | 1/1 | 0.99 | 0.16 | 46,46,46,46 | 0 |
| 5 | MN | D | 1197 | 1/1 | 1.00 | 0.15 | 37,37,37,37 | 0 |

## 6.5  Other polymers ⓘ

There are no such residues in this entry.