# WORLDWIDE PDB

## PROTEIN DATA BANK

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

Nov 26, 2014 – 06:42 AM EST

PDB ID : 4TXV

Title : Crystal structure of the mixed disulfide intermediate between thioredoxin-like TlpAs(C110S) and subunit II of cytochrome c oxidase CoxBPD (C233S)

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Deposited on : 2014-07-07

Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
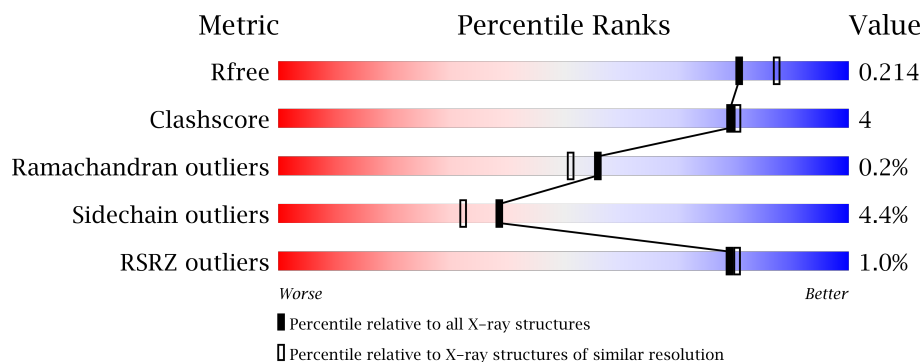
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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# 1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.00 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 | | 0.214 |
| Clashscore | | 4 |
| Ramachandran outliers | | 0.2% |
| Sidechain outliers | | 4.4% |
| RSRZ outliers | | 1.0% |

*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)) |
|---|---|---|
| $R_{free}$ | 66092 | 4888 (2.00-2.00) |
| Clashscore | 79885 | 6188 (2.00-2.00) |
| Ramachandran outliers | 78287 | 6102 (2.00-2.00) |
| Sidechain outliers | 78261 | 6100 (2.00-2.00) |
| RSRZ outliers | 66119 | 4890 (2.00-2.00) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 184 | |
| 1 | C | 184 | |
| 2 | B | 159 | |
| 2 | D | 159 | |

# 2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5267 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thiol:disulfide interchange protein TlpA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 1 | A | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1314 | 836 | 226 | 246 | 6 | | | |
| 1 | C | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1335 | 849 | 230 | 250 | 6 | | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 38 | ALA | - | expression tag | UNP P43221 |
| A | 39 | PRO | - | expression tag | UNP P43221 |
| A | 110 | SER | CYS | engineered mutation | UNP P43221 |
| A | 218 | ALA | - | expression tag | UNP P43221 |
| A | 219 | ALA | - | expression tag | UNP P43221 |
| A | 220 | ALA | - | expression tag | UNP P43221 |
| A | 221 | LEU | - | expression tag | UNP P43221 |
| C | 38 | ALA | - | expression tag | UNP P43221 |
| C | 39 | PRO | - | expression tag | UNP P43221 |
| C | 110 | SER | CYS | engineered mutation | UNP P43221 |
| C | 218 | ALA | - | expression tag | UNP P43221 |
| C | 219 | ALA | - | expression tag | UNP P43221 |
| C | 220 | ALA | - | expression tag | UNP P43221 |
| C | 221 | LEU | - | expression tag | UNP P43221 |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|---------|-------|
| 2 | B | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1127 | 735 | 185 | 202 | 5 | | | |
| 2 | D | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1047 | 684 | 170 | 188 | 5 | | | |

There are 35 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| B | 121 | GLY | - | expression tag | UNP H7C6E5 |
| B | 122 | ALA | - | expression tag | UNP H7C6E5 |
| B | 233 | SER | CYS | engineered mutation | UNP H7C6E5 |
| B | 265 | SER | - | expression tag | UNP H7C6E5 |
| B | 266 | GLY | - | expression tag | UNP H7C6E5 |
| B | 267 | GLY | - | expression tag | UNP H7C6E5 |
| B | 268 | THR | - | expression tag | UNP H7C6E5 |
| B | 269 | GLY | - | expression tag | UNP H7C6E5 |
| B | 270 | THR | - | expression tag | UNP H7C6E5 |
| B | 271 | TYR | - | expression tag | UNP H7C6E5 |
| B | 272 | ALA | - | expression tag | UNP H7C6E5 |
| B | 273 | SER | - | expression tag | UNP H7C6E5 |
| B | 274 | ALA | - | expression tag | UNP H7C6E5 |
| B | 275 | ALA | - | expression tag | UNP H7C6E5 |
| B | 276 | GLY | - | expression tag | UNP H7C6E5 |
| B | 277 | PRO | - | expression tag | UNP H7C6E5 |
| B | 278 | THR | - | expression tag | UNP H7C6E5 |
| B | 279 | GLN | - | expression tag | UNP H7C6E5 |
| D | 121 | GLY | - | expression tag | UNP H7C6E5 |
| D | 122 | ALA | - | expression tag | UNP H7C6E5 |
| D | 233 | SER | CYS | engineered mutation | UNP H7C6E5 |
| D | 266 | GLY | - | expression tag | UNP H7C6E5 |
| D | 267 | GLY | - | expression tag | UNP H7C6E5 |
| D | 268 | THR | - | expression tag | UNP H7C6E5 |
| D | 269 | GLY | - | expression tag | UNP H7C6E5 |
| D | 270 | THR | - | expression tag | UNP H7C6E5 |
| D | 271 | TYR | - | expression tag | UNP H7C6E5 |
| D | 272 | ALA | - | expression tag | UNP H7C6E5 |
| D | 273 | SER | - | expression tag | UNP H7C6E5 |
| D | 274 | ALA | - | expression tag | UNP H7C6E5 |
| D | 275 | ALA | - | expression tag | UNP H7C6E5 |
| D | 276 | GLY | - | expression tag | UNP H7C6E5 |
| D | 277 | PRO | - | expression tag | UNP H7C6E5 |
| D | 278 | THR | - | expression tag | UNP H7C6E5 |
| D | 279 | GLN | - | expression tag | UNP H7C6E5 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | A | 109 | Total 109 | O 109 | 0 | 0 |
| 3 | B | 116 | Total 116 | O 116 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | C | 114 | Total<br>114 | O<br>114 | 0 | 0 |
| 3 | D | 105 | Total<br>105 | O<br>105 | 0 | 0 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

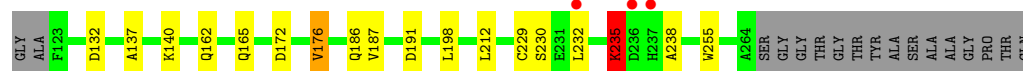• Molecule 1: Thiol:disulfide interchange protein TlpA

Chain A:



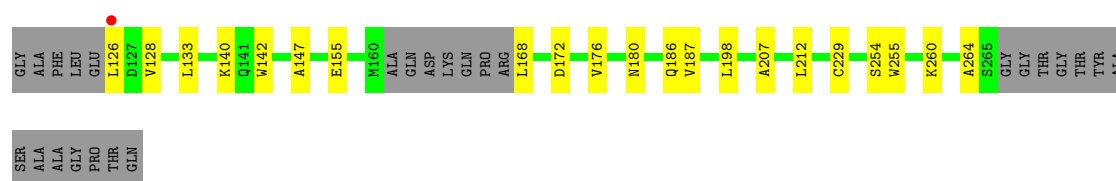• Molecule 1: Thiol:disulfide interchange protein TlpA

Chain C:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain D:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 74.83Å    81.64Å    109.37Å<br>90.00°    90.00°    90.00° | Depositor |
| Resolution (Å) | 65.42   –   2.00<br>49.25   –   2.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.1 (65.42-2.00)<br>99.2 (49.25-2.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.07 (at 2.00Å) | Xtriage |
| Refinement program | REFMAC 5.8.0071 | Depositor |
| R, $R_{free}$ | 0.163   ,   0.212<br>0.172   ,   0.214 | Depositor<br>DCC |
| $R_{free}$ test set | 2304 reflections (5.31%) | DCC |
| Wilson B-factor (Å$^2$) | 33.6 | Xtriage |
| Anisotropy | 0.322 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 41.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $< |L| > = 0.49, < L^2 > = 0.32$ | Xtriage |
| Outliers | 0 of 45681 reflections | Xtriage |
| $F_o,F_c$ correlation | 0.97 | EDS |
| Total number of atoms | 5267 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 39.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

## 5   Model quality ⓘ

### 5.1   Standard geometry ⓘ

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 | 0.82 | 0/1340 | 0.90 | 0/1819 |
| 1 | C | 0.83 | 0/1361 | 0.90 | 0/1847 |
| 2 | B | 0.87 | 0/1157 | 0.92 | 2/1566 (0.1%) |
| 2 | D | 0.90 | 0/1074 | 0.91 | 1/1453 (0.1%) |
| All | All | 0.85 | 0/4932 | 0.91 | 3/6685 (0.0%) |

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 |
| 2 | B | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 2 | B | 172 | ASP | CB-CG-OD1 | 5.57 | 123.32 | 118.30 |
| 2 | B | 132 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 2 | D | 172 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 214 | THR | Peptide |
| 2 | B | 235 | LYS | Peptide |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1314 | 0 | 1343 | 6 | 0 |
| 1 | C | 1335 | 0 | 1368 | 12 | 0 |
| 2 | B | 1127 | 0 | 1122 | 7 | 0 |
| 2 | D | 1047 | 0 | 1042 | 11 | 0 |
| 3 | A | 109 | 0 | 0 | 0 | 0 |
| 3 | B | 116 | 0 | 0 | 1 | 0 |
| 3 | C | 114 | 0 | 0 | 1 | 0 |
| 3 | D | 105 | 0 | 0 | 1 | 0 |
| All | All | 5267 | 0 | 4875 | 33 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (33) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------|--------|-------------|----------|
| 1:C:107:CYS:HG | 2:D:229:CYS:HG | 1.20 | 0.86 |
| 1:A:107:CYS:HG | 2:B:229:CYS:HG | 1.27 | 0.83 |
| 1:C:121:GLN:O | 1:C:125:SER:HB2 | 1.87 | 0.74 |
| 2:D:180:ASN:OD1 | 3:D:397:HOH:O | 2.09 | 0.70 |
| 2:B:235:LYS:O | 2:B:238:ALA:HB3 | 2.00 | 0.60 |
| 1:C:121:GLN:O | 1:C:125:SER:CB | 2.49 | 0.60 |
| 2:B:186:GLN:HB3 | 2:B:212:LEU:HD22 | 1.84 | 0.58 |
| 2:D:187:VAL:CG1 | 2:D:207:ALA:HB2 | 2.35 | 0.56 |
| 2:B:176:VAL:HG13 | 2:B:255:TRP:CZ2 | 2.41 | 0.55 |
| 2:B:230:SER:OG | 2:B:232:LEU:HG | 2.07 | 0.54 |
| 1:C:74:LYS:HE3 | 1:C:188:GLN:O | 2.08 | 0.54 |
| 2:D:187:VAL:HG12 | 2:D:207:ALA:HB2 | 1.93 | 0.50 |
| 1:A:81:GLU:OE2 | 1:A:85:GLY:HA2 | 2.12 | 0.49 |
| 1:C:74:LYS:HE2 | 3:C:351:HOH:O | 2.13 | 0.48 |
| 1:C:143:LYS:N | 1:C:144:PRO:CD | 2.77 | 0.47 |
| 1:A:140:ASP:O | 1:A:142:GLU:N | 2.48 | 0.47 |
| 1:A:138:THR:HG22 | 1:A:162:GLN:O | 2.16 | 0.46 |
| 2:B:137:ALA:HB3 | 2:B:187:VAL:HG12 | 1.99 | 0.45 |
| 2:D:176:VAL:HG13 | 2:D:255:TRP:CZ2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:C:214:THR:HG22 | 1:C:216:LYS:HB2 | 1.99 | 0.44 |
| 2:D:140:LYS:O | 2:D:142:TRP:HA | 2.18 | 0.43 |
| 1:C:56:ALA:N | 1:C:57:PRO:CD | 2.81 | 0.43 |
| 2:B:176:VAL:HG13 | 2:B:255:TRP:CE2 | 2.54 | 0.43 |
| 1:C:97:THR:O | 1:C:129:PHE:HA | 2.18 | 0.43 |
| 2:D:147:ALA:HB2 | 2:D:155:GLU:HG2 | 2.02 | 0.42 |
| 1:A:97:THR:O | 1:A:129:PHE:HA | 2.20 | 0.42 |
| 1:C:74:LYS:HD2 | 1:C:74:LYS:HA | 1.83 | 0.42 |
| 2:D:186:GLN:HB3 | 2:D:212:LEU:HD11 | 2.02 | 0.41 |
| 1:A:110:SER:HB2 | 1:A:180:PRO:HB3 | 2.02 | 0.41 |
| 1:C:209:LEU:HG | 1:C:209:LEU:O | 2.19 | 0.41 |
| 2:D:260:LYS:O | 2:D:264:ALA:HB2 | 2.19 | 0.41 |
| 1:C:109:PRO:HD2 | 2:D:229:CYS:SG | 2.61 | 0.40 |
| 3:B:407:HOH:O | 2:D:128:VAL:CG1 | 2.69 | 0.40 |

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 | 173/184 (94%) | 166 (96%) | 6 (4%) | 1 (1%) | 33 | 24 |
| 1 | C | 176/184 (96%) | 170 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | B | 140/159 (88%) | 135 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | D | 129/159 (81%) | 127 (98%) | 2 (2%) | 0 | 100 | 100 |
| All | All | 618/686 (90%) | 598 (97%) | 19 (3%) | 1 (0%) | 56 | 51 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 141 | PRO |

### 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 | 136/140 (97%) | 129 (95%) | 7 (5%) | 33 | 26 |
| 1 | C | 138/140 (99%) | 135 (98%) | 3 (2%) | 64 | 65 |
| 2 | B | 117/125 (94%) | 110 (94%) | 7 (6%) | 27 | 20 |
| 2 | D | 109/125 (87%) | 104 (95%) | 5 (5%) | 37 | 30 |
| All | All | 500/530 (94%) | 478 (96%) | 22 (4%) | 39 | 32 |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 60 | HIS |
| 1 | A | 74 | LYS |
| 1 | A | 94 | ARG |
| 1 | A | 110 | SER |
| 1 | A | 137 | ASP |
| 1 | A | 149 | LYS |
| 1 | A | 186 | ASP |
| 2 | B | 140 | LYS |
| 2 | B | 162 | GLN |
| 2 | B | 165 | GLN |
| 2 | B | 176 | VAL |
| 2 | B | 191 | ASP |
| 2 | B | 198 | LEU |
| 2 | B | 235 | LYS |
| 1 | C | 186 | ASP |
| 1 | C | 204 | GLU |
| 1 | C | 209 | LEU |
| 2 | D | 126 | LEU |
| 2 | D | 133 | LEU |
| 2 | D | 168 | LEU |
| 2 | D | 198 | LEU |
| 2 | D | 254 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 152 | ASN |
| 1 | A | 168 | GLN |
| 2 | B | 162 | GLN |
| 2 | D | 186 | GLN |
| 2 | D | 194 | HIS |

### 5.3.3   RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6   Ligand geometry ⓘ

There are no ligands in this entry.

## 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 (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 | 175/184 (95%) | -0.30 | 1 (0%) | 86 | 88 | 22, 34, 61, 90 | 0 |
| 1 | C | 178/184 (96%) | -0.39 | 1 (0%) | 86 | 88 | 25, 38, 58, 81 | 0 |
| 2 | B | 142/159 (89%) | -0.26 | 3 (2%) | 60 | 61 | 23, 34, 70, 93 | 0 |
| 2 | D | 133/159 (83%) | -0.31 | 1 (0%) | 83 | 84 | 26, 35, 65, 79 | 0 |
| All | All | 628/686 (91%) | -0.32 | 6 (0%) | 79 | 80 | 22, 35, 64, 93 | 0 |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 236 | ASP | 4.2 |
| 2 | B | 232 | LEU | 3.7 |
| 2 | B | 237 | HIS | 3.4 |
| 2 | D | 126 | LEU | 2.7 |
| 1 | C | 40 | THR | 2.1 |
| 1 | A | 41 | GLY | 2.1 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.