



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 5FTP / pdb\_00005ftp  
Title : sulfur SAD phasing of Cdc23Nterm: data collection with a tailored X- ray  
beam size at 2.69 Å wavelength (4.6 keV)  
Authors : Cianci, M.; Groves, M.R.; Barford, D.; Schneider, T.R.  
Deposited on : 2016-01-14  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

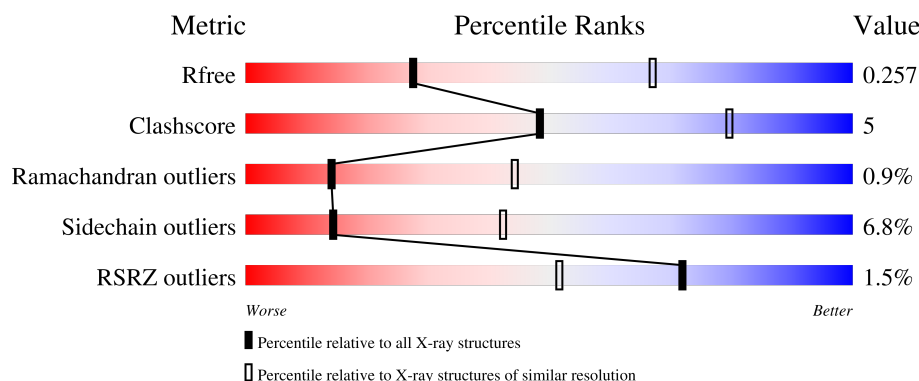
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                             |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------------|
| 1   | A     | 291    | <div> <div>%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>21%</div> </div> </div>              |
| 1   | B     | 291    | <div> <div>%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3866 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1871  | 1207 | 307 | 348 | 9 |         |         |       |
| 1   | B     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1988  | 1280 | 328 | 371 | 9 |         |         |       |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 18      | MET      | -      | expression tag | UNP O94556 |
| A     | 302     | ALA      | -      | expression tag | UNP O94556 |
| A     | 303     | GLU      | -      | expression tag | UNP O94556 |
| A     | 304     | ASN      | -      | expression tag | UNP O94556 |
| A     | 305     | LEU      | -      | expression tag | UNP O94556 |
| A     | 306     | TYR      | -      | expression tag | UNP O94556 |
| A     | 307     | PHE      | -      | expression tag | UNP O94556 |
| A     | 308     | GLN      | -      | expression tag | UNP O94556 |
| A     | 285     | LEU      | ASP    | conflict       | UNP O94556 |
| B     | 18      | MET      | -      | expression tag | UNP O94556 |
| B     | 302     | ALA      | -      | expression tag | UNP O94556 |
| B     | 303     | GLU      | -      | expression tag | UNP O94556 |
| B     | 304     | ASN      | -      | expression tag | UNP O94556 |
| B     | 305     | LEU      | -      | expression tag | UNP O94556 |
| B     | 306     | TYR      | -      | expression tag | UNP O94556 |
| B     | 307     | PHE      | -      | expression tag | UNP O94556 |
| B     | 308     | GLN      | -      | expression tag | UNP O94556 |
| B     | 285     | LEU      | ASP    | conflict       | UNP O94556 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | A     | 5        | Total | O | 0       | 0       |
|     |       |          | 5     | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | B     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

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.

Chain A:

63% 16% 21%

Met GLN LEU R21 R22 R23 R24 S32 R37 V40 R44 L50 N51 G52 M53 N54 P55 I56 E57 Met HIS GLU ILE PRQ PHE SER SER THR PRQ THR GLY GLU PHE ASP LEU ASP PRQ ASP M77 K81 V85 Y91 K95 D99 L110 L121 Y127

G130 LYS SER GLU GLU ASN THR LEU LEU ASN THR LEU LEU THR L148 F155 Y156 Y157 V161 S164 L165 H166 L178 S179 K197 F205 W206 W207 L213 L217 D218 S219 L220 L223 S232 T239 L248 F249 Q250 E257 K258 L260

E263 I264 N268 S269 R270 Y271 K273 K276 T280 R284 L285 PHE ASP ALA GLU SER LEU PHE GLU ASN ILE LEU THR ASN ASP PRO PRO ALA GLU ASN LEU LEU THR PHE GLN

Chain B:

0% 67% 13% 17%

MET GLN L20 C26 P85 ILE GLU MET GLU HIS ILE PRO PHE SER THR PRO THR GLY PHE ASP LEU ASP PRO M77 A78 N79 K81 L82 L83 E84 V85 I90 K95 D99 L110 L121 E135 GLU ASN THR LEU ASN THR LEU

THR LEU SER THR N152 Y157 I158 S159 E160 V161 L165 Q168 G169 N170 L178 Y183 F195 L196 K197 L213 I217 D218 S219 L220 E221 T222 V226 P231 S232 T233 H234 I235 M236 T237 K238 L239 Y243 Q250 S253 E257 K258 L259 A260 E261 Q262

E263 I264 Q275 R276 T280 R284 LEU PHE ASP GLU ALA GLU SER LEU PHE GLU N295 I296 N299 Q308

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 61.25Å 61.25Å 151.56Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 61.25 – 3.10<br>61.25 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (61.25-3.10)<br>99.8 (61.25-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.82 (at 3.13Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0135                                             | Depositor        |
| R, $R_{free}$                                                           | 0.187 , 0.260<br>0.198 , 0.257                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 510 reflections (5.04%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 62.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.010                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 53.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.069 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 3866                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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     | 0.65         | 0/1909      | 1.00        | 4/2577 (0.2%) |
| 1   | B     | 0.65         | 0/2028      | 1.00        | 2/2734 (0.1%) |
| All | All   | 0.65         | 0/3937      | 1.00        | 6/5311 (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                   |
| 1   | B     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | A     | 37  | ARG  | N-CA-C | 10.62 | 125.98                 | 112.92              |
| 1   | B     | 232 | SER  | N-CA-C | -5.99 | 101.42                 | 110.28              |
| 1   | A     | 37  | ARG  | O-C-N  | -5.47 | 115.77                 | 122.34              |
| 1   | A     | 40  | VAL  | N-CA-C | 5.46  | 116.23                 | 110.72              |
| 1   | B     | 168 | GLN  | N-CA-C | -5.24 | 103.11                 | 110.50              |
| 1   | A     | 51  | ASN  | N-CA-C | -5.01 | 103.92                 | 110.53              |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 37  | ARG  | Peptide |
| 1   | B     | 234 | HIS  | 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     | 1871  | 0        | 1870     | 22      | 0            |
| 1   | B     | 1988  | 0        | 1981     | 22      | 0            |
| 2   | A     | 5     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 3866  | 0        | 3851     | 42      | 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 5.

All (42) 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:A:148:LEU:HD21 | 1:A:155:PHE:HE1  | 1.37                     | 0.89              |
| 1:A:148:LEU:HD21 | 1:A:155:PHE:CE1  | 2.17                     | 0.79              |
| 1:A:148:LEU:HD23 | 1:A:148:LEU:C    | 2.21                     | 0.64              |
| 1:B:110:LEU:HD11 | 1:B:121:LEU:HD12 | 1.80                     | 0.63              |
| 1:B:261:GLU:HA   | 1:B:264:ILE:CD1  | 2.32                     | 0.59              |
| 1:A:166:HIS:NE2  | 1:A:179:SER:OG   | 2.36                     | 0.57              |
| 1:B:168:GLN:O    | 1:B:170:ASN:N    | 2.40                     | 0.55              |
| 1:A:81:LYS:O     | 1:A:85:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:213:LEU:O    | 1:A:217:ILE:HG13 | 2.11                     | 0.51              |
| 1:B:261:GLU:O    | 1:B:264:ILE:HD13 | 2.10                     | 0.51              |
| 1:B:81:LYS:O     | 1:B:85:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:157:TYR:O    | 1:B:161:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:273:LYS:N    | 1:A:273:LYS:HD2  | 2.26                     | 0.50              |
| 1:B:220:LEU:HD13 | 1:B:250:GLN:HB3  | 1.94                     | 0.49              |
| 1:A:157:TYR:O    | 1:A:161:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:127:TYR:CZ   | 1:A:148:LEU:HA   | 2.49                     | 0.48              |
| 1:A:207:TRP:CZ2  | 1:A:271:TYR:OH   | 2.65                     | 0.48              |
| 1:A:220:LEU:HD13 | 1:A:250:GLN:HB3  | 1.96                     | 0.48              |
| 1:B:234:HIS:O    | 1:B:237:THR:N    | 2.45                     | 0.48              |
| 1:A:259:LEU:O    | 1:A:263:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:213:LEU:O    | 1:B:217:ILE:HG12 | 2.14                     | 0.47              |
| 1:A:205:PHE:CD1  | 1:B:26:CYS:HB3   | 2.50                     | 0.46              |
| 1:B:261:GLU:C    | 1:B:264:ILE:HD13 | 2.41                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:183:TYR:CE2  | 1:B:195:PHE:CE2  | 3.04                     | 0.46              |
| 1:A:220:LEU:HD13 | 1:A:250:GLN:CB   | 2.46                     | 0.46              |
| 1:B:296:ILE:HA   | 1:B:299:ASN:HD22 | 1.81                     | 0.46              |
| 1:B:296:ILE:HA   | 1:B:299:ASN:ND2  | 2.30                     | 0.45              |
| 1:B:95:LYS:NZ    | 1:B:99:ASP:OD1   | 2.49                     | 0.45              |
| 1:B:259:LEU:O    | 1:B:263:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:95:LYS:NZ    | 1:A:99:ASP:OD1   | 2.49                     | 0.45              |
| 1:A:276:ARG:O    | 1:A:280:THR:HG23 | 2.18                     | 0.44              |
| 1:B:261:GLU:O    | 1:B:264:ILE:CD1  | 2.67                     | 0.43              |
| 1:A:50:LEU:O     | 1:A:53:MET:HG2   | 2.20                     | 0.42              |
| 1:A:223:LEU:HD22 | 1:A:248:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:44:ARG:HH22  | 1:B:308:GLN:C    | 2.28                     | 0.41              |
| 1:A:178:LEU:HD12 | 1:A:178:LEU:HA   | 1.94                     | 0.41              |
| 1:A:269:SER:O    | 1:A:273:LYS:HD3  | 2.20                     | 0.41              |
| 1:A:91:TYR:CZ    | 1:A:121:LEU:HD22 | 2.56                     | 0.41              |
| 1:B:222:THR:O    | 1:B:226:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:220:LEU:HD13 | 1:B:250:GLN:CB   | 2.52                     | 0.40              |
| 1:B:243:TYR:HA   | 1:B:275:GLN:HE22 | 1.86                     | 0.40              |
| 1:B:276:ARG:O    | 1:B:280:THR:HG23 | 2.20                     | 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     | 224/291 (77%) | 207 (92%) | 16 (7%) | 1 (0%)   | 30          | 61 |
| 1   | B     | 234/291 (80%) | 216 (92%) | 15 (6%) | 3 (1%)   | 9           | 35 |
| All | All   | 458/582 (79%) | 423 (92%) | 31 (7%) | 4 (1%)   | 14          | 44 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 235 | ILE  |
| 1   | B     | 169 | GLY  |
| 1   | A     | 54  | ASN  |
| 1   | B     | 231 | 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     | 206/267 (77%) | 194 (94%) | 12 (6%)  | 18          | 48 |
| 1   | B     | 219/267 (82%) | 202 (92%) | 17 (8%)  | 11          | 38 |
| All | All   | 425/534 (80%) | 396 (93%) | 29 (7%)  | 14          | 42 |

All (29) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | ARG  |
| 1   | A     | 32  | SER  |
| 1   | A     | 110 | LEU  |
| 1   | A     | 164 | SER  |
| 1   | A     | 197 | LYS  |
| 1   | A     | 219 | SER  |
| 1   | A     | 232 | SER  |
| 1   | A     | 239 | ILE  |
| 1   | A     | 257 | GLU  |
| 1   | A     | 264 | ILE  |
| 1   | A     | 268 | ASN  |
| 1   | A     | 284 | ARG  |
| 1   | B     | 79  | ASN  |
| 1   | B     | 81  | LYS  |
| 1   | B     | 83  | LEU  |
| 1   | B     | 90  | ILE  |
| 1   | B     | 110 | LEU  |
| 1   | B     | 121 | LEU  |
| 1   | B     | 159 | SER  |
| 1   | B     | 165 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 178 | LEU  |
| 1   | B     | 197 | LYS  |
| 1   | B     | 219 | SER  |
| 1   | B     | 239 | ILE  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 253 | SER  |
| 1   | B     | 257 | GLU  |
| 1   | B     | 264 | ILE  |
| 1   | B     | 296 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 229 | GLN  |
| 1   | A     | 275 | GLN  |
| 1   | B     | 79  | ASN  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 299 | ASN  |
| 1   | B     | 308 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|---------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 230/291 (79%) | -0.19  | 3 (1%)    | 75 56 | 31, 51, 78, 127       | 0       |
| 1   | B     | 242/291 (83%) | -0.08  | 4 (1%)    | 69 48 | 31, 56, 85, 113       | 0       |
| All | All   | 472/582 (81%) | -0.14  | 7 (1%)    | 72 52 | 31, 54, 83, 127       | 0       |

All (7) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 20  | LEU  | 3.5  |
| 1   | A     | 23  | ILE  | 2.9  |
| 1   | B     | 78  | ALA  | 2.5  |
| 1   | B     | 77  | MET  | 2.3  |
| 1   | A     | 56  | ILE  | 2.2  |
| 1   | B     | 235 | ILE  | 2.1  |
| 1   | A     | 147 | THR  | 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 oligosaccharides 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.