



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2014 – 12:55 PM GMT

PDB ID : 2XSM  
Title : Crystal structure of the mammalian cytosolic chaperonin CCT in complex with tubulin  
Authors : Munoz, I.G.; Yebenes, H.; Zhou, M.; Mesa, P.; Serna, M.; Bragado-Nilsson, E.; Beloso, A.; Robinson, C.V.; Valpuesta, J.M.; Montoya, G.  
Deposited on : 2010-10-29  
Resolution : 5.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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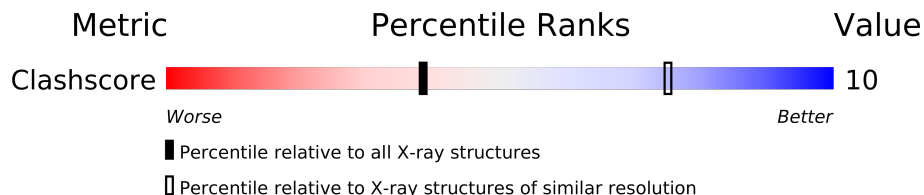
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22699  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22699

# 1 Overall quality at a glance











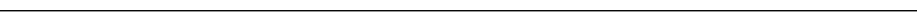
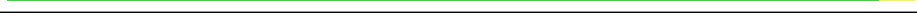




The reported resolution of this entry is 5.50 Å.

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



| Metric     | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 79885                       | 1008 (7.40-3.52)                                      |

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  $\geq 3$ , 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     | 489    |  |
| 2   | B     | 478    |  |
| 3   | C     | 455    |  |
| 4   | D     | 471    |  |
| 5   | E     | 472    |  |
| 6   | F     | 466    |  |
| 7   | G     | 485    |  |
| 8   | H     | 474    |  |
| 9   | I     | 293    |  |
| 10  | J     | 299    |  |
| 11  | K     | 394    |  |
| 12  | L     | 297    |  |
| 12  | O     | 297    |  |
| 13  | M     | 298    |  |
| 14  | N     | 289    |  |
| 15  | P     | 481    |  |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6438 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 CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 1   | A     | 489      | Total C<br>489 489 | 0       | 0       | 489   |

- Molecule 2 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 2   | B     | 478      | Total C<br>478 478 | 0       | 0       | 478   |

- Molecule 3 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 3   | C     | 455      | Total C<br>455 455 | 0       | 0       | 455   |

- Molecule 4 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 4   | D     | 471      | Total C<br>471 471 | 0       | 0       | 471   |

- Molecule 5 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 5   | E     | 472      | Total C<br>472 472 | 0       | 0       | 472   |

- Molecule 6 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 6   | F     | 466      | Total C<br>466 466 | 0       | 0       | 466   |

- Molecule 7 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 7   | G     | 485      | Total C<br>485 485 | 0       | 0       | 485   |

- Molecule 8 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 8   | H     | 474      | Total C<br>474 474 | 0       | 0       | 474   |

- Molecule 9 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 9   | I     | 293      | Total C<br>293 293 | 0       | 0       | 293   |

- Molecule 10 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 10  | J     | 299      | Total C<br>299 299 | 0       | 0       | 299   |

- Molecule 11 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 11  | K     | 394      | Total C<br>394 394 | 0       | 0       | 394   |

- Molecule 12 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 12  | L     | 297      | Total C<br>297 297 | 0       | 0       | 297   |
| 12  | O     | 297      | Total C<br>297 297 | 0       | 0       | 297   |

- Molecule 13 is a protein called CCT.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 13  | M     | 298      | Total C<br>298 298 | 0       | 0       | 298   |

- Molecule 14 is a protein called CCT.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 14  | N     | 289      | Total | C   | 0       | 0       | 289   |
|     |       |          | 289   | 289 |         |         |       |

- Molecule 15 is a protein called CCT.

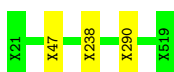
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 15  | P     | 481      | Total | C   | 0       | 0       | 481   |
|     |       |          | 481   | 481 |         |         |       |

### 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.

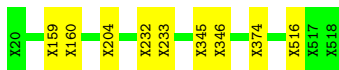
- Molecule 1: CCT

Chain A: 



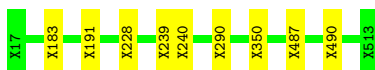
- Molecule 2: CCT

Chain B: 



- Molecule 3: CCT

Chain C: 



- Molecule 4: CCT

Chain D: 



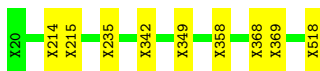
- Molecule 5: CCT

Chain E: 



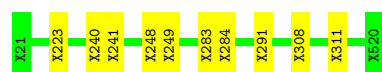
- Molecule 6: CCT

Chain F: 



- Molecule 7: CCT

Chain G: 



- Molecule 8: CCT

Chain H: 



- Molecule 9: CCT

Chain I: 



- Molecule 10: CCT

Chain J: 



- Molecule 11: CCT

Chain K: 



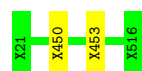
- Molecule 12: CCT

Chain L: 



- Molecule 12: CCT

Chain O: 



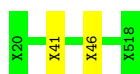
- Molecule 13: CCT

Chain M: 



- Molecule 14: CCT

Chain N: 



- Molecule 15: CCT

Chain P: 





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 21 21 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 272.70Å 313.50Å 158.30Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 100.00 – 5.50<br>97.58 – 5.44                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (100.00-5.50)<br>98.3 (97.58-5.44)           | Depositor<br>EDS |
| $R_{merge}$   | 0.05   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.37 (at 5.41Å)  | Xtriage          |
| Refinement program  | REFMAC 5.5.0099  | Depositor        |
| R, $R_{free}$   | (Not available) , (Not available)<br>0.955 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                       | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 257.8  | Xtriage          |
| Anisotropy  | 0.400  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 58.05 , 838.3  | EDS              |
| Estimated twinning fraction   | No twinning to report.                                       | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.16$  | Xtriage          |
| Outliers  | 0 of 45495 reflections                                       | Xtriage          |
| $F_o, F_c$ correlation  | 0.64   | EDS              |
| Total number of atoms   | 6438   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 26.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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     | 489   | 0        | 0        | 2       | 0            |
| 2   | B     | 478   | 0        | 0        | 5       | 0            |
| 3   | C     | 455   | 0        | 0        | 5       | 0            |
| 4   | D     | 471   | 0        | 0        | 4       | 0            |
| 5   | E     | 472   | 0        | 0        | 11      | 0            |
| 6   | F     | 466   | 0        | 0        | 5       | 0            |
| 7   | G     | 485   | 0        | 0        | 5       | 0            |
| 8   | H     | 474   | 0        | 0        | 2       | 0            |
| 9   | I     | 293   | 0        | 0        | 6       | 0            |
| 10  | J     | 299   | 0        | 0        | 4       | 0            |
| 11  | K     | 394   | 0        | 0        | 8       | 0            |
| 12  | L     | 297   | 0        | 0        | 2       | 0            |
| 12  | O     | 297   | 0        | 0        | 1       | 0            |
| 13  | M     | 298   | 0        | 0        | 3       | 0            |
| 14  | N     | 289   | 0        | 0        | 1       | 0            |
| 15  | P     | 481   | 0        | 0        | 4       | 0            |
| All | All   | 6438  | 0        | 0        | 63      | 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 10.

All (63) close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 11:K:171:UNK:C  | 11:K:172:UNK:CA | 2.24        | 1.15     |
| 7:G:283:UNK:CA  | 7:G:284:UNK:CA  | 2.25        | 1.13     |
| 4:D:448:UNK:CA  | 4:D:449:UNK:CA  | 2.27        | 1.13     |
| 3:C:239:UNK:CA  | 3:C:290:UNK:CA  | 2.30        | 1.10     |
| 2:B:232:UNK:CA  | 2:B:346:UNK:CA  | 2.34        | 1.06     |
| 9:I:99:UNK:CA   | 9:I:100:UNK:CA  | 2.35        | 1.03     |
| 9:I:474:UNK:CA  | 9:I:485:UNK:CA  | 2.37        | 1.02     |
| 7:G:240:UNK:CA  | 7:G:241:UNK:CA  | 2.44        | 0.95     |
| 10:J:144:UNK:CA | 10:J:145:UNK:CA | 2.48        | 0.92     |
| 11:K:347:UNK:CA | 11:K:358:UNK:CA | 2.48        | 0.91     |
| 2:B:233:UNK:CA  | 2:B:345:UNK:CA  | 2.49        | 0.89     |
| 11:K:380:UNK:CA | 11:K:381:UNK:CA | 2.52        | 0.87     |
| 7:G:248:UNK:CA  | 7:G:249:UNK:CA  | 2.52        | 0.87     |
| 15:P:220:UNK:CA | 15:P:221:UNK:CA | 2.56        | 0.83     |
| 13:M:474:UNK:CA | 13:M:485:UNK:CA | 2.59        | 0.80     |
| 6:F:214:UNK:CA  | 6:F:369:UNK:CA  | 2.61        | 0.79     |
| 13:M:406:UNK:CA | 13:M:493:UNK:CA | 2.61        | 0.79     |
| 2:B:159:UNK:CA  | 2:B:160:UNK:CA  | 2.61        | 0.78     |
| 3:C:487:UNK:CA  | 3:C:490:UNK:CA  | 2.61        | 0.78     |
| 14:N:41:UNK:CA  | 14:N:46:UNK:CA  | 2.61        | 0.78     |
| 5:E:214:UNK:CA  | 5:E:369:UNK:CA  | 2.61        | 0.78     |
| 5:E:276:UNK:CA  | 5:E:277:UNK:CA  | 2.63        | 0.77     |
| 5:E:230:UNK:CA  | 5:E:348:UNK:CA  | 2.63        | 0.76     |
| 9:I:480:UNK:CA  | 9:I:481:UNK:CA  | 2.65        | 0.75     |
| 3:C:228:UNK:CA  | 3:C:350:UNK:CA  | 2.65        | 0.75     |
| 9:I:148:UNK:CA  | 9:I:151:UNK:CA  | 2.66        | 0.73     |
| 6:F:349:UNK:CA  | 6:F:358:UNK:CA  | 2.67        | 0.72     |
| 9:I:48:UNK:CA   | 15:P:516:UNK:CA | 2.73        | 0.67     |
| 5:E:41:UNK:CA   | 5:E:46:UNK:CA   | 2.73        | 0.66     |
| 11:K:40:UNK:CA  | 11:K:47:UNK:CA  | 2.73        | 0.66     |
| 11:K:202:UNK:CA | 11:K:218:UNK:CA | 2.76        | 0.63     |
| 7:G:223:UNK:CA  | 7:G:308:UNK:CA  | 2.77        | 0.63     |
| 8:H:474:UNK:CA  | 8:H:484:UNK:CA  | 2.78        | 0.62     |
| 7:G:291:UNK:CA  | 7:G:311:UNK:CA  | 2.79        | 0.60     |
| 8:H:287:UNK:CA  | 8:H:308:UNK:CA  | 2.81        | 0.59     |
| 3:C:239:UNK:CA  | 3:C:240:UNK:CA  | 2.81        | 0.58     |
| 15:P:233:UNK:CA | 15:P:345:UNK:CA | 2.82        | 0.57     |
| 12:L:474:UNK:CA | 12:L:475:UNK:CA | 2.83        | 0.56     |
| 5:E:327:UNK:CA  | 5:E:342:UNK:CA  | 2.83        | 0.56     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 13:M:37:UNK:CA  | 13:M:38:UNK:CA  | 2.86        | 0.53     |
| 9:I:142:UNK:CA  | 9:I:143:UNK:CA  | 2.88        | 0.52     |
| 5:E:347:UNK:CA  | 5:E:360:UNK:CA  | 2.87        | 0.52     |
| 4:D:348:UNK:CA  | 4:D:358:UNK:CA  | 2.89        | 0.50     |
| 5:E:234:UNK:CA  | 5:E:343:UNK:CA  | 2.91        | 0.49     |
| 10:J:476:UNK:CA | 10:J:483:UNK:CA | 2.91        | 0.49     |
| 6:F:235:UNK:CA  | 6:F:342:UNK:CA  | 2.90        | 0.48     |
| 12:O:450:UNK:CA | 12:O:453:UNK:CA | 2.92        | 0.48     |
| 10:J:164:UNK:CA | 10:J:167:UNK:CA | 2.91        | 0.48     |
| 5:E:428:UNK:CA  | 12:L:461:UNK:CA | 2.92        | 0.47     |
| 10:J:405:UNK:CA | 10:J:493:UNK:CA | 2.92        | 0.47     |
| 5:E:51:UNK:CA   | 6:F:518:UNK:CA  | 2.93        | 0.47     |
| 4:D:428:UNK:CA  | 11:K:461:UNK:CA | 2.93        | 0.47     |
| 11:K:214:UNK:CA | 11:K:370:UNK:CA | 2.93        | 0.46     |
| 11:K:49:UNK:CA  | 11:K:63:UNK:CA  | 2.93        | 0.46     |
| 4:D:201:UNK:CA  | 4:D:373:UNK:CA  | 2.94        | 0.46     |
| 2:B:204:UNK:CA  | 2:B:374:UNK:CA  | 2.94        | 0.46     |
| 1:A:47:UNK:CA   | 2:B:516:UNK:CA  | 2.95        | 0.45     |
| 1:A:238:UNK:CA  | 1:A:290:UNK:CA  | 2.96        | 0.44     |
| 6:F:215:UNK:CA  | 6:F:368:UNK:CA  | 2.97        | 0.42     |
| 15:P:288:UNK:CA | 15:P:289:UNK:CA | 2.97        | 0.42     |
| 3:C:183:UNK:CA  | 3:C:191:UNK:CA  | 2.97        | 0.42     |
| 5:E:240:UNK:CA  | 5:E:331:UNK:CA  | 2.99        | 0.41     |
| 5:E:95:UNK:CA   | 5:E:98:UNK:CA   | 2.99        | 0.41     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 ⓘ

### 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<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     | 0/489    | -      | -       | -                     | -     |
| 2   | B     | 0/478    | -      | -       | -                     | -     |
| 3   | C     | 0/455    | -      | -       | -                     | -     |
| 4   | D     | 0/471    | -      | -       | -                     | -     |
| 5   | E     | 0/472    | -      | -       | -                     | -     |
| 6   | F     | 0/466    | -      | -       | -                     | -     |
| 7   | G     | 0/485    | -      | -       | -                     | -     |
| 8   | H     | 0/474    | -      | -       | -                     | -     |
| 9   | I     | 0/293    | -      | -       | -                     | -     |
| 10  | J     | 0/299    | -      | -       | -                     | -     |
| 11  | K     | 0/394    | -      | -       | -                     | -     |
| 12  | L     | 0/297    | -      | -       | -                     | -     |
| 12  | O     | 0/297    | -      | -       | -                     | -     |
| 13  | M     | 0/298    | -      | -       | -                     | -     |
| 14  | N     | 0/289    | -      | -       | -                     | -     |
| 15  | P     | 0/481    | -      | -       | -                     | -     |
| All | All   | 0/6438   | -      | -       | -                     | -     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.